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Sharp lower bounds for the Zagreb indices of unicyclic graphs

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Abstract: The first Zagreb index M_1 is equal to the sum of the squares of the degrees of the vertices, and the second Zagreb index M_2 is equal to the sum of the products of the degrees of pairs of adjacent vertices of the respective graph. In this paper we present the lower bound on M_1 and M_2 among all unicyclic graphs of given order, maximum degree, and cycle length, and characterize graphs for which the bound is attained. Moreover, we obtain some relations between the Zagreb indices for unicyclic graphs.

Key words: First Zagreb index, second Zagreb index, unicyclic graph, maximum degree, cycle length

1. Introduction

Let $G=(V,E)$ be a simple graph with vertex set $V(G)$ and edge set $E(G)$. $d_G(u)$ denotes the degree of the vertex u of G. The maximum degree of G and the average of the degrees of the vertices adjacent to a vertex u are denoted by $\Delta(G)$ and $\mu_G(u)$, respectively. The cycle of a graph G is denoted by $C(G)$. Denote by $\mathcal{U}_n(k,\Delta)$ the set of all simple connected unicyclic graphs of order n with the maximum degree Δ and cycle length k. In $\mathcal{U}_n(k,\Delta)$, we must have $\Delta+k\leq n+2$. A pendant vertex is a vertex of degree one. The path, star, and cycle of order n are denoted by P_n $K_{1,n-1}$, and C_n respectively.

The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined as:

$$M_1(G)=\sum_{u\in V(G)}(d_G(u))^2 \quad \text{and} \quad M_2(G)=\sum_{uv\in E(G)}d_G(u)d_G(v).$$

The Zagreb indices were introduced in [9] and elaborated in [8]. These indices reflect the extent of branching of the molecular carbon-atom skeleton, and can thus be viewed as molecular structure descriptors [1] and [15]. Their main properties were summarized in [4, 7, 13, 19]. Some recent results on the Zagreb indices are reported in [4, 5, 9–12, 14–20]. [18] gave the unicyclic graphs with the first three smallest and largest M_1. [17] characterized the graphs with smallest and largest M_2 among all unicyclic graphs. [6] gave the unicyclic graphs of given order and cycle length with minimum and maximum Zagreb indices.

Recently, it has been conjectured that for each simple graph with n vertices and m edges, it holds that $M_1(G)/n\leq M_2(G)/m$. This conjecture has been disproved in general graphs and has been proved for chemical graphs and trees in [10, 16].

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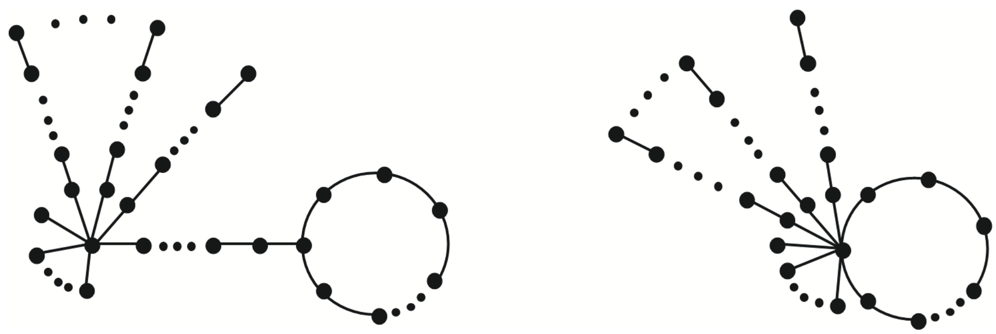
The paper is organized in the following way. In Section 2, we present the lower bound on M_1 in $\mathcal{U}_n(k,\Delta)$ and characterize extremal graphs. In Section 3, we obtain the lower bound on M_2 in $\mathcal{U}_n(k,\Delta)$ and characterize extremal graphs. Finally, in Section 4, we find some relations between M_1 and M_2 for unicyclic graphs and from these results it follows that $M_1(G)/n \leq M_2(G)/m$ for all unicyclic graphs.

2. Lower bound on M_1 in $\mathcal{U}_n(k,\Delta)$

A starlike tree is a tree with exactly one vertex having degree greater than two. Denote by $\mathcal{S}_{n,\Delta}$ the set of all starlike trees of order n with maximum degree Δ.



(a) (b)

Figure 1. (a) One graph in $\mathcal{A}_n(k,\Delta)$, (b) one graph in $\mathcal{B}_n(k,\Delta)$.

$\mathcal{A}_n(k,\Delta)$ denotes the set of unicyclic graphs obtained by identifying a pendant vertex of a starlike tree in $\mathcal{S}_{n-k+1,\Delta}$ with one vertex of C_k (see Figure 1(a)). Denote by $\mathcal{B}_n(k,\Delta)$ the set of graphs of order n obtained by attaching $\Delta-2$ paths to one vertex of C_k (see Figure 1(b)). Let A_n^k be the unicyclic graph obtained by identifying one pendant vertex of P_{n-k+1} with a vertex of C_k.

Lemma 2.1 *Let x be a pendant vertex of a connected graph G, which is adjacent to a vertex v. Also let y be a pendant vertex, different from x. Consider the transformation $G' = G - vx + yx$. Then $M_1(G) \geq M_1(G')$ with equality if and only if vertex x is adjacent to a vertex of degree 2.*

Proof $d_G(w) = d_{G'}(w)$ for $w \neq v, y$ whereas $d_{G'}(v) = d_G(v) - 1$ and $d_{G'}(y) = 2$. Thus

$$M_1(G) - M_1(G') = 2d_G(v) - 4. \tag{1}$$

Since $d_G(v) \geq 2$, $M_1(G) \geq M_1(G')$ with equality holding if and only if $d_G(v) = 2$. □

We have

$$M_1(G) = \begin{cases} \Delta(\Delta-3) + 4n + 4 & \text{if} \quad G \in \mathcal{A}_n(k,\Delta) \\ \Delta(\Delta-3) + 4n + 2 & \text{if} \quad G \in \mathcal{B}_n(k,\Delta). \end{cases} \tag{2}$$

Now we are ready to give a lower bound on M_1 and characterization of extremal graphs.

Theorem 2.2 *Let G be a graph in $\mathcal{U}_n(k,\Delta)$, where $3 \leq k \leq n - \Delta + 2$. Then*

$$M_1(G) \geq \Delta(\Delta-3) + 4n + 2$$

with equality if and only if $G \in \mathcal{B}_n(k,\Delta)$.

Proof If $G \in \mathcal{B}_n(k,\Delta)$ then $M_1(G) = \Delta(\Delta-3)+4n+2$, the equality holds. Now we have to show that

$$M_1(G) > \Delta(\Delta-3)+4n+2 \tag{3}$$

for all $G \notin \mathcal{B}_n(k,\Delta)$. If $G \in \mathcal{A}_n(k,\Delta)$ then from (2) the inequality holds in (3). Now we suppose that $G \notin \mathcal{A}_n(k,\Delta)$. Let u be the maximum degree vertex in G. We consider the following two cases.

Case $1:$ $u \notin V(C(G))$. In this case we find the longest path from vertex u to any pendant vertex v such that its each vertex ($\neq u$) is not contained in the path from vertex u to cycle $C(G)$. Since $G \notin \mathcal{A}_n(k,\Delta)$, there is a pendant vertex x ($x \neq v$), which is adjacent to a vertex y ($y \neq u$). We choose this pendant vertex x from G and consider the transformation $G' = G - yx + vx$; then $G' \in \mathcal{U}_n(k,\Delta)$ and $M_1(G) \geq M_1(G')$ by Lemma 2.1. By the above described transformation we have nonincreased the value of M_1. If $G' \in \mathcal{A}_n(k,\Delta)$ we are done. If not, then we continue the construction as follows. Clearly (u,x) is the longest path of G' in which its each vertex ($\neq u$) is not contained in the path from vertex u to cycle $C(G)$. Since $G' \notin \mathcal{A}_n(k,\Delta)$ we choose one pendant vertex, which is adjacent to a vertex ($\neq u$) of degree greater than or equal to 2 in G'. By applying the same transformation a sufficient number of times (s-times), we arrive at a graph $G^{(s)}$ in $\mathcal{A}_n(k,\Delta)$. Thus we have the following sequence:

$$M_1(G) \geq M_1(G') \geq M_1(G'') \geq \cdots \geq M_1(G^{(s-1)}) \geq M_1(G^{(s)}).$$

Since $G^{(s)} \in \mathcal{A}_n(k,\Delta)$, the inequality holds in (3), by (2).

Case $2:$ $u \in V(C(G))$. In this case we find the longest path from vertex u to any pendant vertex v such that its each vertex ($\neq u$) is not contained in $C(G)$. Using the same procedure as in Case 1, we get

$$M_1(G) \geq M_1(G') \geq M_1(G'') \geq \cdots \geq M_1(G^{(s-1)}) \geq M_1(G^{(s)})$$

where $G^{(s)} \in \mathcal{B}_n(k,\Delta)$. Therefore there exists exactly one pendant vertex in $G^{(s-1)}$, which is adjacent to a vertex of degree three and nonadjacent to the maximum degree vertex u. We choose this pendant vertex in $G^{(s-1)}$ and apply the same transformation, and we arrive at $G^{(s)}$. Thus we have $M_1(G) \geq M_1(G^{(s-1)}) > M_1(G^{(s)})$ by Lemma 2.1. Hence the inequality holds in (3) and the theorem is proved. □

The proof of Corollary 2.3 follows directly from Theorem 2.2.

Corollary 2.3 *[6] Let G be a unicyclic graph of order n and cycle length k. Then*

$$M_1(G) \geq 4n+4$$

with equality if and only G is isomorphic to A_n^k.

3. Lower bound on M_2 in $\mathcal{U}_n(k,\Delta)$

Let B_n^k ($k \leq n$) be the unicyclic graph with $n-k$ pendant vertices and its each pendant vertex is adjacent to one vertex of C_k. In particular, $B_n^n = C_n$, a cycle of order n. Denote by $C_{n,\Delta}^k$ ($\Delta \geq 4$) a unicyclic graph obtained by identifying two pendant vertices of the path $P_{n-\Delta-k+2}$ with the center of star $K_{1,\Delta-1}$ and one vertex of cycle C_k, respectively. Denote by $D_{n,\Delta}^k$ ($\Delta \geq 4$) a unicyclic graph of order n obtained by identifying a pendant vertex of $P_{n-\Delta-k+3}$ with a pendant vertex of $B_{\Delta+k-2}^k$.

Lemma 3.1 *Let G be a connected graph possessing two adjacent vertices u and v both of degree greater than or equal to 2. Also let x be a pendant vertex of G, which is adjacent to a vertex y $(\neq u, v)$. Consider the transformation $G' = G - yx - uv + ux + xv$. Then $M_2(G) \geq M_2(G')$ with equality if and only if $d_G(u) = 2$ or $d_G(v) = 2$, and vertex y is adjacent to a vertex of degree 2 and a vertex of degree 1, respectively, in G.*

Proof Now we have $d_G(w) = d_{G'}(w)$ for $w \neq x, y$ whereas $d_{G'}(y) = d_G(y) - 1$ and $d_{G'}(x) = d_G(x) + 1 = 2$. Thus

$$\begin{aligned} M_2(G) - M_2(G') &= d_G(u)d_G(v) - 2d_G(u) - 2d_G(v) + d_G(y) + \sum_{wy \in E(G')} d_{G'}(w) \\ &= (d_G(u) - 2)(d_G(v) - 2) + d_G(y) + d_G(y)\mu_G(y) - 5. \end{aligned} \tag{4}$$

Since G is connected, $d_G(y)\mu_G(y) \geq 3$. Also we have $(d_G(u) - 2)(d_G(v) - 2) \geq 0$ and $d_G(y) \geq 2$. Thus $M_2(G) \geq M_2(G')$.

Suppose that $M_2(G) = M_2(G')$. Then all inequalities in the above argument must be equalities. Thus $d_G(u) = 2$ or $d_G(v) = 2$, and $d_G(y) = 2$ $d_G(y)\mu_G(y) = 3$. Hence the result. □

The following result is obtained in [6].

Lemma 3.2 *[6] Let G be a unicyclic graph of order n and cycle length k. If G is different from A_n^k then $M_2(G) > M_2(A_n^k)$.*

We have

$$M_2(G) = \begin{cases} \Delta(\Delta - 2) + 4n & \text{if } G \cong B_n^k \\ \Delta(\Delta - 2) + 4n + 4 & \text{if } G \cong C_{n,\Delta}^k \Delta + k = n \\ \Delta(\Delta - 3) + 4n + 6 & \text{if } G \cong C_{n,\Delta}^k \Delta + k < n \\ \Delta(\Delta - 1) + 4n - 2 & \text{if } G \cong D_{n,\Delta}^k \Delta + k \leq n + 1. \end{cases} \tag{5}$$

Let $G \in \mathcal{U}_n(k, \Delta)$, then obviously $\Delta + k \leq n + 2$. If $\Delta + k = n$ and the maximum degree vertex does not lie on the cycle of G then G is isomorphic to $C_{n,\Delta}^k$. If $\Delta + k \geq n$ and G is different from $C_{n,\Delta}^k$ then the maximum degree vertex of G must lie on the cycle. In this case we can easily calculate and characterize graphs with minimum M_2. Therefore we give the lower bound on $M_2(G)$ and obtain some characterization of extremal graphs when $\Delta + k < n$.

Theorem 3.3 *Let G be a graph in $\mathcal{U}_n(k, \Delta)$, where $\Delta + k < n$. Then*

$$M_2(G) \geq \begin{cases} \Delta(\Delta - 3) + 4n + 6 & \text{if } \Delta \geq 5 \\ 4n + 10 & \text{if } \Delta = 4 \\ 4n + 4 & \text{if } \Delta = 3 \end{cases} \tag{6}$$

where Δ is maximum degree in G. Moreover, the equalities hold in (6) if and only if $G \cong C_{n,\Delta}^k$; $G \cong C_{n,4}^k$ or $G \cong D_{n,4}^k$; $G \cong A_n^k$; respectively.

Proof Let u be maximum degree vertex in G and also let $C(G)$ be the unique cycle in G. Since $\Delta + k < n$, we have $\Delta \geq 3$. First we assume that $\Delta = 3$ in G. By Lemma 3.2 we have $M_2(G) \geq 4n + 4$ with equality if and only if $G \cong A_n^k$. Next we assume that $\Delta \geq 4$. Now we consider the following two cases:

Case 1 : $u \notin C(G)$. In this case, we show that if G is different from $C_{n,\Delta}^k$ then $M_2(G) > M_2(C_{n,\Delta}^k)$. Let v be a vertex adjacent to maximum degree vertex u, which lies on the path from u to the cycle $C(G)$. Since G is different from $C_{n,\Delta}^k$, there is a pendant vertex x such that $xy \in E$ $(y \neq u)$. Consider the transformation $G' = G - yx - uv + ux + xv$. By Lemma 3.1, we have $M_2(G) \geq M_2(G')$. Applying the same transformation a sufficient number of times (s-times), we arrive at $G^{(s)}$ such that $G^{(s)} \cong C_{n,\Delta}^k$. Thus $M_2(G) \geq M_2(C_{n,\Delta}^k)$. There is exactly one pendant vertex in $G^{(s-1)}$, which is nonadjacent to the maximum degree vertex and adjacent to a vertex of degree greater than or equal to 2. We choose this pendant vertex and apply the same transformation on $G^{(s-1)}$ to arrive at $G^{(s)}$; then by Lemma 3.1 we have $M_2(G^{(s-1)}) > M_2(G^{(s)})$ that is $M_2(G) > M_2(C_{n,\Delta}^k)$.

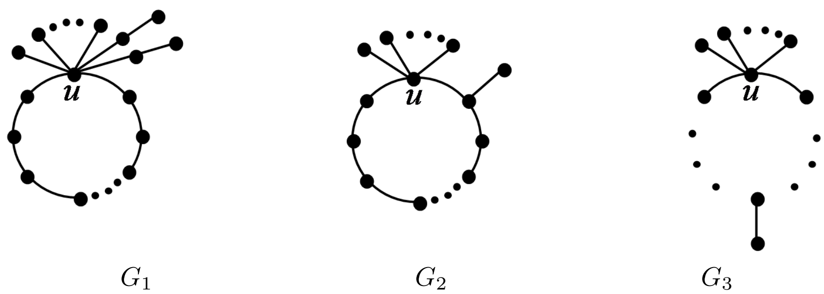


Figure 2. $|V(G_i)| = n$ and $d_{G_i}(u) = \Delta$, $i = 1, 2, 3$.

Case 2 : $u \in C(G)$. In this case, we show that if G is different from $D_{n,\Delta}^k$ then $M_2(G) > M_2(C_{n,\Delta}^k)$. Let v be a vertex adjacent to maximum degree vertex u, which lies on the cycle $C(G)$. Also let x be a pendant vertex such that $xy \in E$ $(y \neq u)$. We choose this pendant vertex from G and consider the transformation $G' = G - yx - uv + ux + xv$. Then by Lemma 3.1 we have $M_2(G) \geq M_2(G')$ where $G' \in \mathcal{U}_n(k+1, \Delta)$ i.e. the cycle length is increasing. Repeating the same transformation, we can always arrive at a graph G^* such that $G^* = G_1$ or $G^* = G_2$ or $G^* = G_3$ (see Figure 2) and $M_2(G) \geq M_2(G^*)$.

(i) If $G^* \cong G_1$, then

$$M_2(G^*) = \Delta^2 + 4n - 4. \tag{7}$$

Hence $M_2(G^*) > M_2(C_{n,\Delta}^k)$ as $\Delta > 3$. Thus $M_2(G) > M_2(C_{n,\Delta}^k)$.

(ii) If $G^* \cong G_2$, then

$$M_2(G^*) = \Delta^2 - \Delta + 4n + 1. \tag{8}$$

Hence $M_2(G^*) > M_2(C_{n,\Delta}^k)$ by (5). Thus $M_2(G) > M_2(C_{n,\Delta}^k)$.

(iii) If $G^* \cong G_3$, then

$$M_2(G^*) = \Delta^2 - 2\Delta + 4n + 3. \tag{9}$$

Thus $M_2(G^*) > M_2(C_{n,\Delta}^k)$ by (5), that is, $M_2(G) > M_2(C_{n,\Delta}^k)$. Since $\Delta + k < n$, we have $M_2(C_{n,\Delta}^k) \leq M_2(D_{n,\Delta}^k)$ with equality if and only if $\Delta = 4$. From above, Case 1 and Case 2, we get the required result. $\square$

Denote $\mathcal{C}_\Delta = \{C_{n,\Delta}^k \mid 3 \leq k \leq n - \Delta - 1\}$. Note that if $G \in \mathcal{C}_\Delta$ then $M_2(G) = \Delta(\Delta - 3) + 4n + 6$.

Corollary 3.4 *Let G be a unicyclic graph of order n and maximum vertex degree Δ. Then*

$$M_2(G) \geq \begin{cases} \Delta(\Delta-3)+4n+6 & \text{if } \Delta > 6 \\ \Delta(\Delta-2)+4n & \text{if } \Delta \leq 6 \end{cases} \tag{10}$$

with equality if and only if $G \in \mathcal{C}_\Delta$, $G \cong B_n^k$ or $G \in \mathcal{C}_6$, respectively.

Proof Let u be maximum degree vertex in G and k be the length of $C(G)$. First, we suppose that $u \notin V(C(G))$. Then $\Delta+k \leq n$. If $\Delta+k=n$ then $G \cong C_{n,\Delta}^k$ and from (5), we have $M_2(G)=\Delta(\Delta-3)+4n+6$. Otherwise, if G is different from $C_{n,\Delta}^k$ then by Case 1 of Theorem 3.3 we have $M_2(G) > M_2(C_{n,\Delta}^k)$, that is,

$$M_2(G) > \Delta(\Delta-3)+4n+6. \tag{11}$$

Now suppose that $u \in V(C(G))$ and G is different from B_n^k. Then by Case 2 of Theorem 3.3 we have $M_2(G) \geq M_2(G^*)$. From (7), (8), and (9), $M_2(G^*) > M_2(B_n^k)$ by (5). Hence $M_2(G) > M_2(B_n^k)$, that is,

$$M_2(G) > \Delta(\Delta-2)+4n. \tag{12}$$

From (11) and (12), we get the required result. □

4. Relations between Zagreb indices

$S(m_1, m_2, \ldots, m_k)$ is a unicyclic graph of order n with girth k and $n-k$ pendant vertices, where m_i is the number of pendant vertices adjacent to i-th vertex of the cycle [2]. We consider that the vertices in the cycle are numbered clockwise (see Figure 3). Clearly $\sum_{i=1}^{k} m_i = n-k$ and $S(0,0,\ldots,0)=C_n$.

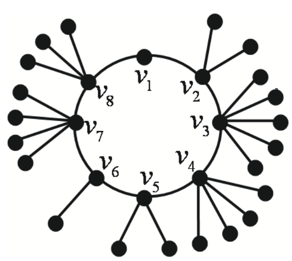


Figure 3. $S(0,2,5,4,2,1,4,3)$.

A cyclic graph is a graph containing at least one graph cycle. Denote $h(G)=M_2(G)-M_1(G)$ for a graph G.

Lemma 4.1 *Let G be a cyclic graph possessing two adjacent vertices u and v both of degree greater than or equal to 2. Also let x be pendant vertex of G, which is adjacent to a vertex y ($\neq u, v$). Consider the transformation $G' = G - yx - uv + ux + xv$.*

(i) If $y \notin V(C(G))$, then $h(G) \geq h(G')$.

(ii) If $y \in V(C(G))$, then $h(G) \geq h(G')+1$.

Proof Now we have $d_G(w) = d_{G'}(w)$ for $w \neq x, y$ whereas $d_{G'}(y) = d_G(y) - 1$ and $d_{G'}(x) = d_G(x) + 1 = 2$. Thus

$$M_1(G') - M_1(G) = -2d_G(y) + 4.$$

Combining the above equation and (4), we get

$$\begin{aligned} h(G) - h(G') &= M_2(G) - M_2(G') + M_1(G') - M_1(G) \\ &= (d_G(u) - 2)(d_G(v) - 2) - d_G(y) + d_G(y)\mu_G(y) - 1. \end{aligned} \tag{13}$$

If $y \notin V(C(G))$, then $d_G(y)\mu_G(y) \geq d_G(y) + 1$. Otherwise $d_G(y)\mu_G(y) \geq d_G(y) + 2$. From the above and (13), we get the required results. □

Denote $\mathcal{S} = \{S(m_1, m_2, \ldots, m_k) | \ m_{i-1} = m_{i+1} = 0 \text{ for } m_i \neq 0 \ 2 \leq i \leq k, \text{ where } m_{k+1} = m_1\}$.

Theorem 4.2 *Let G be a unicyclic graph with cycle length k. Then*

$$M_2(G) - M_1(G) \geq \sum_{u \in V(C(G))} d_G(u) - 2k \tag{14}$$

with equality if and only if $G \in \mathcal{S}$.

Proof We distinguish the following two cases.

Case 1 : $G \cong S(m_1, m_2, \ldots, m_k)$. If $m_i = 0$ for all $1 \leq i \leq k$, then $G \cong C_n$ and the equality in (14) holds. Otherwise, there is a pendant vertex x adjacent to a vertex y, $y \in V(C(G))$. Let u and v be the adjacent vertices on the cycle C_k. We choose pendant vertex x from G and consider the transformation $G' = G - yx - uv + ux + xv$. Then by Lemma 4.1(ii) we have $h(G) \geq h(G') + 1$. Clearly, the number of pendant vertices in G is $n - k$. Therefore, repeating the same transformation $n - k$ times, we arrive at C_n. Then we have

$$h(G) \geq h(C_n) + n - k = \sum_{u \in V(C(G))} d_G(u) - 2k$$

since $h(C_n) = 0$ and $n - k = \sum_{u \in V(C(G))} d_G(u) - 2k$. The equality holds in Lemma 4.1(ii) if and only if $d_G(y)\mu_G(y) = d_G(y) + 2$ and $d_G(u) = 2$ and/or $d_G(v) = 2$. Thus, two adjacent vertices to y in the cycle have degree 2. Hence $G \in \mathcal{S}$.

Case 2 : $G \ncong S(m_1, m_2, \ldots, m_k)$. Then there is a pendant vertex x adjacent to a vertex y, $y \notin V(C(G))$. Let u and v be the adjacent vertices on the cycle C_k. We choose pendant vertex x from G and consider the transformation $G' = G - yx - uv + ux + xv$. Then by Lemma 4.1(i) we have $h(G) \geq h(G')$. Repeating this transformation s $(= n - \sum_{u \in V(C(G))} d_G(u) + k)$ times, we arrive at a graph $G^{(s)}$, such that $G^{(s)} \cong S(l_1, l_2, \ldots, l_{k+s})$. Thus $h(G) \geq h(G^{(s)})$ and the number of pendant vertices in $G^{(s)}$ is $n - k - s$. Hence, similarly to Case 1, we have

$$h(G^{(s)}) \geq h(C_n) + n - k - s = \sum_{u \in V(C(G))} d_G(u) - 2k$$

since $h(C_n) = 0$ and $s = n - \sum_{u \in V(C(G))} d_G(u) + k$.

Clearly, there is exactly one pendant vertex in $G^{(s-1)}$, which is adjacent to a vertex w where $d_{G^{(s-1)}}(w) = 2$ and $w \notin V(C(G^{(s-1)}))$. We choose this pendant vertex and apply the same transformation on $G^{(s-1)}$ to arrive at $G^{(s)}$; then from (13) we have $h(G^{(s-1)}) > h(G^{(s)})$ because $d_{G^{(s-1)}}(w)\mu_{G^{(s-1)}}(w) \geq 4$. Therefore $h(G) > h(G^{(s)}) \geq \sum_{u\in V(C(G))} d_G(u) - 2k$ and in this case the inequality in (14) is strict. □

Theorem 4.3 *Let G be a unicyclic graph of order n with maximum degree Δ. Then*

$$M_2(G) - M_1(G) \geq \begin{cases} \Delta - 2 & \text{if } d = 0 \\ \Delta & \text{if } d = 1 \\ 2 & \text{if } d > 1 \end{cases} \tag{15}$$

where d is the length of the shortest path from the maximum degree vertex u to the cycle $C(G)$. The equalities hold in (15) if and only if $G \cong B_n^k$, $G \cong C_{n,\Delta}^k$, $\Delta + k = n$, and $G \in \mathcal{C}_\Delta$, respectively.

Proof (i) The proof of the first inequality in (15) can be done from Theorem 4.2 as

$$\sum_{u\in V(C(G))} d_G(u) \geq \Delta + 2(k-1).$$

We can see easily that the first equality holds in (15) if and only if $G \cong B_n^k$.

(ii) Now we give a proof of the second inequality. Let $d = 1$. Then $\Delta + k \leq n$. If $\Delta + k = n$, then $G \cong C_{n,\Delta}^k$ and we have $M_2(G) - M_1(G) = \Delta$, by (2) and (5). Otherwise, $\Delta + k < n$ and hence $G \ncong C_{n,\Delta}^k$ as $d = 1$. Let u be the maximum degree vertex of G. Then there is a pendant vertex x, which is adjacent to a vertex y and nonadjacent to u. Also, let v and w be adjacent vertices in the cycle $C(G)$. We choose pendant vertex x from G and consider the transformation $G' = G - yx - vw + vx + xw$. Then by Lemma 4.1 (i) we have $h(G) \geq h(G')$. Repeating the above transformation a sufficient number of times (s-times), we arrive at a graph $G^{(s)}$ such that $G^{(s)} \cong C_{n,\Delta}^{k'}$, $\Delta + k' = n$, where $k' = k + s$. Therefore $h(G) \geq h(C_{n,\Delta}^{k'})$, $\Delta + k' = n$, that is, $M_2(G) - M_1(G) \geq \Delta$.

If $G \ncong C_{n,\Delta}^k$, $\Delta + k < n$ then from the above there exists exactly one pendant vertex in $G^{(s-1)}$, which is nonadjacent to the maximum degree vertex. We choose this pendant vertex and apply the same transformation on $G^{(s-1)}$ to arrive at $G^{(s)}$; then from (13) one can easily see that $h(G^{(s-1)}) > h(C_{n,\Delta}^{k'})$, $\Delta + k' = n$. Hence $h(G) > h(C_{n,\Delta}^{k'})$, $\Delta + k' = n$, that is, $M_2(G) - M_1(G) > \Delta$.

(iii) Using the same technique as in (ii), we get the third inequality in (15) and equality holds in (15) if and only if $G \in \mathcal{C}_\Delta$. □

Corollary 4.4 *[3, 11] Let G be a unicyclic graph of order n. Then $M_2(G) \geq M_1(G)$ with equality holding if and only if G is isomorphic to C_n.*

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