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Extremal Modified Schultz Index of Bicyclic Graphs

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Abstract

For a graph $G = (V, E)$, the modified Schultz index of G is defined as

$$S^*(G) = \sum_{\{u,v\} \subseteq V(G)} (d_G(u) \cdot d_G(v)) d_G(u, v)$$

where $d_G(u)$ (or $d(u)$) is the degree of the vertex u of G, and $d_G(u, v)$ is the distance between u and v. Let $\mathcal{B}(n)$ be the set of bicyclic graph with n vertices. In this paper, we study the modified Schultz index of $\mathcal{B}(n)$, graphs in $\mathcal{B}(n)$ with the smallest modified Schultz index $S^*(G)$ are determined. The corresponding extremal graphs are characterized as well.

1 Introduction

We use Bondy and Murty [1] for terminology and notions not defined here. Let $G = (V, E)$ be a simple connected graph with the vertex set V and the edge set E. For any $u, v \in V$, $d_G(u)$ (or simply by $d(u)$) and $d_G(u, v)$ denote the degree of u and the distance (i.e.,the number of edges on the shortest path) between u and v, respectively. The distance $d(x, y)$ from a vertex x to another vertex y is the minimum number of edges in an $x - y$ path. The distance $d_G(x, S)$ from a vertex x to the set S is $\min_{y \in S} d(x, y)$. A leaf is a vertex of degree one and a stem is a vertex adjacent to at least one leaf, pendant edges are edges incident to a leaf and stem, denote it simply as K_2. Let P_n, C_n and $K_{1,n-1}$(or S_n) be the path, cycle and the star on n vertices.

The oldest and most thoroughly examined use of a topological index in chemistry was by Wiener [2] in the study of paraffin boiling points, and the topological index was called Wiener index or Wiener number. The Wiener index of the graph G, is equals to the sum of distances between all pairs of vertices of the respective molecular graph, i.e.,

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v) \tag{1}$$

In connection with certain investigations in mathematical chemistry, Schultz [3] in 1989 introduced a graph-theoretical descriptor for characterizing alkanes by an integer, namely the *Schultz index*, defined as

$$S(G) = \sum_{\{u,v\} \subseteq V(G)} (d_G(u) + d_G(v)) d_G(u, v) \tag{2}$$

The Schultz index attracted much attention after it was discovered. It has been demonstrated that $S(G)$ and $W(G)$ are closely mutually related for certain classes of molecular graphs [4-10]. Klein *et al* [6] derived an explicit relation between $S(G)$ and $W(G)$ for trees:

$$S(G) = 4W(G) - n(n-1) \tag{3}$$

Motivated by equations (2) and (3), I. Gutman [9] defined the modification of $S(G)$, i.e.,

$$S^*(G) = \sum_{\{u,v\} \subseteq V(G)} (d_G(u) \cdot d_G(v)) d_G(u, v) \tag{4}$$

which here we refer to as *the modified Schultz index*. A result analogous to equation (3) applies [9]:

$$S^*(G) = 4W(G) - (n-1)(2n-1) \tag{5}$$

In [11], the authors derived relations between $W(G)$ and $S(G)$, $S^*(G)$ for the (unbranched) hexagonal chain composed of n fused hexagons, i.e.,

$$S(G) = \frac{25}{4} W(G) - \frac{3}{4}(2n+1)(20n+7)$$

$$S^*(G) = 5W(G) - 3(2n+1)^2$$

In [12-15], the authors derived the formulas for calculating the modified Schultz index of nanotubes covered by C_4 and polyhex nanotubes, C_4C_8 nanotubes. More results in this direction can be found in Refs. [16-23].

The cyclomatic number of a connected graph G is defined as $c(G) = m - n + 1$. A graph G with $c(G) = k$ is called a k cyclic graph, for $c(G) = 2$, we named G as a bicyclic graph. Let $\mathcal{B}(n)$ be the set of all bicyclic graphs with n vertices. For any graph $G \in \mathcal{B}(n)$, there are two fundamental cycles C_p and C_q in G. As described in [24, 25], we divide all the $\mathcal{B}(n)$ with two cycles of lengths p and q into three classes.

(1) $\mathbb{A}(p, q)$ is the set of $G \in \mathcal{B}(n)$ in which the cycles C_p and C_q have only one common vertex;

(2) $\mathbb{B}(p, q)$ is the set of $G \in \mathcal{B}(n)$ in which the cycles C_p and C_q have no common vertex;

(3) $\mathbb{C}(p, q, l)$ is the set of $G \in \mathcal{B}(n)$ in which the cycles C_p and C_q have a common path of length l.

Note that the induced subgraph of vertices on the cycles of $G \in \mathbb{C}(p, q)$ (or $\mathbb{C}(q, p)$), $\mathbb{C}(p, q, l)$) is showed in Fig. 1(a) (or (b),(c)) and $\mathbb{C}(p, q, l) = \mathbb{C}(p, p + q - 2l, p - l) = \mathbb{C}(p + q - 2l, q, q - l)$.

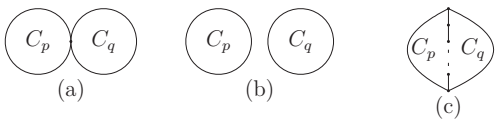


Fig 1.

In this paper, we shall study the modified Schultz index of $\mathcal{B}(n)$ by introducing two grafting transformations, the lower bounds for $S^*(G)$ are determined. We also characterize the corresponding extremal graphs.

2 Preliminaries

Let $E' \subseteq E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E'. $W \subseteq V(G)$, $G - W$ denotes the subgraph of G obtained by deleting the vertices of W and the edges incident with them.

For any two graphs G_1 and G_2, if there exists a common vertex v between them, we denote this graph as $G_1 v G_2$, i.e., the vertex set of $G_1 v G_2$ is $V(G_1) \cup V(G_2)$, $V(G_1) \cap V(G_2) = \{v\}$, and $E(G_1 v G_2) = E(G_1) \cup E(G_2)$, Obviously, if $|V(G_1)| = n_1 + 1$ and

$|V(G_2)| = n_2 + 1$, then $|V(G_1vG_2)| = n_1 + n_2 + 1$. If there exists a bridge uv between them such that $u \in V(G_1)$ and $v \in V(G_2)$, we denote this graph as G_1uvG_2. If there are a copies of graphs $G_1, G_2, \cdots, G_l (l \geq 2)$ with all graphs sharing one common vertex v, then, we denote this graph as $G_1vG_2v \cdots vG_l$.

For convenience, we provide some grafting transformations, which will decrease the modified Schultz index of graphs in the following:

Grafting transformations 1. Let uv is an edge of G_1uvG_2, G_1 and G_2 are 2-edge-connected graphs, $G_1uG_2uK_2$ is the graph transformed from G_1uvG_2 , depicted in Fig 2. with $|V(G_1)|, |V(G_2)| \geq 2$

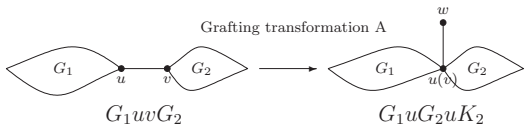


Fig 2. The grafting transformation A

Lemma 1. Let $G_1uG_2uK_2$ be obtained from G_1uvG_2 by grafting transformation A, then $S^*(G_1uG_2uK_2) < S^*(G_1uvG_2)$.

Proof. Let $G = G_1uvG_2$, $G' = G_1uG_2uK_2$. By the definition of modified Schultz index, we have

$$
\begin{aligned}
S^* \quad & (G') - S^*(G) = [d(u) + d(v) - 1] \\
+ \quad & \sum_{x \in V(G_1)\backslash u} d(x)(d_G(x,u) + 1) + \sum_{y \in V(G_2)\backslash v} d(y)(d_G(y,v) + 1) \\
+ \quad & [d(u) + d(v) - 1] \left(\sum_{x \in V(G_1)\backslash u} d(x) d_G(x,u) + \sum_{y \in V(G_2)\backslash v} d(y) d_G(y,v) \right) \\
+ \quad & \sum_{x \in V(G_1)\backslash u} \sum_{y \in V(G_2)\backslash v} d(x)d(y)(d_G(x,y) - 1) - d(u) \cdot d(v) \\
- \quad & d(u) \sum_{x \in V(G_1)\backslash u} d(x) d_G(x,u) - d(v) \sum_{y \in V(G_2)\backslash v} d(y) d_G(y,v) \\
- \quad & d(u) \sum_{y \in V(G_2)\backslash v} d(y)(d_G(y,v) + 1) - d(v) \sum_{x \in V(G_1)\backslash u} d(x)(d_G(x,u) + 1)
\end{aligned}
$$

$$
\begin{aligned}
&- \sum_{x\in V(G_1)\setminus u}\sum_{y\in V(G_2)\setminus v} d(x)d(y)d_G(x,y)\\
&= d(u)+d(v)-1-d(u)d(v)+\sum_{x\in V(G_1)\setminus u} d(x)d_G(x,u)+\sum_{x\in V(G_1)\setminus u} d(x)\\
&+ \sum_{y\in V(G_2)\setminus v} d(y)d_G(y,v)+\sum_{y\in V(G_2)\setminus v} d(y)+d(u)\sum_{x\in V(G_1)\setminus u} d(x)d_G(x,u)\\
&+ d(v)\sum_{x\in V(G_1)\setminus u} d(x)d_G(x,u)+d(v)\sum_{y\in V(G_2)\setminus v} d(y)d_G(y,v))-\sum_{x\in V(G_1)\setminus u} d(x)d_G(x,u)\\
&- \sum_{y\in V(G_2)\setminus v} d(y)d_G(y,v)-d(v)\sum_{y\in V(G_2)\setminus v} d(y)d_G(y,v)-d(u)\sum_{y\in V(G_2)\setminus v} d(y)d_G(y,v)\\
&- d(v)\sum_{x\in V(G_1)\setminus u} d(x)d_G(x,u)-d(u)\sum_{y\in V(G_2)\setminus v} d(y)-d(v)\sum_{x\in V(G_1)\setminus u} d(x)\\
&- \sum_{x\in V(G_1)\setminus u}\sum_{y\in V(G_2)\setminus v} d(x)d(y)\\
&= d(u)+d(v)-1-d(u)d(v)+(1-d(v))\sum_{x\in V(G_1)\setminus u} d(x)+(1-d(u))\sum_{y\in V(G_2)\setminus v} d(y)\\
&= -(d(u)-1)(d(v)-1)+(1-d(v))\sum_{x\in V(G_1)\setminus u} d(x)+(1-d(u))\sum_{y\in V(G_2)\setminus v} d(y)\\
&- \sum_{x\in V(G_1)\setminus u}\sum_{y\in V(G_2)\setminus v} d(x)d(y)<0
\end{aligned}
$$

The proof is completed.

Remark 1. Repeating grafting transformation A, any tree can changed into a star, any unicyclic or bicyclic graph can be changed into an unicyclic or bicyclic graph such that all the edges not on the cycles are pendant edges.

Grafting transformations 2. Let u and v be two vertices in G. $u_1, u_2, \cdots, u_s$ are the leaves adjacent to u, $v_1, v_2, \cdots, v_t$ are the leaves adjacent to v. $G' = G - \{vv_1, vv_2, \cdots, vv_t\} + \{uv_1, uv_2, \cdots, uv_t\}$, $G'' = G - \{uu_1, uu_2, \cdots, uu_s\} + \{vu_1, vu_2, \cdots, vu_s\}$, and $|V(G_0)| \geq 3$, as shown in Fig 3.

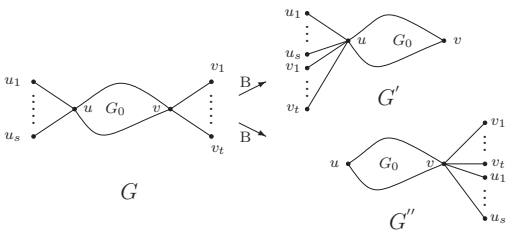


Fig 3. Grafting transformation B

Lemma 2. Let G' and G'' be obtained from G by grafting transformation B. Then,

$$S^*(G) > \min\{S^*(G'), S^*(G'')\}$$

Proof. Let $G_0^* = G_0 \setminus \{u, v\}$. By the definition of modified Schultz index, we have

$$\begin{aligned}
S^* \quad & (G') - S^*(G) = 2\binom{s+t}{2} + \sum_{x\in G_0^*} d(x)(d(u)+t)d_G(x,u) \\
+ \quad & \sum_{x\in G_0^*} d(x)(d(v)-t)d_G(x,v) + (d(u)+t)(d(v)-t)d_G(u,v) + (s+t)(d(u)+t) \\
+ \quad & (s+t)(d(v)-t)(d_G(u,v)+1) + t\sum_{x\in G_0^*} d(x)(d_G(x,u)+1) - 2\binom{s}{2} - 2\binom{t}{2} \\
- \quad & st(d_G(u,v)+2) - \sum_{x\in G_0^*} d(x)d(u)d_G(x,u) - \sum_{x\in G_0^*} d(x)d(v)d_G(x,v) \\
- \quad & d(u)d(v)d_G(u,v) - sd(u) - td(v) - sd(v)(d_G(u,v)+1) - td(u)(d_G(u,v)+1) \\
- \quad & t\sum_{x\in G_0^*} d(x)(d_G(x,v)+1) \\
= \quad & s^2 + 2st + t^2 - s - t + \sum_{x\in G_0^*} d(x)d(u)d_G(x,u) + t\sum_{x\in G_0^*} d(x)d_G(x,u) \\
+ \quad & \sum_{x\in G_0^*} d(x)d(v)d_G(x,v) - t\sum_{x\in G_0^*} d(x)d_G(x,v) + d(u)d(v)d_G(u,v) \\
+ \quad & td(v)d_G(u,v) - td(u)d_G(u,v) - t^2 d_G(u,v) + sd(u) + st + td(u) + t^2 \\
+ \quad & sd(v)d_G(u,v) + sd(v) - std_G(u,v) - st + td(v)d_G(u,v) + td(v) - t^2 d_G(u,v)
\end{aligned}$$

$$
\begin{aligned}
- \quad & t^2 + t\sum_{x\in G_0^*} d(x)d_G(x,u) + t\sum_{x\in G_0^*} d(x) - s^2 - t^2 + s + t - 2st - std_G(u,v) \\
- \quad & \sum_{x\in G_0^*} d(x)d(u)d_G(x,u) - \sum_{x\in G_0^*} d(x)d(v)d_G(x,v) - d(u)d(v)d_G(u,v) \\
- \quad & sd(u) - td(v) - sd(v)d_G(u,v) - sd(v) - td(u)d_G(u,v) - td(u) \\
- \quad & t\sum_{x\in G_0^*} d(x)d_G(x,v) - t\sum_{x\in G_0^*} d(x) \\
= \quad & 2t\{\sum_{x\in G_0^*} d(x)[d_G(x,u) - d_G(x,v)] + d_G(u,v)[d(v) - d(u)] - (s+t)d_G(u,v)\}
\end{aligned}
$$

Similarly, we have

$$
\begin{aligned}
S^* \quad & (G^{''}) - S^*(G) = 2\binom{s+t}{2} + \sum_{x\in G_0^*} d(x)(d(v)+s)d_G(x,v) \\
+ \quad & \sum_{x\in G_0^*} d(x)(d(u)-s)d_G(x,u) + (d(u)-s)(d(v)+s)d_G(u,v) + (s+t)(d(v)+s) \\
+ \quad & (s+t)(d(u)-s)(d_G(u,v)+1) + s\sum_{x\in G_0^*} d(x)(d_G(x,v)+1) - 2\binom{s}{2} - 2\binom{t}{2} \\
- \quad & st(d_G(u,v)+2) - \sum_{x\in G_0^*} d(x)d(u)d_G(x,u) - \sum_{x\in G_0^*} d(x)d(v)d_G(x,v) \\
- \quad & d(u)d(v)d_G(u,v) - sd(u) - td(v) - sd(v)(d_G(u,v)+1) - td(u)(d_G(u,v)+1) \\
- \quad & t\sum_{x\in G_0^*} d(x)(d_G(x,v)+1) \\
= \quad & 2s\left\{\sum_{x\in G_0^*} d(x)[d_G(x,v) - d_G(x,u)] + d_G(u,v)[d(u) - d(v)] - (s+t)d_G(u,v)\right\}
\end{aligned}
$$

If $S^*(G^{'}) - S^*(G) > 0$, then

$$
\sum_{x\in G_0^*} d(x)d_G(x,v) + d(u)d_G(u,v) < \sum_{x\in G_0^*} d(x)d_G(x,u) + d(v)d_G(u,v) - (s+t)d_G(u,v)
$$

Thus,

$$
\begin{aligned}
& S^* \quad (G^{''}) - S^*(G) \\
= \quad & 2s \left\{ \sum_{x \in G_0^*} d(x) \left[d_G(x,v) - d_G(x,u) \right] + d_G(u,v) \left[d(u) - d(v) \right] - (s+t) d_G(u,v) \right\} \\
= \quad & 2s \left\{ \sum_{x \in G_0^*} d(x) d_G(x,v) + d(u) d_G(u,v) - \sum_{x \in G_0^*} d(x) d_G(x,u) \right\} \\
- \quad & 2s \left\{ d_G(u,v) d(v) - (s+t) d_G(u,v) \right\} < -4s(s+t) d_G(u,v) < 0
\end{aligned}
$$

The proof is completed.

Remark 2. Repeating grafting transformation B, any bicyclic graph can be changed into a bicyclic graph such that all the pendant edges are attached to the same vertex.

Lemma 3. Let G' and G'' be the graphs depicted in Fig 3. Let $G_0^* = G_0 \backslash \{u, v\}$. Then $S^*(G') > S^*(G'')$ if $d_{G_0}(u) > d_{G_0}(v)$ and $\sum_{x \in G_0^*} d_{G_0^*}(x) d_{G_0^*}(x,u) < \sum_{x \in G_0^*} d_{G_0^*}(x) d_{G_0^*}(x,v)$; otherwise $S^*(G') < S^*(G'')$.

Proof. By the definition of modified Schultz index, we have

$$
\begin{aligned}
& S^*(G^{'}) \\
= \quad & 2\binom{s+t}{2} + \sum_{x \in G_0^*} d_{G_0^*}(x) d_{G_0}(v) d_{G_0^*}(x,v) + \sum_{x \in G_0^*} d_{G_0^*}(x) [d_{G_0}(u) + s + t] d_{G_0^*}(x,u) + \\
& (s+t)[d_{G_0}(u) + s + t] + (s+t) d_{G_0}(v)[1 + d_{G_0}(u,v)] + d_{G_0}(v)[d_{G_0}(u) + s + \\
& t] d_{G_0}(u,v) + (s+t) \sum_{x \in G_0^*} d_{G_0^*}(x)[d_{G_0^*}(x,u) + 1] + \sum_{x,y \in G_0^*} d_{G_0^*}(x) d_{G_0^*}(y)(d_{G_0^*}(x,y) \\
& S^*(G^{''}) \\
= \quad & 2\binom{s+t}{2} + \sum_{x \in G_0^*} d_{G_0^*}(x) d_{G_0}(u) d_{G_0^*}(x,u) + \sum_{x \in G_0^*} d_{G_0^*}(x) [d_{G_0}(v) + s + t] d_{G_0^*}(x,v) + \\
& (s+t)[d_{G_0}(v) + s + t] + (s+t) d_{G_0}(u)[1 + d_{G_0}(u,v)] + d_{G_0}(u)[d_{G_0}(v) + s + \\
& t] d_{G_0}(u,v) + (s+t) \sum_{x \in G_0^*} d_{G_0^*}(x)[d_{G_0^*}(x,v) + 1] + \sum_{x,y \in G_0^*} d_{G_0^*}(x) d_{G_0^*}(y)(d_{G_0^*}(x,y)
\end{aligned}
$$

Thus,

$$
\begin{aligned}
& S^*(G^{'}) - S^*(G^{''}) \\
= \quad & 2(s+t)\{ \sum_{x \in G_0^*} d_{G_0^*}(x)[d_{G_0^*}(x,u) - d_{G_0^*}(x,v)] + d_{G_0}(u,v)[d_{G_0}(v) - d_{G_0}(u)]\}
\end{aligned}
$$

Therefore, if $d_{G_0}(u) > d_{G_0}(v)$ and $\sum_{x \in G_0^*} d_{G_0^*}(x) d_{G_0^*}(x,u) < \sum_{x \in G_0^*} d_{G_0^*}(x) d_{G_0^*}(x,v)$, we have $S^*(G^{'}) < S^*(G'')$; otherwise $S^*(G^{'}) > S^*(G'')$.

The proof is completed.

3 The Modified Schultz Index In Bicyclic Graphs

In this section we shall give lower bounds for the Modified Schultz index in bicyclic graphs.

Before our main results, we need a known results, which is useful to our proof.

Lemma 4. Let C_n be the cycle of order n, v is a vertex on C_n. Then

$$\sum_{x\in V(C_n)} d_{C_n}(v,x) = \begin{cases} \frac{1}{4}n^2, & \text{if } n \text{ is even;} \\ \frac{1}{4}(n^2-1), & \text{if } n \text{ is odd.} \end{cases}$$

$$W(C_n) = \begin{cases} \frac{1}{8}n^3, & \text{if } n \text{ is even;} \\ \frac{1}{8}(n^3-n), & \text{if } n \text{ is odd.} \end{cases}$$

Similar to the Lemma 4, for the modified Schultz index of C_n, we have

Theorem 1. Let C_n be the cycle of order n, then

$$S^*(C_n) = 4W(C_n) = \begin{cases} \frac{1}{2}n^3, & \text{if } n \text{ is even;} \\ \frac{1}{2}(n^3-n), & \text{if } n \text{ is odd.} \end{cases}$$

3.1 The Smallest Modified Schultz Index In $\mathbb{A}(p,q)$

In this section, we shall find the bicyclic graph with the smallest modified Schultz index in $\mathbb{A}(p,q)$.

Let $S_n(p,q)$ be a graph in $\mathbb{A}(p,q)$ such that $n+1-(p+q)$ pendent edges are attached to the common vertex of C_p and C_q. $S'_n(p,q)$ be a graph in $\mathbb{A}(p,q)$ such that $n+1-(p+q)$ pendent edges are attached to one vertex of C_p or C_q. See Fig 4.

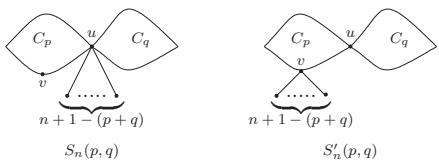


Fig 4. The graph $S_n(p,q)$ and $S'_n(p,q)$

Theorem 2. $S_n(p,q)$ is the graph with the smallest $S^*(G)$ in $\mathbb{A}(p,q)$.

Proof. First, repeating the transformations A and B on graph G, we can get a graph G' such that all the edges not on the cycles are the pendant edges attached to the same vertex v. By Lemmas 1 and 2, we have $S^*(G) \geq S^*(G')$ with the equality if and only if

all the edges not on the cycles are also the pendant edges attached to the same vertex in G. If $G' \ncong S_n(p,q)$, then $v \neq u$, where u is the common vertex of C_p and C_q.

Without loss of the generality, we assume that v is on the cycle C_p.

Let $G_0 = C_p u C_q$, $G_0^* = G_0 \setminus \{u,v\}$ in $S_n(p,q)$ and $S'_n(p,q)$.

From the proof of Lemma 3, it is easily to see that

$$d_{G_0}(u) = 4 > d_{G_0}(v) = 2$$

and

$$\sum_{x \in G_0^*} d_{G_0^*}(x) d_{G_0^*}(x,u) = 2 \sum_{x \in G_0^*} d_{G_0^*}(x,u) < 2 \sum_{x \in G_0^*} d_{G_0^*}(x,v)$$

, we have

$$S^*(S_n(p,q)) < S^*(S'_n(p,q))$$

This completes the proof.

Remark 3. Given $p \geq 3$ and $q \geq 3$, from the theorem above, it is suffice to see that $S_n(p,q)$ is the unique graph with the smallest modified Schultz index in $\mathbb{A}(p,q)$.

Theorem 3. (i)If $G \in \mathbb{A}(p,q)$, then

(i) $S^*(S_n(p,q)) \geq S^*(S_n(p-1,q))$;

(ii) For all $p \geq 3$ and $q \geq 3$, $S_n(3,3)$ is the unique graph with the smallest modified Schultz index in $\mathbb{A}(p,q)$.

Proof. By the Remark 3, $S_n(p,q)$ is the unique graph with the smallest modified Schultz index in $\mathbb{A}(p,q)$. Firstly, Let $e = uv$ be an edge of the cycle C_p(by the symmetry of p and q), applying grafting transformation A on $S_n(p,q)$, then $S_n(p,q)$ can be changed into the graph G'(see Fig 5.) and e is changed into a pendent edge adjacent to $u(v)$. By the Lemma 1, we have

$$S^*(S_n(p,q)) > S^*(G').$$

Secondly, applying grafting transformation B on G', then G' can be changed into $G''(G'' \cong S_n(p-1,q))$, such that

$$S^*(G') > S^*(G'').$$

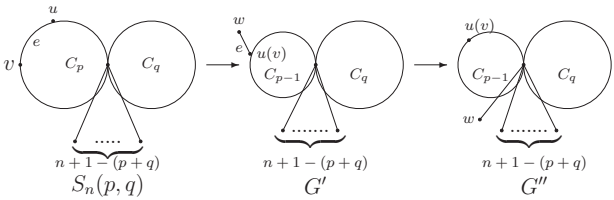


Fig 5. Graph transformations

Repeating grafting transformations A and B on $S_n(p,q)$, then $S_n(p,q)$ is changed into $S_n(3,3)$, and

$$S^*(S_n(p,q)) > S^*(S_n(3,3)) \text{ if } p \geq 3 \text{ and } q > 3, \text{ or } p > 3 \text{ and } q \geq 3.$$

Lastly, we have

$$S^*(S_n(p,q)) \geq S^*(S_n(3,3))$$

for all graphs in $\mathbb{A}(p,q)$ with $p \geq 3$ and $q \geq 3$. The equality holds if and only if $G \cong S^*(S_n(3,3))$.

This completes the proof.

Theorem 4. The modified Schultz index of $S_n(3,3)$ is

$$S^*(S_n(3,3)) = 2n^2 + 7n - 13$$

Proof. Let $G_1^* = C_p \setminus \{u\}$, $G_2^* = C_q \setminus \{u\}$ in $S_n(p,q)$. Then by the definition of modified Schultz index, we have

$$\begin{aligned} & S^*(S_n(p,q)) \\ = \; & 2n^2 + 3n + 1 - (2n+1)(p+q) + 4W(C_p) + 4W(C_q) \\ & +4(n+1-q) \sum_{x \in G_1^*} d_{G_1^*}(x,u) + 4(n+1-p) \sum_{x \in G_2^*} d_{G_2^*}(x,u) \end{aligned}$$

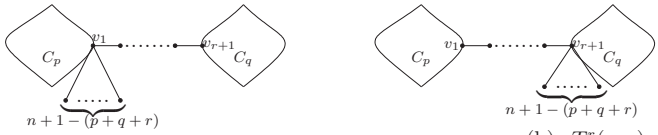
By combing Lemma 4 and Theorem 1, when $p = 3$ and $q = 3$, it is easily to get the result.

This completes the proof.

3.2 The Smallest Modified Schultz Index In $\mathbb{B}(p,q)$

In this section, we shall find the bicyclic graph with the smallest modified Schultz index in $\mathbb{B}(p,q)$.

Let $T_n^r(p,q)$ be the $(n,n+1)-$graph obtaining from connecting C_p and C_q by a path of length r and the other $n+1-p-q-r$ edges are all attached to the common vertex of the path and C_p, see Fig. 6(a). $T_n^r(q,p)$ is showed in Fig. 6(b).



(a). $T_n^r(p,q)$ (b). $T_n^r(q,p)$

Fig. 6. The graphs $T_n^r(p,q)$ and $T_n^r(q,p)$

Firstly, similar to the discussion way of section 3.1, we have

Theorem 5. If $G \in \mathbb{B}(p,q)$, the length of the shortest path connecting C_p and C_q in G is r, then

(i) $S^*(G) > S^*(T_n^r(p,q))$ with the equality if and only if $G \cong T_n^r(p,q)$; or

(ii) $S^*(G) \geq S^*(T_n^r(q,p))$ with the equality if and only if $G \cong T_n^r(q,p)$.

Proof. We omit the proof of the theorem here.

Similarly, we have

Theorem 6. If $r \geq 2$, then $S^*(T_n^r(p,q) < S^*(T_n^{r-1}(p,q))$.

Theorem 7. $S^*(T_n^1(p,q)) \geq S^*(T_n^1(3,3))$, with the equality if and only if $p = q = 3$.

Theorem 8. The $T_n^1(3,3)$ is the unique graph with the smallest modified Schultz index among all graphs in $\mathbb{B}(p,q)$ for all $p \geq 3$ and $q \geq 3$.

Theorem 9. The modified Schultz index of $T_n^1(3,3)$ is

$$S^*(T_n^1(3,3)) = 2n^2 + 17n - 37$$

Proof. By the definition of modified Schultz index, we have

$$\begin{aligned} & S^*(T_n^1(3,3)) \\ = \; & 2\binom{n-6}{2} + 2\times 2\times 2 + 2\times(n-3)\times 2 + 2\times 3\times 2 + (n-6)\times(n-3) \\ & +(n-6)\times 3\times 2 + 2\times 2\times(n-6)\times 2 + 2\times(n-6)\times 3\times 2 + 3\times(n-3) \\ & +2\times 3\times 2\times 2 + 2\times 2\times 3\times 4 + 2\times(n-3)\times 2\times 2 \\ = \; & 2n^2 + 17n - 37 \end{aligned}$$

This completes the proof.

3.3 The Smallest Modified Schultz Index In $\mathbb{B}(p,q)$

In this section, we shall find the bicyclic graph with the smallest modified Schultz index in $\mathbb{C}(p,q,l)$.

Let $\theta_n^l(p,q)$ be the graph obtaining from the graph in Fig 1(c) by attaching $n+1+l-(p+q)$ to one of its vertices with degree 3 (see Fig 8(a)).

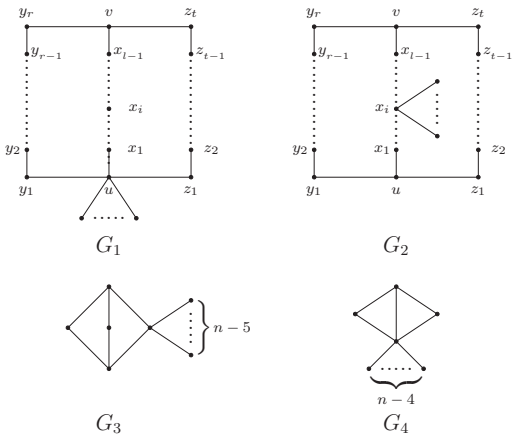


Fig 7. The graphs G_i $(i = 1, 2, 3, 4)$

Theorem 10. Let $G \in \mathbb{C}(p, q, l)$. Then $S^*(G) \geq S^*(G_4)$ with the equality if and only if $G \cong G_4$, where G_4 is the graph in Fig 8.

Proof. Repeating the transformations A and B on graph G, we can get a graph G' such that all the edges not on the cycles are the pendant edges attached to the same vertex v_0, i.e., G' is one of the graphs in Fig 8. By Lemmas 1 and 2, we have $S^*(G) \geq S^*(G')$ with the equality if and only if all the edges not on the cycles are also the pendant edges attached to the same vertex in G.

Let $W_1 = ux_1x_2 \cdots x_{l-1}v$ be the common path of C_p and C_q of the graph G' in Fig 8, $W_2 = uy_1y_2 \cdots y_rv$ and $W_3 = uz_1z_2 \cdots z_tv$ the other paths from u to v on C_p and C_q, respectively; $r = p - l - 1$, $t = q - l - 1$, $r \geq 0$, $t \geq 0$, $l \geq 1$ and $r + t + l \geq 3$.

If there is an edge $e = xy$ in G_1 such that the degrees of x and y are equal two, then we can obtain a graph G_1' by contracting the edge e and attaching a pendant edge $e' = uu'$ to u, and we have $S^*(G_1) > S^*(G_1')$ by Lemma 1, repeating grafting transformation B on G_1', G_1' is changed into the graph G_1'' such that the pendent edge is transferred to the vertex u and $S^*(G_1') > S^*(G_1'')$ by Lemma 2. Repeating above operations, then graph G will changed into G_4. $S^*(G) \geq S^*(G_4)$, the equality holds if and only if $G \cong G_4$.

If there are two edges e_1 and e_2 in G_2 such that the degrees of their end-vertices are equal two, then we can obtain a graph G_2' by contracting the edges e_1 and e_2 and

attaching two pendant edges to x_i; or if there an edge e in G_2 such that the degrees of its end-vertices and e_2 are equal two, then we can obtain a graph G_2' by contracting the edge e and attaching a pendant edge to x_i. By Lemma 1 and 2, we have $S^*G_2) > S^*(G_2')$. Repeating above operations, we shall get that $S^*(G_2) \geq S^*(G_3)$ and equality holds if and only if $G \cong G_3$.

It is easily to computed out that

$$\begin{aligned} & S^*(G_3) \\ = \; & 2\tbinom{n-5}{2} + (n-5)\times(n-3) + (n-5)\times 3\times 2\times 2 + (n-5)\times 2\times 3\times 2 \\ & +(n-3)\times 3\times 2 + (n-3)\times 2\times 2\times 2 + 3\times 3\times 2 + 3\times 2\times 4 + 2\times 2\times 2 \\ = \; & 2n^2 + 19n - 67 \\ & S^*(G_4) \\ = \; & 2\tbinom{n-4}{2} + 2\times 3\times 2 + 2\times(n-3)\times 2 + 3\times(n-1) + 2\times 2\times(n-4)\times 2 \\ & +3\times 2\times(n-4) + (n-4)\times(n-1) + 4\times 2 \\ = \; & 2n^2 + 7n - 19 \end{aligned}$$

And

$$\begin{aligned} & S^*(G_3) - S^*(G_4) \\ = \; & 2n^2 + 19n - 67 - 2n^2 - 7n + 19 \\ = \; & 12n - 48 > 0 \qquad (\text{since } n \geq 5) \end{aligned}$$

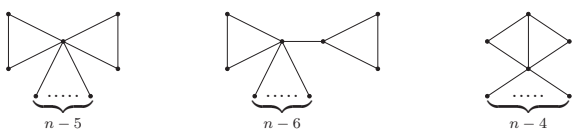
This completes the proof.

Note that $G_4 \cong \theta_n^1(3,3)$, in next following, we use this notion for it.

4 Bicyclic Graphs With The Smallest Modified Schultz Index

Finally, we give the bicyclic graphs with the smallest modified Schultz index.

Theorem 11. $S_n(3,3)$ is the unique graph with the the smallest modified Schultz index among all bicyclic graphs with n vertices.



$S_n(3,3)$ $\quad$ $T_n^1(3,3)$ $\quad$ $\theta_n^1(3,3)$

Fig 8. The graphs $S_n(3,3)$, $T_n^1(3,3)$, $\theta_n^1(3,3)$

Proof. From Theorem 3, Theorem 8 and Theorem 10, we only need to compare the modified Schultz index of $S_n(3,3)$, $T_n^1(3,3)$ and $\theta_n^1(3,3)$.

Computing immediately, we have

(i) when $n \geq 15$, $S^*(\theta_n^1(3,3)) > S^*(T_n^1(3,3)) > S^*(S_n(3,3))$;

(ii) when $6 \leq n < 15$, $S^*(T_n^1(3,3)) > S^*(\theta_n^1(3,3)) > S^*(S_n(3,3))$.

Therefore, $S_n(3,3)$ has the smallest modified Schultz index among all bicyclic graphs with n vertices.

The result follows.

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