On the Nullity of Bicyclic Graphs

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- **Background**
- **Definition and Known results**
- **The nullity set of $\mathcal{B}_n$**
- **The bicyclic graph with maximal nullity**

Background

- ⋆ 1957, Collatz and Sinogowitz first posed the problem of characterizing all graphs which satisfy $\eta(G) > 0$. This question is of great interest in both chemistry and mathematics. For a bipartite graph G, which correspond 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 $A(G)$. The problem has not yet been solved completely. Some results on trees, bipartite graphs and unicyclic graphs are known.

1 Definition and Known results

- ⋆ The adjacency matrix $A(G)$ of a graph G with the vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ 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.
- ⋆ A graph is said to be singular(nonsingular) if its adjacency matrix A is a singular(nonsingular) matrix.
- ⋆ The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of $A(G)$ are said to be the eigenvalues of the graph G, and to form the spectrum of this graph.
- ⋆ The number of zero eigenvalues in the spectrum of the graph G is called its nullity and is denoted by $\eta(G)$.
- ⋆ $\gamma(A(G))$ be the rank of $A(G)$. Clearly, $\eta(G) = n - \gamma(A(G))$.
- ⋆ Let $\mathcal{G}_n$ be the set of all graphs of order n, and let $[0, n] = \{0, 1, 2, \ldots, n\}$. 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 $\eta(G) = k$.
- ⋆ An elementary graph is a simple graph, each component of which is regular has degree 1 or 2. In other words, each component is a single edge(K_2) or a cycle(C_r). A spanning elementary subgraph of G is an elementary subgraph which contains all vertices of G

- $\star$ A unicyclic graph is a simple connected graph with equal number of vertices and edges. Denote by $\mathcal{U}_n$ the set of all unicyclic graphs of order n.
- $\star$ A bicyclic graph is a simple connected graph in which the number of edges equals the number of vertices plus one. Denoted by $\mathcal{B}_n$ the set of all bicyclic graphs of order n.
- $\star$ $\mathcal{B}_n$ consists of three types of graphs: first type denoted by B_n^+ is the set of those graphs each of which is an $\infty-$graph with trees attached when $q > 1$; second type denoted by B_n^{++} is the set of those graphs each of which is an $\infty-$graph with trees attached when $q = 1$; third type denoted by θ_n is the set of those graphs each of which is an $\theta-$graph with trees attached. Then $\mathcal{B}_n$=$B_n^+ \bigcup B_n^{++} \bigcup \theta_n$.

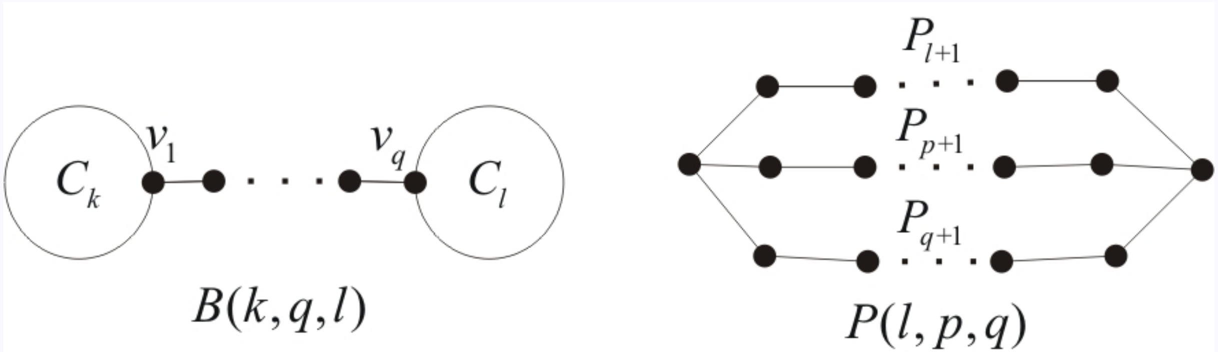


Fig.1.2

⋆ **Proposition 1.1.** Let G be a graph of order n. Then $\eta(G) = n$ if and only if G is a null graph.

⋆ **Proposition 1.2.** 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 $\eta(G) = \sum_{i=1}^{t} \eta(G_i)$.

⋆ **Proposition 1.3.** Let A be the adjacency matrix of a graph G. Then

$$detA = \sum (-1)^{r(H)} 2^{s(H)},$$

where the summation is over all spanning elementary subgraphs H of G.

⋆ **Theorem 1.1.** If T is a tree of order n and m is the size of its maximum matchings, then $\eta(T) = n - 2m$.

⋆ **Corollary 1.1.** Let T be a tree of order n. The nullity $\eta(T)$ of T is zero if and only if T is a PM-tree.

⋆ **Theorem 1.2.**(Tan Xuezhong, Liu Bolian, 2005) For any $U \in \mathcal{U}_n$ $(n \geq 5)$, $\eta(U) \leq n-4$.

⋆ **Theorem 1.3.**(Tan Xuezhong, Liu Bolian, 2005) The nullity set of $\mathcal{U}_n (n \geq 5)$ is $[0, n-4]$.

⋆ **Theorem 1.4.**(Tan Xuezhong, Liu Bolian, 2005) Let $U \in \mathcal{U}_n$ $(n \geq 5)$. Then $\eta(U) = n-4$ if and only if $U \cong U_1^*$ or $U \cong U_2^*$ or $U \cong U_3^*$, where U_1^*, U_2^* and U_3^* are shown in $Fig.1.1$.

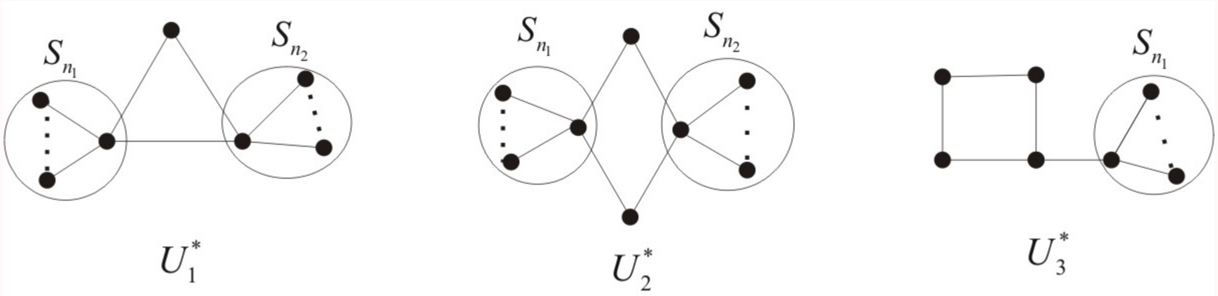


Fig.1.1

2 The nullity set of $\mathcal{B}_n$

⋆ **Lemma 2.1.** A path with four vertices of degree 2 in a bipartite graph G can be replaced by an edges without changing the value of $\eta(G)$.

⋆ **Lemma 2.2.** For a graph G containing a vertex of degree 1, if the induced subgraph H of G is obtained by deleting this vertex together with the vertex adjacent to it, then the relation $\eta(H) = \eta(G)$ holds.

⋆ **Lemma 2.3.** Let G_1, G_2 and G_3 be the graphs of order n shown in $Fig.2.1$, respectively. Then $\eta(G_1) = 0$, $\eta(G_2) = 1$ and $\eta(G_3) = \begin{cases} 2 & n \equiv 0(mod2) \\ 3 & n \equiv 1(mod2) \end{cases}$.

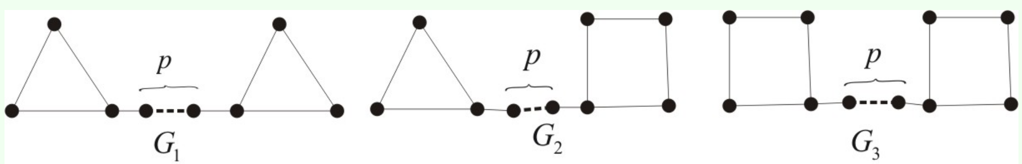


Fig.2.1

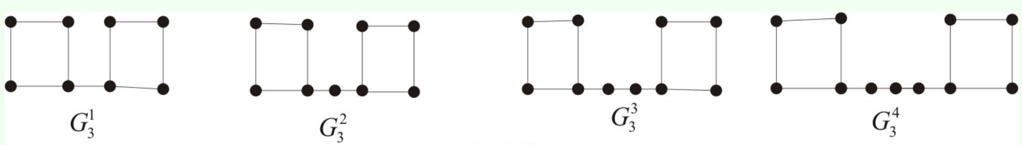


Fig.2.2

⋆ **Lemma 2.4.** $\eta(C_n) = \begin{cases} 2 & n \equiv 0(mod4) \\ 0 & otherwise \end{cases}$.

⋆ **Proof:** When $n \equiv 0(mod2)$, by Lemma 2.1, since C_n is a bipartite graph, we can get that

$$\eta(C_n) = \begin{cases} 2 & \text{if } n \equiv 0(mod4) \\ 0 & \text{if } n \equiv 2(mod4) \end{cases}$$

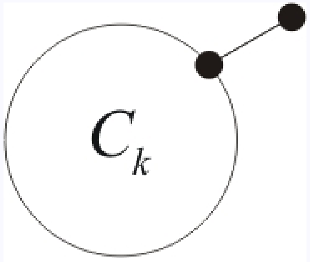
When $n \equiv 1(mod2)$, the spanning elementary subgraph of C_n is itself. Since $r(C_n) = n-1$, $s(C_n) = 1$, $detA(C_n) = 2 \neq 0$ by Proposition 1.3. Thus $\eta(C_n) = 0$.

⋆ **Lemma 2.5.** $\gamma(A(C_n)) = \begin{cases} n-2 & n \equiv 0(mod4) \\ n & otherwise \end{cases}$.

⋆ **Lemma 2.6.** For any $G \in B_n^+$ $(n \geq 7)$, $\eta(G) \leq n - 6$.

⋆ **Proof:** Let C_k, C_l are two vertex-disjoint cycles in G

- Case 1. $k, l \in \{3, 4\}$. There must exists one of graphs shown in $Fig.2.1$ as a vertex-induced subgraph of G since $G \in B_n^+$. By Lemma 2.3, for each G_i $(i = 1, 2, 3)$, we have $\gamma(A(G_i)) \geq 6$. Hence $\gamma(A(G)) \geq \gamma(A(G_i)) \geq 6$. Thus $\eta(G) \leq n - \gamma(A(G_i)) \leq n - 6$
- Case 2. $k \geq 5$ or $l \geq 5$. Without loss of generally, we assume that $k \geq 5$. There must exists H_1 as a vertex-induced subgraph of G since $G \in B_n^+$. By Lemma 2.2, it is easy to get that $\eta((H_1)) = \begin{cases} 1 & \text{if } k \equiv 0(mod2) \\ 0 & \text{if } k \equiv 1(mod2) \end{cases}$ Hence $\gamma(A(H_1)) = \begin{cases} k & \text{if } n \equiv 0(mod2) \\ k+1 & \text{if } n \equiv 1(mod2) \end{cases}$ Since $k \geq 5$, we have $\gamma(A(H_1)) \geq 6$. Therefore $\gamma(A(G)) \geq \gamma(A(H_1)) \geq 6$. Thus $\eta(G) \leq n - \gamma(A(H_1)) \leq n - 6$



H_1

⋆ **Theorem 2.1.** The nullity set of $B_n^+ (n \geq 7)$ is $[0, n-6]$.

⋆ **Proof:** By Lemma 2.6, it suffices to show that for each $k \in [0, n-6]$, there exist a graph $G \in B_n^+$ such that $\eta(G) = k$.

- When $k = 0$, let $G = G_1$ shown in $Fig.2.1$, we have $\eta(G_1) = 0$.

- When $1 \leq k \leq n-7$, let $G = G_4$ shown in $Fig.2.3$. Using Lemma 2.2 repeatedly, if $n \not\equiv k (mod 2)$, after $\frac{n-k-5}{2}$ steps, we get $P_2 \bigcup C_3 \bigcup kK_1$. Hence $\eta(G) = \eta(P_2 \bigcup C_3 \bigcup kK_1) = k$. If $n \equiv k (mod 2)$, after $\frac{n-k-4}{2}$ steps, we get $P_2 \bigcup P_2 \bigcup kK_1$. Hence $\eta(G) = \eta(P_2 \bigcup P_2 \bigcup kK_1) = k$.

- When $k = n-6$, let $G = G_5$ shown in $Fig.2.3$. By Lemma 2.2, we get $P_2 \bigcup C_4 \bigcup (n-8)K_1$. Hence $\eta(G) = \eta(P_2 \bigcup C_4 \bigcup (n-8)K_1) = n - 8 + 2 = n - 6$

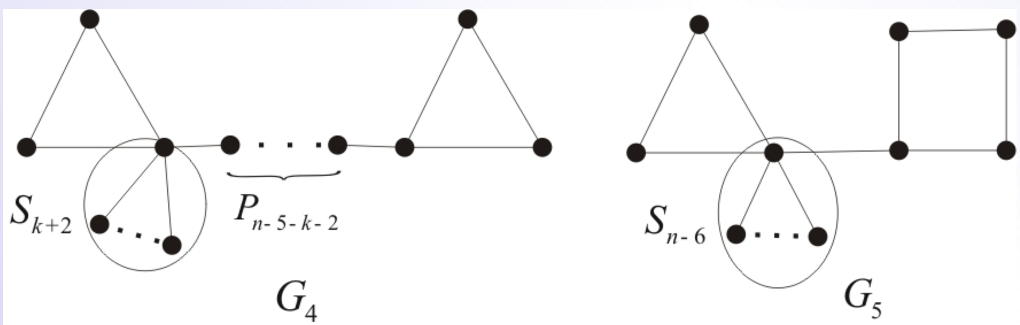


Fig.2.3

$\star$ **Lemma 2.7.** For any $G \in B_n^{++}$ $(n \geq 8)$, $\eta(G) \leq n-6$.

$\star$ **Theorem 2.2.** The nullity set of $B_n^{++}(n \geq 8)$ is $[0, n-6]$.

$\star$ **Lemma 2.8.** For any $G \in \theta_n$ $(n \geq 6)$, $\eta(G) \leq n-4$.

$\star$ **Theorem 2.3.** The nullity set of $\theta_n(n \geq 6)$ is $[0, n-4]$.

3 The bicyclic graph with maximal nullity

⋆ **Theorem 3.1.** Let $G \in B_n^+$ $(n \geq 10)$. Then $\eta(G) = n - 6$ if and only if $G \cong G_1^*$ or $G \cong G_2^*$ or $G \cong G_3^*$, where G_1^*, G_2^* and G_3^* are shown in $Fig.3.1$.

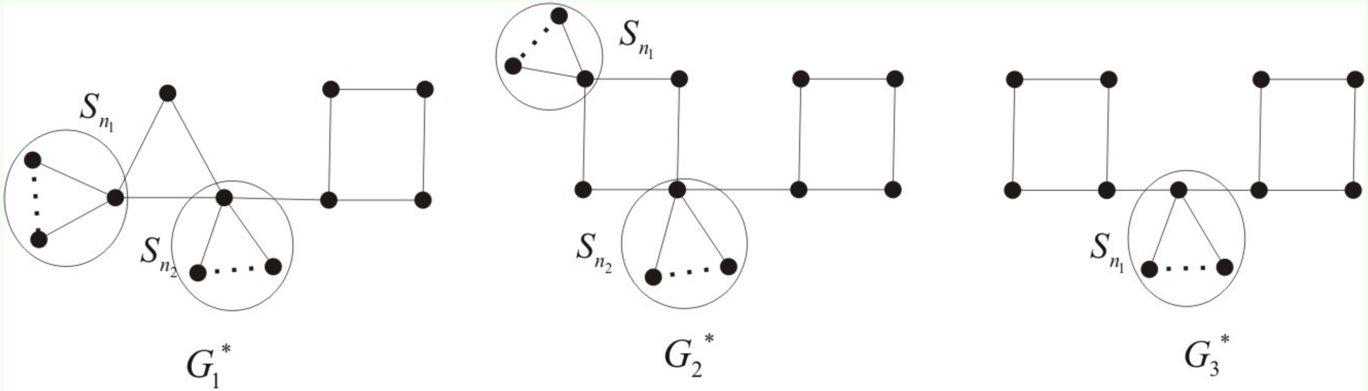


Fig.3.1

⋆ **Proof:** If $G \cong G_i^*$ $(i = 1, 2, 3)$, it is easy to check that $\eta(G) = n - 6$. So it is suffices to prove the converse side of the theorem.

Let C_k, C_l be two vertex-disjoint cycles in G.

- **Claim 1.** If $G \in B_n^+$ $(n \geq 10)$, $\eta(G) = n - 6$, then $k, l \in \{3, 4\}$.
- **Claim 2.** If $\eta(G) = n - 6$ $(n > 9)$ and $k, l \in \{3, 4\}$, then there exists at least one pendent vertex in G.

- Let x be a pendant vertex in G and y the adjacent vertex of x. Let $G_1 = G_{11} \bigcup G_{12} \bigcup \ldots \bigcup G_{1t}$ be the graph obtained by deleting x, y from G, where $G_{11}, G_{12}, \ldots, G_{1t}$ are connected components of G_1. At least one of G_{1i} $(i = 1, 2, \ldots, t)$ is nontrivial. Otherwise, G would be a star.
- In fact, there are at most two nontrivial components in G_1.
- Case 1. There is a unique nontrivial component in G_1.
- Case 2. There are two nontrivial components in G_1.
- Subcase 2.1. Both G_{11} and G_{12} contain pendent vertex.
- Subcase 2.2. Only one of G_{11}, G_{12} contains pendent vertices.
- subcase 2.3. G_{11} and G_{12} no contain pendent vertices.

⋆ **Theorem 3.2.** Let $G \in B_n^{++}$ $(n \geq 8)$. Then $\eta(G) = n - 6$ if and only if $G \cong G_1^*$ or $G \cong G_2^*$ or $G \cong G_3^*$ or $G \cong G_4^*$ or $G \cong G_5^*$ or $G \cong G_6^*$ or $G \cong G_7^*$ or $G \cong G_8^*$, where G_1^*, G_2^*, G_3^*, G_4^*, G_5^*, G_6^*, G_7^* and G_8^* are shown in $Fig.3.3$.

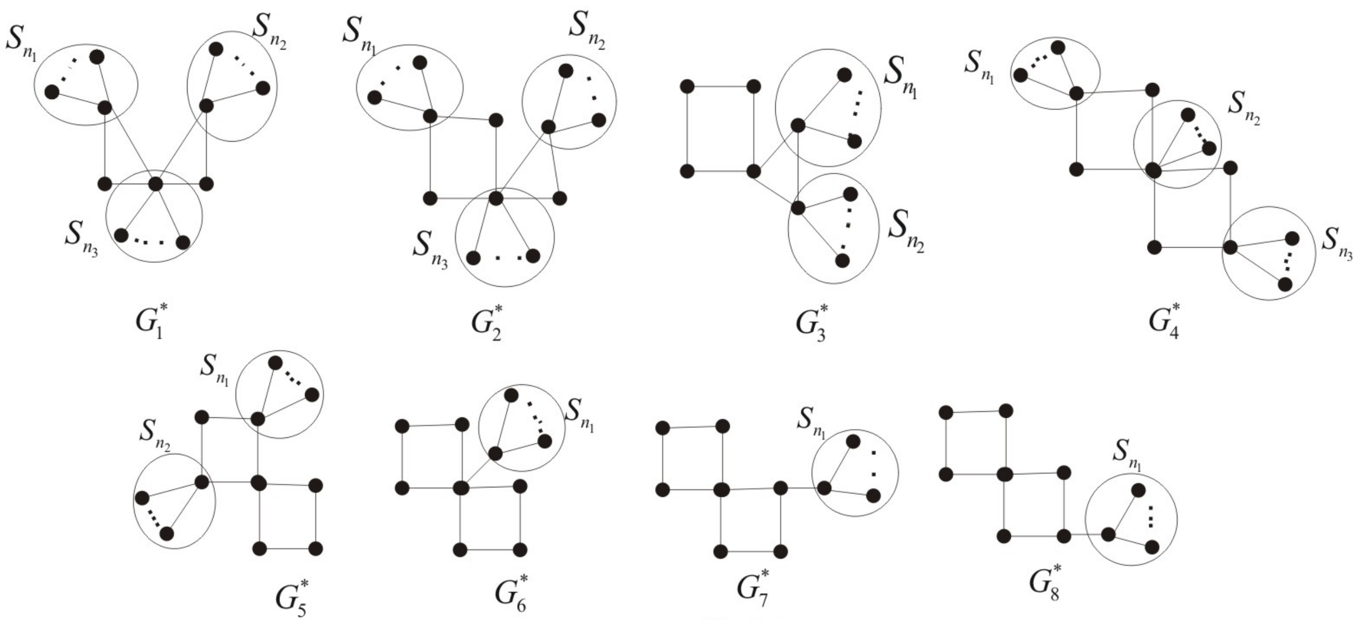


Fig.3.3

⋆ **Theorem 3.3.** Let $G \in \theta_n$ $(n \geq 6)$. Then $\eta(G) = n - 4$ if and only if $G \cong G_1^*$ or $G \cong G_2^*$ or $G \cong G_3^*$ or $G \cong G_4^*$ or $G \cong G_5^*$ or $G \cong G_6^*$, where G_1^*, G_2^*, G_3^*, G_4^*, G_5^* and G_6^* are shown in $Fig.3.6$.

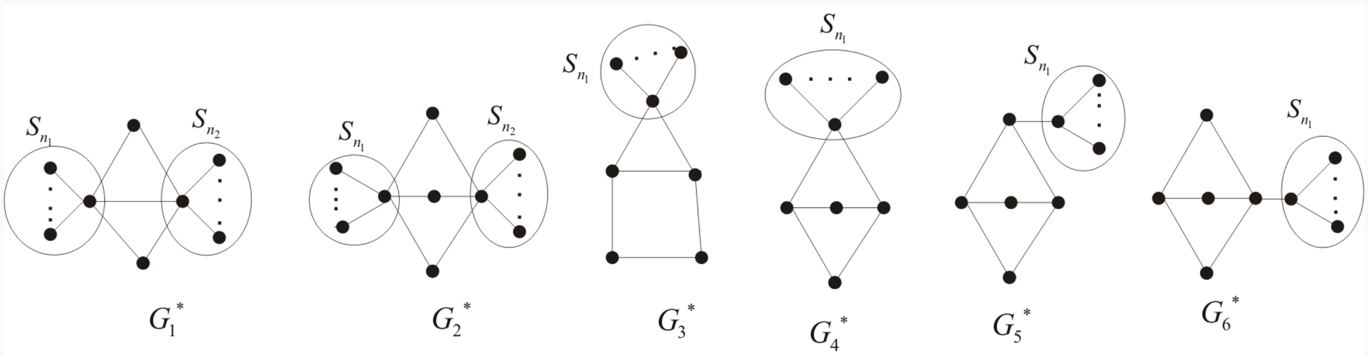


Fig.3.6

Thank You!