Extremal cactuses for the Schultz and modified Schultz indices*

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Abstract

Let G be a cactus, which all of blocks of G are either edges or cycles. Denote $\mathscr{G}(n,r)$ the set of cactuses of order n and with r cycles. In this paper, we present a unified approach to the extremal cactuses, for Schultz and the modified Schultz indices.

1 Introduction

Let $G=(V,E)$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$ and $|V|=n$, $|E(G)|=m$ are the number of vertices and edges G, respectively. For any $u,v \in V$, $d_G(u)$ (or simply by $d(u)$) and $d_G(u,v)$ (or simply by $d(u,v)$) denote the degree of u and the distance (i.e.,the number of edges on the shortest path) between u and v, respectively. Let P_n, C_n and $S_n(K_{1,n-1})$ 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 [1] 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.,

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

In connection with certain investigations in mathematical chemistry, Schultz [2] in 1989 introduced firstly in connection with certain chemical applications. Soon after, I. Gutman [3] named it the *Schultz index*, defined as

$$\mathcal{W}_+(G):=S(G):=\sum_{\{u,v\}\subset V(G)} (d_G(u)+d_G(v))d_G(u,v) \tag{2}$$

This name was eventually accepted by most authors.

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Motivated by equation (2), I. Gutman [4] defined the modification of $\mathcal{W}_+(G)$, i.e.,

$$\mathcal{W}_*(G) := S^*(G) := \sum_{\{u,v\}\subseteq V(G)} (d_G(u) \cdot d_G(v))d_G(u,v) \quad (3)$$

which here we refer to as *the modified Schultz index*. The Schultz and modified Schultz indices attracted much attention after them were discovered. It has been demonstrated that $\mathcal{W}_+(G)$, $\mathcal{W}_*(G)$ and $W(G)$ are closely mutually related for certain classes of molecular graphs [5-9]. Klein *et al* [6] derived an explicit relation between $\mathcal{W}_+(G)$ and $W(G)$ for trees:

$$\mathcal{W}_+(G) = 4W(G) - n(n-1) \quad (4)$$

A result analogous to equation (4) applies [3]:

$$\mathcal{W}_*(G) = 4W(G) - (n-1)(2n-1) \quad (5)$$

In [8], the authors derived relations between $W(G)$ and $\mathcal{W}_+(G)$, $\mathcal{W}_*(G)$ for the (unbranched) hexagonal chain composed of n fused hexagons, i.e.,

$$\mathcal{W}_+(G) = \frac{25}{4}W(G) - \frac{3}{4}(2n+1)(20n+7) \quad (6)$$

$$\mathcal{W}_*(G) = 5W(G) - 3(2n+1)^2 \quad (7)$$

In [10], A. I. Tomescu characterized the connected unicyclic and bicyclic graphs in terms of the degree sequence, as well as the graphs in these classes minimal with respect to the Schultz index are given. In [11], O. Bucicovschi and S. M. Cioabă studied the Schultz index of graphs with given order and size, and determined the minimum degree distance of a connected graph of order n and size m. 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. In [16], the authors investigated bicyclic graphs with extremal modified Schultz index. More results in these directions can be found in Refs. [17-20].

We say that the graph G is a cactus if any two of its cycles have at most one common vertex. If all cycles of the cactus G have exactly one common vertex we say that they form a bundle. Denote $\mathscr{G}(n,r)$ the set of cacti of order n and with r cycles. Obviously, $\mathscr{G}(n,0)$ is the set of all trees and $\mathscr{G}(n,1)$ is the set of all unicyclic graphs. We use $G^0(n,r)$ to denote the cactus obtained from the $n-$vertex star by adding r mutually independent edges (see Figure 1).

In this paper, we present a unified approach to the extremal Schultz and modified Schultz indices for cactuses.

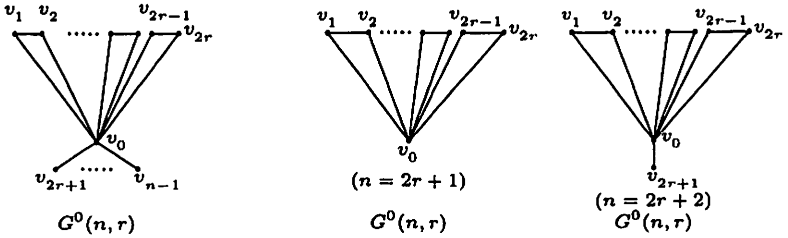

Figure 1. The graphs $G^0(n, r)$

2 Three transformations which decrease the Schultz and modified Schultz indices

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.

Firstly, We introduce some known Lemmas, which are useful to our proof.

Lemma 2.1. 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 2.1, we have

Lemma 2.2. Let C_n be the cycle of order n, then

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

Lemma 2.3. Let $G^0(n, r)$ be the cacti depicted in Figure 1, then

(i) $\mathcal{W}_+(G^0(n, r)) = 4rn - 10r + 3n^2 - 7n + 4$;

(ii) $\mathcal{W}_*(G^0(n, r)) = 4r^2 + 6rn - 16r + 2n^2 - 5n + 3$.

Proof. For all pairs (x, y) of vertices in $G^0(n, r)$, we have $d(x, y) = 1$ or $d(x, y) = 2$. We divided the vertices into two groups-the center v_0, the neighbors $v_1, v_2, \cdots, v_{2r}$ of the center, and the leaves $v_{2r+1}, \cdots, v_{n-2r-1}$.

Case (i) By the definition of Schultz index, we have

(1) Obviously, there are $n + r - 1$ pairs with $d(x, y) = 1$, all the total pairs for the contribution to the Schultz index are:

$$4 \times r + n \times (n - 2r - 1) + 2r \times (n + 1)$$

(2) All pairs of the form $(x,y)=(v_i,v_j)(v_i \not\sim v_j)$, $(x,y)=(v_i,v_j)$ for $1\leq i\leq 2r$, $2r+1\leq j\leq n-2r-1)$ satisfy $d(x,y)=2$. The total pairs for the contribution to the Schultz index are:

$$2\times\binom{n-2r-1}{2}+4[\binom{2r}{2}-r]+3\times 2r\times(n-2r-1)$$

Summing up, the Schultz index of $G^0(n,r)$ is

$$\begin{aligned}&\mathcal{W}_+(G^0(n,r))\\ =\ & 4\times r+n\times(n-2r-1)+2r\times(n+1)+2\times\{2\times\tbinom{n-2r-1}{2}\\ &+4[\tbinom{2r}{2}-r]+3\times 2r\times(n-2r-1)\}\\ =\ & 4rn+3n^2-10r-7n+4\end{aligned}$$

Case (ii) By the definition of modified Schultz index, we have

(1)All the total pairs with $d(x,y)=1$ for the contribution to the modified Schultz index are:

$$4\times r+(n-1)\times(n-2r-1)+2r\times 2(n-1)$$

(2)All pairs satisfy $d(x,y)=2$ for the contribution to the modified Schultz index are:

$$\binom{n-2r-1}{2}+4[\binom{2r}{2}-r]+2\times 2r\times(n-2r-1)$$

Summing up, the Schultz index of $G^0(n,r)$ is

$$\begin{aligned}&\mathcal{W}_+(G^0(n,r))\\ =\ & 4\times r+(n-1)\times(n-2r-1)+2r\times 2(n-1)+2\times\{\tbinom{n-2r-1}{2}\\ &+4[\tbinom{2r}{2}-r]+2\times 2r\times(n-2r-1)\}\\ =\ & 4r^2+6rn+2n^2-16r-5n+3\end{aligned}$$

Nextly, We give three transformations which will decrease the Schultz and modified Schultz indices as follows.

Transformation A: Let uv be an edge in G, $d_G(v)\geq 2$, $N_G(v)=\{u,w_1,w_2,\cdots,w_s\}$, and $w_1,w_2,\cdots,w_s$ are leaves adjacent to v. $G'=G-\{vw_1,vw_2,\cdots,vw_s\}+\{uw_1,uw_2,\cdots,uw_s\}$.

Lemma 2.4. Let G' be obtained from G by transformation A, then (i). $\mathcal{W}_+(G')<\mathcal{W}_+(G)$; (ii)[16]. $\mathcal{W}_*(G')<\mathcal{W}_*(G)$.

Proof. (i) Let $G_0=G-\{v,w_1,w_2,\cdots,w_s\}$, $G_0'=G_0-u$. By the definition of the Schultz index, we have

$$\begin{aligned}&\mathcal{W}_+(G)\\ =\ & \sum_{x,y\in G_0'}(d_{G_0'}(x)+d_{G_0'}(y))d_{G_0'}(x,y)+(s+2)\sum_{x\in G_0'}d_{G_0'}(x)d_{G_0'}(x,u)\\ &+(d_G(u)+2s+1)\sum_{x\in G_0'}d_{G_0'}(x,u)+(2s+1)\sum_{x\in G_0'}d_{G_0'}(x)\\ &+(3s+1)|G_0'|+(2s+1)d_G(u)+3s^2+3s+1\end{aligned}$$

$$\begin{aligned}
&\mathcal{W}_+(G') \\
= &\sum_{x,y\in G_0'}(d_{G_0'}(x)+d_{G_0'}(y))d_{G_0'}(x,y)+(s+2)\sum_{x\in G_0'}d_{G_0'}(x)d_{G_0'}(x,u) \\
&+(d_G(u)+2s+1)\sum_{x\in G_0'}d_{G_0'}(x,u)+(s+1)\sum_{x\in G_0'}d_{G_0'}(x) \\
&+(s+1)|G_0'|+(s+1)d_G(u)+3s^2+4s+1
\end{aligned}$$

Therefore,

$$\mathcal{W}_+(G)-\mathcal{W}_+(G')=s\sum_{x\in G_0'}d_{G_0'}(x)+2s|G_0'|+sd_G(u)-s>0.$$

Remark 1. Repeating Transformation A, any cyclic graph can be changed into a cyclic graph such that all the edges not on the cycles are pendant edges.

Transformations B. 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. $G'=G-\{vv_1,vv_2,\cdots,vv_t\}+\{uv_1,uv_2,\cdots,uv_t\}$, $G''=G-\{uu_1,uu_2,\cdots,uu_s\}+\{vu_1,vu_2,\cdots,vu_s\}$.

Lemma 2.5. Let G' and G'' be obtained from G by transformation B. Then

(i). $\mathcal{W}_+(G)>\mathcal{W}_+(G')$ or $\mathcal{W}_+(G)>\mathcal{W}_+(G'')$;

(ii)[16]. $\mathcal{W}_*(G)>\mathcal{W}_*(G')$ or $\mathcal{W}_*(G)>\mathcal{W}_*(G'')$.

Proof. (i) Let $G_0^*=G_0-\{u,v\}$. By the definition of Schultz index, we have

$$\begin{aligned}
&\mathcal{W}_+(G')-\mathcal{W}_+(G) \\
= &4\binom{s+t}{2}+\sum_{x\in G_0^*}[d_{G_0^*}(x)+d_G(u)+t]d_G(x,u)+\sum_{x\in G_0^*}[d_{G_0^*}(x)+d_G(v) \\
&-t]d_G(x,v)+(d_G(u)+d_G(v))d_G(u,v)+(s+t)[1+d_G(u)+t]+ \\
&(s+t)[1+d_G(v)-t](d_G(u,v)+1)+t\sum_{x\in G_0^*}(1+d_{G_0^*}(x))(d_G(x,u) \\
&+1)-4\binom{s}{2}-4\binom{t}{2}-2st(d_G(u,v)+2)-\sum_{x\in G_0^*}[d_{G_0^*}(x)+d_G(u)] \\
&d_G(x,u)-\sum_{x\in G_0^*}[d_{G_0^*}(x)+d_G(v)]d_G(x,v)-[d_G(u)+d_G(v)]d_G(u,v) \\
&-s[1+d_G(u)]-t[1+d_G(v)]-s[1+d_G(v)](d_G(u,v)+1) \\
&-t[1+d_G(u)](d_G(u,v)+1)-t\sum_{x\in G_0^*}[1+d_{G_0^*}(x)](d_G(x,v)+1) \\
= &t\{\sum_{x\in G_0^*}(2+d_{G_0^*}(x))[d_G(x,u)-d_G(x,v)]+td_G(u,v)[d_G(v)-d_G(u)] \\
&-t(3s+t)d_G(u,v)\}
\end{aligned}$$

Similarly, we have

$$\begin{aligned}
&\mathcal{W}_+(G'')-\mathcal{W}_+(G) \\
= &s\{\sum_{x\in G_0^*}(2+d_{G_0^*}(x))[d_G(x,v)-d_G(x,u)]+sd_G(u,v)[d_G(u)-d_G(v)] \\
&-s(3t+s)d_G(u,v)\}
\end{aligned}$$

If $\mathcal{W}_+(G')-\mathcal{W}_+(G)>0$, thus

$$\sum_{x\in G_0^*}(2+d_{G_0^*}(x))d_G(x,u)+d_G(v)d_G(u,v)$$
$$> \sum_{x\in G_0^*}(2+d_{G_0^*}(x))d_G(x,v)+d_G(u)d_G(u,v)+(3s+t)d_G(u,v)$$

Then

$$\begin{aligned}&\mathcal{W}_+(G'')-\mathcal{W}_+(G)\\ =\ & s\{\sum_{x\in G_0^*}(2+d_{G_0^*}(x))d_G(x,v)-\sum_{x\in G_0^*}(2+d_{G_0^*}(x))d_G(x,u)\\ &+d_G(u)d_G(u,v)-d_G(v)d_G(u,v)-(3t+s)d_G(u,v)\}\\ <\ & -4s(s+t)d_G(u,v)<0\end{aligned}$$

Otherwise, $\mathcal{W}_+(G'')-\mathcal{W}_+(G)>0$, thus

$$\sum_{x\in G_0^*}(2+d_{G_0^*}(x))d_G(x,v)+d_G(u)d_G(u,v)$$
$$> \sum_{x\in G_0^*}(2+d_{G_0^*}(x))d_G(x,u)+d_G(v)d_G(u,v)+(3t+s)d_G(u,v)$$

Then

$$\begin{aligned}&\mathcal{W}_+(G')-\mathcal{W}_+(G)\\ =\ & t\{\sum_{x\in G_0^*}(2+d_{G_0^*}(x))d_G(x,u)-\sum_{x\in G_0^*}(2+d_{G_0^*}(x))d_G(x,v)\\ &+d_G(v)d_G(u,v)-d_G(u)d_G(u,v)-(3s+t)d_G(u,v)\}\\ <\ & -4t(s+t)d_G(u,v)<0\end{aligned}$$

Remark 2. After repeating transformation A, repeating transformation B, any cyclic graph can be changed into a cyclic graph such that all the pendant edges are attached to the same vertex.

Lemma 2.6. Suppose that G is a graph of order $n\geq 7$ obtained from a connected graph $G_0\ncong P_1$ and a cycle $C_p=v_0v_1\cdots v_{p-1}v_0(p\geq 4$ for p is even; otherwise $p\geq 5)$ by identifying v_0 with a vertex v of the graph G_0. Let $G'=G-v_{p-1}v_{p-2}+vv_{p-2}$. We name above operation as grafting transformation C. Then (i). $\mathcal{W}_+(G)>\mathcal{W}_+(G')$; (ii)[16]. $\mathcal{W}_*(G)>\mathcal{W}_*(G')$.

Proof.(i) Let $G_0'=G_0-v$, $C_p'=C_p-\{v,v_{p-1}\}$, $C_{p-1}'=C_{p-1}-v$. By the definition of Schultz index, we have

Case (1). p is even.

$$\begin{aligned}&\mathcal{W}_+(G)\\ =\ & \sum_{x,y\in G_0'}d_{G_0'}(x)d_{G_0'}(y)d_{G_0'}(x,y)+\sum_{x\in G_0'}(d_{G_0'}(x)+d_G(v))d_{G_0'}(x,v)\\ &+4\sum_{x,y\in C_p'}d_{C_p'}(x,y)+(2+d_G(v))\sum_{x\in C_p'}d_{C_p'}(x,v)\\ &+4\sum_{x\in C_p'}d_{C_p'}(x,v)+2+d_G(v)+\sum_{x\in G_0'}(2+d_{G_0'}(x))\\ &\sum_{y\in C_p'}[d_{G_0'}(x,v)+\sum_{x\in G_0'}(2+d_{G_0'}(x))[d_{G_0'}(x,v)+1]\\ =\ & \sum_{x,y\in G_0'}[d_{G_0'}(x)+d_{G_0'}(y)]d_{G_0'}(x,y)+p\sum_{x\in G_0'}d_{G_0'}(x)d_{G_0'}(x,v)+\\ &[d_G(v)+2p-2]\sum_{x\in G_0'}d_{G_0'}(x,v)+\frac{p^2}{4}\sum_{x\in G_0'}d_{G_0'}(x)+\frac{p^2}{4}d_G(v)\\ &+\frac{p^3}{2}-\frac{p^2}{2}+\frac{p^2}{2}(|V(G_0')|-1)\end{aligned}$$

Similarly, we have

$$\begin{aligned}
& \mathcal{W}_+(G') \\
= & \sum_{x,y\in G'_0} [d_{G'_0}(x)+d_{G'_0}(y)]d_{G'_0}(x,y) + p\sum_{x\in G'_0} d_{G'_0}(x)d_{G'_0}(x,v) \\
& +[d_G(v)+2p-2]\sum_{x\in G'_0} d_{G'_0}(x,v) + (\tfrac{p^2}{4}-\tfrac{p}{2}+1)\sum_{x\in G'_0} d_{G'_0}(x) \\
& +(\tfrac{p^2}{4}-\tfrac{p}{2}+1)d_G(v) + \tfrac{p^3}{2} - p^2 + 3p - 4 \\
& +(\tfrac{p^2}{2}-p+1)(|V(G'_0)|-1)
\end{aligned}$$

Thus,

$$\begin{aligned}
& \mathcal{W}_+(G') - \mathcal{W}_+(G) \\
= & (1-\tfrac{p}{2})\sum_{x\in G'_0} d_{G'_0}(x) + (1-\tfrac{p}{2})d_G(v) + (1-p)(|V(G'_0)|-1) \\
& -\tfrac{1}{2}(p-3)^2 + \tfrac{1}{2} \\
< & \ 0 \quad (\text{since } p \geq 4)
\end{aligned}$$

Case (2). p is odd.

Similar to case (i), we have

$$\begin{aligned}
& \mathcal{W}_+(G') - \mathcal{W}_+(G) \\
= & (\tfrac{3}{2}-\tfrac{p}{2})\sum_{x\in G'_0} d_{G'_0}(x) + (\tfrac{3}{2}-\tfrac{p}{2})d_G(v) + (2-p)(|V(G'_0)|-1) \\
& -\tfrac{1}{2}(p-4)^2 + \tfrac{7}{2} \\
< & \ 0 \quad (\text{since } p \geq 5)
\end{aligned}$$

The completes the proof.

3 Results

In this section, we determine the extremal cactuses for the Schultz and modified Schultz indices.

In [21], Borovićanin and Petrović showed that $G^0(n,r)$ is the maximal spectral radius in the set $\mathscr{G}(n,r)$. In [22], H. Liu and M. Lu derived a unified approach to extremal cacti for Wiener index, Merrifield-Simmons index, Hosoya index and spectral radius. In [23], Lu, Zhang and Tian prove that $G^0(n,r)$ is the minimal Randić index in the set $\mathscr{G}(n,r)$.

Let $C(a_1,a_2,\cdots,a_r;k)$ be a graph obtained from r cycles $C_{a_i}(1\leq i\leq r)$ and k edges by taking one vertex of each cycle and each edge, and combining them as one vertex. Denote $\mathscr{C}^0(n,r) = \{C(a_1,a_2,\cdots,a_r;k) : a_i \geq 3, 1\leq i\leq r, \sum_{i=1}^{r}(a_i-1)+k+1 = n\}$. Then $\mathscr{C}^0(n,r)\subseteq \mathscr{G}(n,r)$ and $G^0(n,r) = C(\underbrace{3,3,\cdots,3}_{r};n-2r-1)$.

Theorem 3.1. Let $G\in\mathscr{G}(n,r)$, then

$$\mathcal{W}_+(G)\geq \mathcal{W}_+(G^0(n,r)); \quad \mathcal{W}_*(G)\geq \mathcal{W}_*(G^0(n,r)).$$

The equalities hold if and only if $G \cong G^0(n,r)$.

Proof. Choose $G \in \mathscr{G}(n,r)$ such that the Schultz index and modified Schultz index of G are as small as possible.

Let $V_c = \{v \in V(G) : v \text{ is a cut-vertex of } G\}$

We first prove that the graph $|V_c| = 1$. In order to do that we will prove the following claim.

Claim 1. $G \in \mathscr{C}^0(n,r)$.

Proof of Claim 1.

Assume that $|V_c| > 1$. Let $u, v \in V_c$ and H is a component containing u, v such that $N_G(u) \setminus N_H(u) \neq \emptyset$ and $N_G(v) \setminus N_H(v) \neq \emptyset$. Denote by $N_G(u) \setminus N_H(u) = \{u_1, u_2, \cdots, u_s\}$, $N_G(v) \setminus N_H(v) = \{v_1, v_2, \cdots, v_t\}$ for $s, t \geq 1$. Let $G_1^* = G - \{uu_1, uu_2, \cdots, uu_s\} + \{vu_1, vu_2, \cdots, vu_s\}$ and $G_2^* = G - \{vv_1, vv_2, \cdots, vv_t\} + \{uv_1, uv_2, \cdots, uv_t\}$, then $G_1^*, G_2^* \in \mathscr{G}(n,r)$. By Lemma 2.5, $\mathcal{W}_+(G_1^*) < \mathcal{W}_+(G)$, $\mathcal{W}_*(G_1^*) < \mathcal{W}_*(G)$ and $\mathcal{W}_+(G_2^*) < \mathcal{W}_+(G)$, $\mathcal{W}_*(G_2^*) < \mathcal{W}_*(G)$, which contradict to the choice of G. Therefore, $|V_c| = 1$, such that $G \in \mathscr{C}^0(n,r)$.

Follows from Claim 1, the graph G is a bundle and denote the only cut-vertex of G by v.

Secondly, we prove that if G contains a tree T attached to a cycle at some vertex u (called the root of T) then T consists only of edges containing u, i.e.,

Claim 2. Any tree T attached to a vertex v of one of the cycles in the graph G contains only vertices at distance one from its root u.

Proof of Claim 2.

In the opposite case, there exists a tree T_i(with root $v_i \in C_i$) and a vertex v_j of T_i whose distance from v_i is greater than one. We will get a graph $G^* = G - v_{j-1}v_j + v_{j-2}v_j$ (suppose that the path between v_i, v_j is $v_i \cdots v_{j-2}v_{j-1}v_j$), and $G^* \in \mathscr{G}(n,r)$. Further, by Lemma 2.4, we have $\mathcal{W}_+(G^*) < \mathcal{W}_+(G)$ and $\mathcal{W}_*(G^*) < \mathcal{W}_*(G)$, which contradict to the choice of G.

Hence, any tree T attached to a vertex of some cycle of G consists only of edges with exactly one common vertex.

Thirdly, We shall prove the following claim.

Claim 3. Any tree T of the graph G is attached to the common vertex v of all cycles of the bundle.

Proof of Claim 3.

This can be resulted directly from Lemma 2.5.

Hence G is a bundle with a unique tree attached to the common vertex of all cycles of G, and this tree contains only vertices at distance one from the root.

Finally, we prove

Claim 4. $G \cong G^0(n,r)$.

Proof of Claim 4.

Suppose that $G \ncong G^0(n,r)$. Then there exists a cycle

$$C_p = ww_1w_2 \cdots w_{p-1}w$$

with $p \geq 4$. Let $G^* = G - w_1w_2 + ww_2$, then $G^* \in G^0(n,r)$ and by Lemma 2.6, $\mathcal{W}_+(G^*) < \mathcal{W}_+(G)$ and $\mathcal{W}_*(G^*) < \mathcal{W}_*(G)$, a contradiction.

Combining arguments from **Claims** 1-4, we have that $G \cong G^0(n,r)$.

Follows from Lemma 2.3 and Theorem 3.1, we arrive at the following result.

Theorem 3.2. The minimal Schultz and modified Schultz indices in the set $\mathscr{G}(n,r)(1 \leq r \leq \lfloor \frac{n-1}{2} \rfloor)$ are obtained uniquely at $G^0(n,r)$.

Note that $G^0(n,0) = K_{1,n-1}$ and by Lemma 2.3, we have

Theorem 3.3. (i) $\mathcal{W}_+(G_0) > \mathcal{W}_+(G_1) > \cdots > \mathcal{W}_+(G_{\lfloor \frac{n-1}{2} \rfloor})$;
(ii) $\mathcal{W}_*(G_0) > \mathcal{W}_*(G_1) > \cdots > \mathcal{W}_*(G_{\lfloor \frac{n-1}{2} \rfloor})$.

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