# Tricyclic graphs with maximal revised Szeged index 

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#### Abstract

The revised Szeged index of a graph $G$ is defined as $S z^{*}(G)=\sum_{e=u v \in E}\left(n_{u}(e)+\right.$ $\left.n_{0}(e) / 2\right)\left(n_{v}(e)+n_{0}(e) / 2\right)$, where $n_{u}(e)$ and $n_{v}(e)$ are, respectively, the number of vertices of $G$ lying closer to vertex $u$ than to vertex $v$ and the number of vertices of $G$ lying closer to vertex $v$ than to vertex $u$, and $n_{0}(e)$ is the number of vertices equidistant to $u$ and $v$. In this paper, we give an upper bound of the revised Szeged index for a connected tricyclic graph, and also characterize those graphs that achieve the upper bound.


Keywords: Wiener index, Szeged index, Revised Szeged index, tricyclic graph.

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## 1 Introduction

All graphs considered in this paper are finite, undirected and simple. We refer the reader to [2] for terminology and notation not given here. Let $G$ be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For $u, v \in V(G), d_{G}(u, v)$ denotes the distance between $u$ and $v$ in $G$, we use $d(u, v)$ for short, if there is no ambiguity. The Wiener index of $G$ is defined as

$$
W(G)=\sum_{\{u, v\} \subseteq V(G)} d_{G}(u, v)
$$

This topological index has been extensively studied in the mathematical literature; see, e.g., [6, 8]. Let $e=u v$ be an edge of $G$, and define three sets as follows:

$$
\begin{aligned}
& N_{u}(e)=\left\{w \in V(G): d_{G}(u, w)<d_{G}(v, w)\right\} \\
& N_{v}(e)=\left\{w \in V(G): d_{G}(v, w)<d_{G}(u, w)\right\} \\
& N_{0}(e)=\left\{w \in V(G): d_{G}(u, w)=d_{G}(v, w)\right\}
\end{aligned}
$$

Thus, $\left\{N_{u}(e), N_{v}(e), N_{0}(e)\right\}$ is a partition of the vertices of $G$ respect to $e$. The number of vertices of $N_{u}(e), N_{v}(e)$ and $N_{0}(e)$ are denoted by $n_{u}(e), n_{v}(e)$ and $n_{0}(e)$, respectively. A
long time known property of the Wiener index is the formula [7, 16]:

$$
W(G)=\sum_{e=u v \in E(G)} n_{u}(e) n_{v}(e)
$$

which is applicable for trees. Motivated by the above formula, Gutman 5 introduced a graph invariant, named as the Szeged index, as an extension of the Wiener index and defined by

$$
S z(G)=\sum_{e=u v \in E(G)} n_{u}(e) n_{v}(e)
$$

Randić [14] observed that the Szeged index does not take into account the contributions of the vertices at equal distances from the endpoints of an edge, and so he conceived a modified version of the Szeged index which is named as the revised Szeged index. The revised Szeged index of a connected graph $G$ is defined as

$$
S z^{*}(G)=\sum_{e=u v \in E(G)}\left(n_{u}(e)+\frac{n_{0}(e)}{2}\right)\left(n_{v}(e)+\frac{n_{0}(e)}{2}\right) .
$$

Some properties and applications of these two topological indices have been reported in [3, 4, 9 -13, 15. In [1, Aouchiche and Hansen showed that for a connected graph $G$ of order $n$ and size $m$, an upper bound of the revised Szeged index of $G$ is $\frac{n^{2} m}{4}$. In [17], Xing and Zhou determined the unicyclic graphs of order $n$ with the smallest and the largest revised Szeged indices for $n \geq 5$, and they also determined the unicyclic graphs of order $n$ with the unique cycle of length $r(3 \leq r \leq n)$, with the smallest and the largest revised Szeged indices. In [11], we identified those graphs whose revised Szeged index is maximal among bicyclic graphs. In this paper, we give an upper bound of the revised Szeged index for a connected tricyclic graph, and also characterize those graphs that achieve the upper bound.

Theorem 1.1 Let $G$ be a connected tricyclic graph $G$ of order $n \geq 29$. Then

$$
S z^{*}(G) \leq \begin{cases}\left(n^{3}+2 n^{2}-16\right) / 4, & \text { if } n \text { is even }, \\ \left(n^{3}+2 n^{2}-18\right) / 4, & \text { if } n \text { is odd. }\end{cases}
$$

with equality if and only if $G \cong F_{n}$ (see Figure 1.1).

## 2 Main result

It is easy to check that

$$
S z^{*}\left(F_{n}\right)= \begin{cases}\left(n^{3}+2 n^{2}-16\right) / 4, & \text { if } n \text { is even }, \\ \left(n^{3}+2 n^{2}-18\right) / 4, & \text { if } n \text { is odd. }\end{cases}
$$

i.e., $F_{n}$ satisfies the equality of Theorem 1.1,

So, we are left to show that for any connected tricyclic graph $G_{n}$ of order $n \geq 29$, other than $F_{n}, S z^{*}\left(G_{n}\right)<S z^{*}\left(F_{n}\right)$. Using the fact that $n_{u}(e)+n_{v}(e)+n_{0}(e)=n$ and $m=n+2$,

$F_{n}(n$ is even $)$

$F_{n}(n$ is odd $)$

Figure 1.1: The graph for Theorem 1.1
we have

$$
\begin{aligned}
S z^{*}(G) & =\sum_{e=u v \in E(G)}\left(n_{u}(e)+\frac{n_{0}(e)}{2}\right)\left(n_{v}(e)+\frac{n_{0}(e)}{2}\right) \\
& =\sum_{e=u v \in E(G)}\left(\frac{n+n_{u}(e)-n_{v}(e)}{2}\right)\left(\frac{n-n_{u}(e)+n_{v}(e)}{2}\right) \\
& =\sum_{e=u v \in E(G)} \frac{n^{2}-\left(n_{u}(e)-n_{v}(e)\right)^{2}}{4} \\
& =\frac{m n^{2}}{4}-\frac{1}{4} \sum_{e=u v \in E(G)}\left(n_{u}(e)-n_{v}(e)\right)^{2} . \\
& =\frac{n^{3}+2 n^{2}}{4}-\frac{1}{4} \sum_{e=u v \in E(G)}\left(n_{u}(e)-n_{v}(e)\right)^{2}
\end{aligned}
$$

For convenience, let $\delta(e)=\left|n_{u}(e)-n_{v}(e)\right|$, where $e=u v$. We have

$$
\begin{equation*}
S z^{*}(G)=\frac{n^{3}+2 n^{2}}{4}-\frac{1}{4} \sum_{e=u v \in E(G)} \delta^{2}(e) \tag{1}
\end{equation*}
$$

### 2.1 Proof for tricyclic graphs with connectivity 1

Lemma 2.1 Let $G$ be a connected tricyclic graph of order $n \geq 12$ with at least one pendant edge. Then

$$
S z^{*}\left(G_{n}\right)<S z^{*}\left(F_{n}\right)
$$

Proof. Let $e^{\prime}=x y$ be a pendant edge and $d(y)=1$. Then, for $n \geq 12$, we have

$$
\begin{aligned}
\sum_{e=u v \in E}\left(n_{u}(e)-n_{v}(e)\right)^{2} & \geq\left(n_{x}\left(e^{\prime}\right)-n_{y}\left(e^{\prime}\right)\right)^{2} \\
& =(n-1-1)^{2} \\
& >18 .
\end{aligned}
$$

Combining with equality (1), the result follows.
Lemma 2.2 Let $G$ be a connected tricyclic graph of order $n \geq 12$ without pendant edges but with a cut vertex. Then, we have

$$
S z^{*}(G)<S z^{*}\left(F_{n}\right)
$$

Proof. Suppose that $u$ is a cut vertex. Since $G$ is a tricyclic graph without pendant edge, $G$ is composed of a bicyclic graph $B$ and a cycle $C$ and $V(B) \cap V(C)=\{u\}$. It is obvious that $|V(B)| \geq 4$. If $C$ is even, for every edge $e$ in $C$, we have $\delta(e)=|V(B)|-1=n-|V(C)|$. So

$$
\sum_{e \in E(G)} \delta^{2}(e) \geq \sum_{e \in E(C)} \delta^{2}(e)=|E(C)|(|V(B)|-1)^{2} \geq 4 \times 3^{2}>18
$$

If $C$ is odd, for all edges in $C$ but the edge $x y$ such that $d(u, x)=d(u, y)$, we have $\delta(e)=$ $|V(B)|-1=n-|V(C)|$. So

$$
\sum_{e \in E(G)} \delta^{2}(e) \geq \sum_{e \in E(C)} \delta^{2}(e)=(|E(C)|-1)(|V(B)|-1)^{2}
$$

If $|E(C)| \geq 5$, then $\sum_{e \in E(G)} \delta^{2}(e)>18$. If $|E(C)|=3$, then $|V(B)|-1=n-|V(C)| \geq 9$, so $\sum_{e \in E(G)} \delta^{2}(e)>18$.

Combining with equality (1), this completes the proof.

### 2.2 Proof for 2-connected tricyclic graphs

In this section, $\kappa(G) \geq 2$, then it must be one of the graphs depicted in Figure 2.2, The letters $a, b, \ldots, f$ stand for the lengths of the corresponding paths between vertices of degree greater than 2. For the sake of brevity, we refer to these paths as $P(a), P(b), \ldots, P(f)$, respectively. In the statement of the following lemmas, we call these four graphs in Figure 2.2 as $\Theta_{1}, \Theta_{2}, \Theta_{3}$ and $\Theta_{4}$, respectively.
 $E(G)$. Then $\left|n_{u}(e)-n_{v}(e)\right| \leq 1$ if and only if $e$ is in the middle of an odd path of the four paths $P_{1}, P_{2}, P_{3}$ and $P_{4}$.

Proof. Assume that $e=u v$ belongs to $P_{i}(1 \leq i \leq 4)$, the $i$ th path connecting $x$ and $y$. Then, with respect to $N_{u}(e)$ and $N_{v}(e)$, there are three cases to discuss.


Figure 2.2: Four cases for 2-connected tricyclic graphs.

Case 1. $x, y$ are in different sets. We claim that

$$
\left|n_{u}(e)-n_{v}(e)\right|=2\left|b_{i}-a_{i}\right|,
$$

where $a_{i}$ (resp. $b_{i}$ ) is the distance between $x$ (resp. $y$ ) and the edge $e$.
To see this, assume that $x \in N_{u}(e), y \in N_{v}(e)$. Then we have $a_{i}-b_{i}$ vertices more in $N_{u}(e)$ than in $N_{v}(e)$ on the path $P_{i}$, but on each path $P_{j}(j \neq i)$, we have $b_{i}-a_{i}$ vertices more in $N_{u}(e)$ than in $N_{v}(e)$. Hence $\left|n_{u}(e)-n_{v}(e)\right|=\left|3\left(b_{i}-a_{i}\right)+\left(a_{i}-b_{i}\right)\right|=2\left|b_{i}-a_{i}\right|$.

Case 2. $x, y$ are in the same set. We claim that

$$
\left|n_{u}(e)-n_{v}(e)\right|=|V(G)|-g,
$$

where $g$ is the length of the shortest cycle of $G$ that contains $e$.
To see this, assume that $x, y \in N_{u}(e)$. Thus all vertices from the paths $P_{j}(j \neq i)$ are in $N_{u}(e)$. Therefore, $n_{v}(e)=\left\lfloor\frac{g}{2}\right\rfloor$, while $n_{u}(e)=\left\lfloor\frac{g}{2}\right\rfloor+|V(G)|-g$. So $\left|n_{u}(e)-n_{v}(e)\right|=|V(G)|-g$.
Case 3. One of $x, y$ is in $N_{0}(e)$. We claim that

$$
\left|n_{u}(e)-n_{v}(e)\right| \geq 2(a-1)
$$

with equality if and only if two paths of $P_{i}(i=1,2,3,4)$ have length $a$, where $a$ is the length of a shortest path of the four paths $P_{i}(i=1,2,3,4)$.

To see this, assume that $x \in N_{u}(e), y \in N_{0}(e)$. Then the shortest cycle $C$ of $G$ that contains $e$ is odd. Let $z_{j} \in P_{j}\left(P_{j} \nsubseteq C\right)$ be the furthest vertex from $e$ such that $z_{j} \in N_{0}(e)$. Then $\left|n_{u}(e)-n_{v}(e)\right|=\sum_{j}\left(d\left(x, z_{j}\right)-1\right) \geq \sum_{j}\left(a+d\left(y, z_{j}\right)-1\right) \geq 2(a-1)$.

From the above, we know that $\left|n_{u}(e)-n_{v}(e)\right| \geq 2$ in Case 2. In Case $3,\left|n_{u}(e)-n_{v}(e)\right| \leq 1$ if two paths of $P_{i}(i=1,2,3,4)$ have length 1 , which is impossible since $G$ is simple. So, $\left|n_{u}(e)-n_{v}(e)\right| \leq 1$ if and only if $x, y$ are in different sets and $\left|b_{i}-a_{i}\right|=0$, that is, $e$ is in the middle position of an odd path of $P_{i}(i=1,2,3,4)$.

Lemma 2.4 If $G$ is a $\Theta_{1-\text { graph of order } n \geq 12 \text {. Then, we have }}^{\text {a }}$

$$
S z^{*}(G)<S z^{*}\left(F_{n}\right)
$$

Proof. Without loss of generality, assume that $a \leq b \leq c \leq d$, then $b \geq 2$. Now consider the six edges which are incident with $x$ and $y$ but do not belong to $P(a)$. Let $e_{1}=x z$ be one of them, by Lemma 2.3, $\delta\left(e_{1}\right) \geq 2$. Similar thing is true for the other five edges. Hence

$$
\sum_{e \in E(G)} \delta^{2}(e) \geq 6 \times 2^{2}=24>18
$$

Combining with equality (1), this completes the proof.
Lemma 2.5 If $G$ is a $\Theta_{2}$-graph of order $n \geq 12$. Then, we have

$$
S z^{*}(G)<S z^{*}\left(F_{n}\right)
$$

Proof. Without loss of generality, let $d \geq b, e \geq c$. In order to complete the proof, we consider the following four cases.

Case 1. $d \geq b+2$.
Consider the two edges $x x_{1}, y y_{1}$ which belong to $P(d)$, then

$$
\delta\left(x x_{1}\right)=\delta\left(y y_{1}\right)= \begin{cases}a+c+e-2, & b \leq a+c, \\ b+e-2, & b \geq a+c .\end{cases}
$$

Therefrom, we get

$$
\delta\left(x x_{1}\right)=\delta\left(y y_{1}\right) \geq a+c+e-2 .
$$

Since $c+e \geq 3, a+c+e \geq 4$. If $a+c+e \geq 6$, then $\delta\left(x x_{1}\right)=\delta\left(y y_{1}\right) \geq 4$, so $\sum_{e \in E(G)} \delta^{2}(e) \geq$ $2 \times 4^{2}>18$.

If $a=2, c=1, e=2$, then $\delta\left(x x_{1}\right)=\delta\left(y y_{1}\right) \geq 3$. Now consider the edge $x x^{\prime} \in$ $P(e), \delta\left(x x^{\prime}\right) \geq 2$. So $\sum_{e \in E(G)} \delta^{2}(e) \geq 2 \times 3^{2}+2^{2}>18$.

If $a=1, c=1, e=3$, since $n \geq 12, b+d-1 \geq 8$. Now consider the edge $x x^{\prime} \in$ $P(e), \delta\left(x x^{\prime}\right) \geq b+d-1 \geq 8$. So $\sum_{e \in E(G)} \delta^{2}(e) \geq 8^{2}>18$.

If $a=1, c=2, e=2$, then $\delta\left(x x_{1}\right)=\delta\left(y y_{1}\right) \geq 3$. Now consider the edge $x x^{\prime} \in$ $P(e), \delta\left(x x^{\prime}\right) \geq 2$. So $\sum_{e \in E(G)} \delta^{2}(e) \geq 2 \times 3^{2}+2^{2}>18$.

If $a=1, c=1, e=2$, if $b \geq 4>2=a+c$, then $\delta\left(x x_{1}\right)=\delta\left(y y_{1}\right) \geq 4$, so $\sum_{e \in E(G)} \delta^{2}(e) \geq$ $2 \times 4^{2}>18$. If $b=3$ or $2, \delta\left(x x_{1}\right)=\delta\left(y y_{1}\right) \geq 2, d \geq 7$. Now consider the edge $z z^{\prime} \in$ $P(e), \delta\left(z z^{\prime}\right) \geq 4$. So $\sum_{e \in E(G)} \delta^{2}(e) \geq 2 \times 2^{2}+4^{2}>18$. If $b=1$, then $d \geq 9$. Now consider the edge $x x^{\prime} \in P(e), \delta\left(x x^{\prime}\right) \geq d \geq 9$. So $\sum_{e \in E(G)} \delta^{2}(e) \geq 9^{2}>18$.
Case 2. $d=b+1, e=c+1$.
Subcase 2.1. $a+c-1 \geq b$.
Consider two edges $x x_{1} \in P(c)$ and $x x_{2} \in P(e), \delta\left(x x_{1}\right) \geq d-1+e-2=b+e-2$,

$$
\delta\left(x x_{2}\right)= \begin{cases}d+b-1, & c \leq a+b, \\ d-1+c-1, & c \geq a+b .\end{cases}
$$

Therefrom, we get $\delta\left(x x_{2}\right) \geq d+b-1=2 b$. So, $\delta^{2}\left(x x_{1}\right)+\delta^{2}\left(x x_{2}\right)=(b+e-2)^{2}+4 b^{2}=$ $5 b^{2}+2(e-1) b+(e-1)^{2}+3$.

If $b \geq 2$ or $e \geq 4, \sum_{e \in E(G)} \delta^{2}(e) \geq \delta^{2}\left(x x_{1}\right)+\delta^{2}\left(x x_{2}\right)>18$.
If $b=1$, and $e \leq 3$, Now consider the edge $x x^{\prime} \in P(d), \delta\left(x x^{\prime}\right) \geq 4$. So $\sum_{e \in E(G)} \delta^{2}(e) \geq$ $1^{2}+2^{2}+4^{2}>18$.

Subcase 2.2. $b \geq a+c+1$.
Consider the edge $x x_{1} \in P(c)$, since $b \geq a+c+1, y \in N_{x_{1}}\left(x x_{1}\right)$. Let $u$ be the furthest vertex in $P(d)$ such that $u \in N_{x}\left(x x_{1}\right), u^{\prime}$ be the vertex incident with $u$ but not in $N_{x}\left(x x_{1}\right)$. If the cycle $P(d) \cup P(c) \cup P(a)$ is even, then $d(u, x)=d\left(u^{\prime}, y\right)+a+c-1$, that is $d(u, x)-d\left(u^{\prime}, y\right)=$ $a+c-1$. If the cycle $P(d) \cup P(c) \cup P(a)$ is odd, then $d(u, x)+1=d\left(u^{\prime}, y\right)+a+c-1$, that is $d(u, x)-\left(d\left(u^{\prime}, y\right)-1\right)=a+c-1$. So we have $\delta\left(x x_{1}\right)=e-2+a+c-1=a+2 c-2$.

Then consider the edge $x x_{2} \in P(e)$, since $b \geq a+c+1, y \in N_{x_{2}}\left(x x_{2}\right)$. Let $u_{i}(i=$ $1,2)$ be the furthest vertex in $P(b)$ and $P(d)$ such that $u_{i} \in N_{x}\left(x x_{2}\right), u_{i}^{\prime}(i=1,2)$ be the vertex incident with $u_{i}$ but not in $N_{x}\left(x x_{2}\right)$. If the cycle $P(b) \cup P(c) \cup P(a)$ is even, then $d\left(u_{1}, x\right)=d\left(u_{1}^{\prime}, y\right)+a+c, d\left(u_{2}, x\right)+1=d\left(u_{2}^{\prime}, y\right)+a+c$. If the cycle $P(b) \cup P(c) \cup P(a)$ is odd, then $d\left(u_{1}, x\right)+1=d\left(u_{1}^{\prime}, y\right)+a+c, d\left(u_{2}, x\right)=d\left(u_{2}^{\prime}, y\right)+a+c$. So we have $\delta\left(x x_{2}\right)=$ $d\left(u_{1}, x\right)+d\left(u_{2}, x\right) \geq 2 a+2 c-1$.

From above, we have

$$
\sum_{e \in E(G)} \delta^{2}(e) \geq(a+2 c-2)^{2}+(2 a+2 c-1)^{2}>18 .
$$

unless $a=c=1$. If $a=c=1$, now consider the edge $z z^{\prime}$ belonging to $P(e), \delta\left(z z^{\prime}\right) \geq 3$, so $\sum_{e \in E(G)} \delta^{2}(e) \geq 1^{2}+3^{2}+3^{2}>18$.
Subcase 2.3. $b=a+c$.
Consider the edge $x x_{1} \in P(e)$, then $\delta\left(x x_{1}\right)=d-1+b-1=2 b-1$.
If $b \geq 3$, then $\sum_{e \in E(G)} \delta^{2}(e) \geq 5^{2}>18$.
If $b=2$, then $a=c=1, e=2, d=3$, which is impossible since $n \geq 12$.
Case 3. $d=b+1, e=c$.

First, we know that $e=c \geq 2$.
Subcase 3.1. $a+c-1 \geq b$.
Consider the edges $x x_{1} \in P(c)$ and $x x_{2} \in P(e)$, then

$$
\delta\left(x x_{1}\right)=\delta\left(x x_{2}\right) \geq d-1+e-1=d+e-2 .
$$

Since $d \geq 2$ and $e \geq 2, d+e \geq 4$.
If $d+e \geq 6$, then $\sum_{e \in E(G)} \delta^{2}(e) \geq 2 \times 4^{2}>18$.
If $4 \leq d+e \leq 5$, now consider the edge $x x^{\prime} \in P(d)$. If $d=3, e=2$, then $b=c=2, a \geq$ $5, \delta\left(x x^{\prime}\right) \geq 3$. If $d=2, e=3$, then $b=1, c=3, a \geq 5, \delta\left(x x^{\prime}\right) \geq 5$. If $d=2, e=2$, then $b=1, c=2, a \geq 7, \delta\left(x x^{\prime}\right) \geq 4$. So $\sum_{e \in E(G)} \delta^{2}(e)>18$.
Subcase 3.2. $b>a+c-1$.
Consider the edge $x x_{1} \in P(c)$, since $b>a+c-1$, then $y \in N_{x_{1}}\left(x x_{1}\right)$. Let $u$ be the furthest vertex in $P(d)$ such that $z \in N_{x}\left(x x_{1}\right), u^{\prime}$ be the vertex incident with $u$ but not in $N_{x}\left(x x_{1}\right)$. If the cycle $P(d) \cup P(c) \cup P(a)$ is even, then $d(u, x)=d\left(u^{\prime}, y\right)+a+c-1, d(u, x)-d\left(u^{\prime}, y\right)=$ $a+c-1$. If the cycle $P(b) \cup P(c) \cup P(a)$ is odd, then $d(u, x)+1=d(u, y)+a+c-1$, $d(u, x)-\left(d\left(u^{\prime}, y\right)-1\right)=a+c-1$. So we have $\delta\left(x x_{1}\right)=(e-1)+(a+c-1)=a+2 c-2$.

Similarly

$$
\delta\left(x x_{2}\right)=a+2 c-2
$$

where $x x_{2}$ is the edge belonging to $P(e)$.
Since $c \geq 2, a+2 c \geq 5$.
If $a+2 c \geq 6$, then $\sum_{e \in E(G)} \delta^{2}(e) \geq 2 \times 4^{2}>18$.
If $a+2 c=5$, that is $a=1, c=e=2$, then $b \geq 4$. Now consider $y y^{\prime} \in P(d)$, then $\delta\left(y y^{\prime}\right) \geq 3$. So $\sum_{e \in E(G)} \delta^{2}(e)>18$.
Case 4. $d=b, e=c$.
Subcase 4.1. $b=d=c=e \geq 2$.
Consider the edge $x x_{1} \in P(b)$, then $\delta\left(x x_{1}\right)=2(e-1)$. Similarly for the other three edges incident with $x$.

If $e \geq 3$, then $\sum_{e \in E(G)} \delta^{2}(e) \geq 4 \times 4^{2}>18$.
If $e=2$, since $n \geq 12, a \geq 6$. Now consider the edges $y y^{\prime}, z z^{\prime}$ belonging to $P(a), \delta\left(y y^{\prime}\right)=$ $\delta\left(z z^{\prime}\right) \geq 2$, so $\sum_{e \in E(G)} \delta^{2}(e) \geq 4 \times 2^{2}+2^{2}>18$.
Subcase 4.2. $b=d>c=e \geq 2$.
Consider the edge $x x_{1} \in P(b), \delta\left(x x_{1}\right)=d-1+e-1=d+e-2$. For $x x_{2} \in P(d)$, we also have $\delta\left(x x_{2}\right)=d+e-2$.

If $d+e \geq 6$, then $\sum_{e \in E(G)} \delta^{2}(e) \geq 2 \times 4^{2}>18$.
If $d+e=5$, that is $d=3, e=2$, then $a \geq 4$. Now consider $x x^{\prime} \in P(c)$, then $\delta\left(x x^{\prime}\right) \geq 4$. So $\sum_{e \in E(G)} \delta^{2}(e)>18$.

Combining with equality (1), this completes the proof.

Lemma 2.6 If $G$ is a $\Theta_{3}$-graph of order $n \geq 12$. Then, we have

$$
S z^{*}(G)<S z^{*}\left(F_{n}\right)
$$

Proof. Without loss of generality, let $f \geq d, e \geq c$. In order to complete the proof, we consider the following four cases.

Case 1. $e \geq c+2$.
Consider the edge $w w_{1}, y y_{1} \in P(e)$,

$$
\delta\left(y y_{1}\right)=\delta\left(w w_{1}\right)= \begin{cases}a+b+d+f-2, & c \leq a+b+d, \\ c+f-2, & c \geq a+b+d .\end{cases}
$$

Therefrom we get

$$
\delta\left(y y_{1}\right)=\delta\left(w w_{1}\right) \geq a+b+d+f-2 .
$$

Since $d+f \geq 3, a+b+d+f \geq 5$.
If $a+b+d+f \geq 6$, then $\sum_{e \in E(G)} \delta^{2}(e) \geq 2 \times 4^{2}>18$.
If $a+b+d+f=5$, that is $a=b=d=1, f=2$. Now consider the edge $z z^{\prime} \in P(f)$ then $\delta\left(z z^{\prime}\right) \geq 2$, so $\sum_{e \in E(G)} \delta^{2}(e) \geq 2 \times 3^{2}+2^{2}>18$.
Case 2. $e=c+1, f=d+1$.
Subcase 2.1. $a+c-1 \geq b+d$.
Consider the edge $y y_{1} \in P(c)$, $y y_{2} \in P(e)$, then $\delta\left(y y_{1}\right)=e-2+f-1=c+d-1$,

$$
\delta\left(y y_{2}\right)= \begin{cases}b+d+f-1, & c \leq a+b+d \\ c+f-2, & c \geq a+b+d\end{cases}
$$

Therefrom, we get $\delta\left(y y_{2}\right) \geq b+d+f-1=b+2 d$.
If $d \geq 2$ or $b \geq 3$ or $c \geq 4$, then $\sum_{e \in E(G)} \delta^{2}(e)>18$.
If $d=1, b \leq 3, c \leq 3$, then consider the edge $x x^{\prime} \in P(f)$, we have $\delta\left(x x^{\prime}\right) \geq 3$, so $\sum_{e \in E(G)} \delta^{2}(e) \geq 1^{2}+3^{2}+3^{2}>18$.
Subcase 2.2. $a+c \leq b+d-1$.
It's similar to the Subcase 2.1.
Subcase 2.3. $a+c=b+d$.
Consider the edge $y y_{1} \in P(e), x x_{1} \in P(f)$, then $\delta\left(y y_{1}\right)=b+d+f-2=b+2 d-1$, $\delta\left(x x_{1}\right)=a+c+e-2=a+2 c-1$. Since $n=a+b+c+d+e+f-2 \geq 12$, then $(a+2 c-1)+(b+2 d-1) \geq 10$, so $\sum_{e \in E(G)} \delta^{2}(e) \geq(a+2 c-1)^{2}+(b+2 d-1)^{2}>18$.
Case 3. $e=c+1, f=d$.
Subcase 3.1. $a+d-1 \geq b+c$.

Consider the edge $z z_{1} \in P(d), \delta\left(z z_{1}\right) \geq e-1+f-1=c+d-1$. Similarly $\delta\left(z z_{2}\right) \geq c+d-1$, where $z z_{2}$ is the edge belonging to $P(f)$.

Since $d \geq 2$, otherwise $G$ is not simple, then $c+d \geq 3$.
If $c+d \geq 5$, then $\sum_{e \in E(G)} \delta^{2}(e) \geq 2 \times 4^{2}>18$.
If $c=1, d=3$, then $\delta\left(z z_{1}\right), \delta\left(z z_{2}\right) \geq 3$. Now consider the edge $y y^{\prime} \in P(e), \delta\left(y y^{\prime}\right) \geq 3$, so $\sum_{e \in E(G)} \delta^{2}(e) \geq 2 \times 3^{2}+3^{2}>18$.

If $c=2, d=2$, then $\delta\left(z z_{1}\right), \delta\left(z z_{2}\right) \geq 3$. Now consider the edge $y y^{\prime} \in P(e), \delta\left(y y^{\prime}\right) \geq 3$, so $\sum_{e \in E(G)} \delta^{2}(e) \geq 2 \times 3^{2}+3^{2}>18$.

If $c=1, d=2$, then $\delta\left(z z_{1}\right), \delta\left(z z_{2}\right) \geq 2$ and $e=f=2$. Now consider the edge $y y^{\prime} \in P(e)$, no matter $b \geq 2$ or $b=1$, we both have $\delta\left(y y^{\prime}\right) \geq 4$, so $\sum_{e \in E(G)} \delta^{2}(e) \geq 2 \times 2^{2}+4^{2}>18$.
Subcase 3.2. $a+d \leq b+c$.
Now consider the edge $w w_{1} \in P(e)$, then

$$
\delta\left(w w_{1}\right)= \begin{cases}a+d+f-2, & c \leq a+b+d, \\ c+f-2, & c \geq a+b+d .\end{cases}
$$

Therefrom, we get $\delta\left(w w_{1}\right)=a+d-1+f-1=a+2 d-2$.
Since $d \geq 2, a+2 d \geq 5$.
If $a+2 d \geq 7$, then $\delta\left(w w_{1}\right) \geq 5$. So $\sum_{e \in E(G)} \delta^{2}(e) \geq 5^{2}>18$.
If $a+2 d=6$, that is $a=2, d=2$, then $\delta\left(w w_{1}\right) \geq 4$. Now consider the edge $y y^{\prime} \in P(e)$, $\delta\left(y y^{\prime}\right) \geq 2$. So $\sum_{e \in E(G)} \delta^{2}(e) \geq 4^{2}+2^{2}>18$.

If $a+2 d=5$, that is $a=1, d=2$, then $\delta\left(w w_{1}\right) \geq 3$. Now consider the edge $y y^{\prime} \in P(e)$, then we have $\delta\left(y y^{\prime}\right) \geq\left\lceil\frac{b+c+3}{2}\right\rceil-1$. Since $n \geq 12, b+2 c \geq 8$. Then we have $b+c \geq 6$ unless $b=1, c=4$. When $b=1, c=4$, we can draw the graph exactly, we also have $\delta\left(y y^{\prime}\right) \geq 4$. So $\sum_{e \in E(G)} \delta^{2}(e) \geq 3^{2}+4^{2}>18$.
Case 4. $d=f, e=c$.
We may assume that $a \leq b$.
Subcase 4.1. $c=e>d=f \geq 2$.
Consider the edge $w w_{1} \in P(e), \delta\left(w w_{1}\right)=f-1+c-1=c+f-2$. For $w w_{2} \in P(c)$, we also have $\delta\left(w w_{2}\right)=c+f-2$.

Since $c \geq 3$ and $f \geq 2, c+f \geq 5$.
If $c+f \geq 6$, then $\delta\left(w w_{1}\right)=\delta\left(w w_{2}\right) \geq 4$, so $\sum_{e \in E(G)} \delta^{2}(e) \geq 2 \times 4^{2}>18$.
If $c+f=5$, that is $c=3, f=2$, then $\delta\left(w w_{1}\right)=\delta\left(w w_{2}\right) \geq 3$. Now consider the edge $y y^{\prime} \in P(e)$, then we have $\delta\left(y y^{\prime}\right) \geq 1$. So $\sum_{e \in E(G)} \delta^{2}(e) \geq 2 \times 3^{2}+1^{2}>18$.
Subcase 4.2. $c=e=d=f \geq 3$.
Consider the edge $w w_{1} \in P(e), w w_{2} \in P(c), \delta\left(w w_{1}\right)=\delta\left(w w_{2}\right)=f-1+c-1=2(c-1) \geq 4$. So $\sum_{e \in E(G)} \delta^{2}(e) \geq 2 \times 4^{2}>18$.

Subcase 4.3. $c=e=d=f=2$.
If $b \geq a+4$, then we consider the edge $w w_{1} \in P(e), \delta\left(w w_{1}\right)=2$. Similar for $w w_{2} \in$ $P(c), x x_{1} \in P(d), x x_{2} \in P(f)$. Then consider the edge $y y^{\prime} \in P(b), \delta\left(y y^{\prime}\right) \geq 2$, so $\sum_{e \in E(G)} \delta^{2}(e) \geq$ $5 \times 2^{2}>18$.

If $a \leq b \leq a+1$, then we consider the edge $w w_{1} \in P(e), \delta\left(w w_{1}\right)=2$. Similar for $w w_{2} \in P(c), x x_{1} \in P(d), x x_{2} \in P(f)$. Then consider the edge $y w_{i}, z x_{i},(i=1,2), \delta\left(y w_{i}\right) \geq$ $1, \delta\left(z x_{i}\right) \geq 1$, so $\sum_{e \in E(G)} \delta^{2}(e) \geq 4 \times 2^{2}+4 \times 1^{2}>18$.

If $b=a+3$, then we get $T_{n}$ with $n$ being odd. If $b=a+2$, then we get $T_{n}$ with $n$ being even.

Combining with equality (1), this completes the proof.

Lemma 2.7 If $G$ is a $\Theta_{4}$-graph of order $n \geq 29$. Then, we have

$$
S z^{*}(G)<S z^{*}\left(F_{n}\right)
$$

Proof. Without loss of generality, assume that $a=\max \{a, b, c, d, e, f\}$. Since $n \geq 29$, then $a \geq 6$. Now consider the edge $w w_{1} \in P(a)$. Then $z \in N_{w}\left(w w_{1}\right)$ or $z \in N_{0}\left(w w_{1}\right)$, since $d(z, w) \leq d\left(z, w_{1}\right)$ by the choice of $a$. And $z \in N_{0}\left(w w_{1}\right)$ if and only if $a=c \leq b+d$ and $e=1$. We can obtain the similar result for $y$. Next, let $C$ be the shortest cycle containing $w w_{1}$. Then $x \in N_{w}\left(w w_{1}\right)$, if $a>\frac{|C|+1}{2} ; x \in N_{0}\left(w w_{1}\right)$, if $a=\frac{|C|+1}{2} ; x \in N_{w_{1}}\left(w w_{1}\right)$, if $a<\frac{|C|+1}{2}$.
Case 1. $a>\frac{|C|+1}{2}$.
Since $x \in N_{w}\left(w w_{1}\right)$, we can easily get $y, z \in N_{w}\left(w w_{1}\right)$. So we have $\delta\left(w w_{1}\right)=n-|C|$. Similarly, $\delta\left(x x_{1}\right)=n-|C|$, where $x x_{1} \in P(a)$.

If $n-|C| \geq 4$, then $\sum_{e \in E(G)} \delta^{2}(e) \geq 2 \times 4^{2}>18$.
If $n-|C|=1$ and $C$ is composed of paths $P(a), P(f)$ and $P(b)$, then $V(G)-V(C)=\{z\}$, and $e=c=d=1$. Since $P(a) \cup P(f) \cup P(b)$ is the shortest cycle, then $f=b=1$ and $a \geq 26$, by $n \geq 29$. Now consider every edge $e$ in $P(a)$ except the middle one in $\mathrm{P}(\mathrm{a})$ when $a$ is odd, we have $\delta(e)=1$. So $\sum_{e \in E(G)} \delta^{2}(e) \geq a-1>18$.

If $n-|C|=1$ and $C$ is composed of paths $P(a), P(f), P(d)$ and $P(c)$, which is impossible.
If $n-|C|=2$ and $C$ is composed of paths $P(a), P(f)$ and $P(b)$, then $e+c+d \leq 4, f+b \leq 3$. Since $n \geq 29, a \geq 24$. Now consider the six edges $e_{i}(1 \leq i \leq 6)$ in $P(a)$ such that the distance between $e_{i}$ and $x$ or $w$ no more than 2 , then we have $\delta\left(e_{i}\right)=2$. So $\sum_{e \in E(G)} \delta^{2}(e) \geq 6 \times 2^{2}>18$.

If $n-|C|=2$ and $C$ is composed of paths $P(a), P(f), P(d)$ and $P(c)$, then one of the two vertices is in $P(b)$, another vertex is in $P(e)$. It is the case when $C$ is composed of paths $P(a), P(f)$ and $P(b)$.

If $n-|C|=3$ and $C$ is composed of paths $P(a), P(f)$ and $P(b)$, then $e+c+d \leq 5, f+b \leq 4$. Since $n \geq 29, a \geq 22$. Now consider the four edges $e_{i}(1 \leq i \leq 4)$ in $P(a)$ such that the distance between $e_{i}$ and $x$ or $w$ no more than 1 , then we have $\delta\left(e_{i}\right)=3$. So $\sum_{e \in E(G)} \delta^{2}(e) \geq 4 \times 3^{2}>18$.

If $n-|C|=3$ and $C$ is composed of paths $P(a), P(f), P(d)$ and $P(c)$, then either one of the two vertices in $P(b)$, another two vertices are in $P(e)$, or one of the two vertices in $P(e)$,
another two vertices are in $P(b)$. It is the case when $C$ is composed of paths $P(a), P(f)$ and $P(b)$.
Case 2. $a=\frac{|C|+1}{2}$.
Subcase 2.1. $C$ is composed of paths $P(a), P(f), P(d)$ and $P(c)$.
In this case, $y, z \in N_{w}\left(w w_{1}\right)$ and $b>d+c$. Let $u$ be the furthest vertex in $P(e)$ such that $u \in N_{w}\left(w w_{1}\right), u^{\prime}$ be the vertex incident with $u$ but not in $N_{w}\left(w w_{1}\right)$. If the cycle $P(a) \cup P(c) \cup P(e)$ is even, then $d\left(x, u^{\prime}\right)+a-1=d(u, z)+c$, that is $d(u, z)=a-c-1+d\left(x, u^{\prime}\right)$. If the cycle $P(a) \cup P(c) \cup P(e)$ is odd, then $d\left(x, u^{\prime}\right)+a-1=d(u, z)+1+c$, that is $d(u, z)=a-c-2+d\left(x, u^{\prime}\right)$. Then $\delta\left(w w_{1}\right)=b-1+d(u, z) \geq a+b-c-3 \geq a-1 \geq 5$, since $b>d+c$. So $\sum_{e \in E(G)} \delta^{2}(e) \geq 5^{2}>18$.
Subcase 2.2. $C$ is composed of paths $P(a), P(f)$ and $P(b)$.
In this case, $y \in N_{w}\left(w w_{1}\right)$ and $b \leq d+c$.
If $z \in N_{0}\left(w w_{1}\right)$, then $a=c \leq b+d$ and $e=1$. So $\delta\left(w w_{1}\right) \geq c-1=a-1 \geq 5$. Hence $\sum_{e \in E(G)} \delta^{2}(e) \geq 5^{2}>18$.

If $z \in N_{w}\left(w w_{1}\right)$, similar to Subcase 2.1, we have

$$
d(u, z) \geq \begin{cases}a-c-2, & c \leq b+d \\ a-(b+d)-2, & c \geq b+d\end{cases}
$$

Then $\delta\left(w w_{1}\right)=d-1+c+d(u, z) \geq a+d-3 \geq a-2 \geq 4$. Now consider the edge $x x_{1} \in P(a)$. In this case, $w \in N_{0}\left(x x_{1}\right), y \in N_{x}\left(x x_{1}\right)$. By the above analysis, if $z \in N_{0}\left(x x_{1}\right)$, then $\delta\left(x x_{1}\right) \geq 5$. Hence $\sum_{e \in E(G)} \delta^{2}(e) \geq 5^{2}>18$. If $z \in N_{x}\left(x x_{1}\right)$, then $\delta\left(x x_{1}\right) \geq 4$. Hence $\sum_{e \in E(G)} \delta^{2}(e) \geq 2 \times 4^{2}>18$.
Case 3. $a<\frac{|C|+1}{2}$.
Subcase 3.1. Both of $y$ and $z$ are in $N_{0}\left(w w_{1}\right)$.
In this case, $a=b=c, e=f=1$. Then $\delta\left(w w_{1}\right)=c-1=a-1 \geq 5$. Hence $\sum_{e \in E(G)} \delta^{2}(e) \geq 5^{2}>18$.
Subcase 3.2. Both of $y$ and $z$ are in $N_{w}\left(w w_{1}\right)$.
In this case, we get

$$
\delta\left(w w_{1}\right) \geq \begin{cases}a+d-2, & d \geq|b-c|, \\ a+|b-c|-2, & d \leq|b-c| .\end{cases}
$$

Then $\delta\left(w w_{1}\right) \geq a+d-2 \geq a-1 \geq 5$. Hence $\sum_{e \in E(G)} \delta^{2}(e) \geq 5^{2}>18$.
Subcase 3.3. One of $y, z$ is in $N_{0}\left(w w_{1}\right)$.
We may assume that $z \in N_{0}\left(w w_{1}\right)$, then $a=c \leq b+d, e=1$.
If $z \notin V(C)$, then $C=P(a) \cup P(f) \cup P(b)$. So $\delta\left(w w_{1}\right) \geq c-1=a-1 \geq 5$. Hence $\sum_{e \in E(G)} \delta^{2}(e) \geq 5^{2}>18$.

If $z \in V(C)$, for $y \in N_{w}\left(w w_{1}\right)$, then $C=P(a) \cup P(e) \cup P(c)$. Otherwise $C=P(a) \cup$ $P(f) \cup P(d) \cup P(c)$, since $z \in N_{0}\left(w w_{1}\right)$, then $y \in N_{w_{1}}\left(w w_{1}\right)$, a contradiction. Let $u_{1}$ be the furthest vertex in $P(f)$ such that $u_{1} \in N_{w}\left(w w_{1}\right), u_{1}^{\prime}$ be the vertex incident with $u_{1}$ but not in $N_{w}\left(w w_{1}\right)$. If the cycle $P(a) \cup P(f) \cup P(b)$ is even, then $d\left(u_{1}, y\right)+b=d\left(u_{1}^{\prime}, x\right)+a-1$, that is $d\left(u_{1}, y\right)-d\left(u_{1}^{\prime}, x\right)=a-b-1$. If the cycle $P(a) \cup P(f) \cup P(b)$ is odd, then $d\left(u_{1}, y\right)+b+1=$ $d\left(u_{1}^{\prime}, x\right)+a-1$, that is $d\left(u_{1}, y\right)-\left(d\left(u_{1}^{\prime}, x\right)-1\right)=a-b-1$. Let $u_{2}$ be the furthest vertex in $P(d)$ such that $u_{2} \in N_{w}\left(w w_{1}\right), u_{2}^{\prime}$ be the vertex incident with $u_{2}$ but not in $N_{w}\left(w w_{1}\right)$. If the cycle $P(c) \cup P(e) \cup P(b)$ is even, then $d\left(u_{2}, y\right)+b=d\left(u_{2}^{\prime}, z\right)+c=d\left(u_{2}^{\prime}, z\right)+a$, that is $d\left(u_{2}, y\right)=$ $a-b+d\left(u_{2}^{\prime}, z\right)$. If the cycle $P(c) \cup P(e) \cup P(b)$ is odd, then $d\left(u_{2}, y\right)+b+1=d\left(u_{2}^{\prime}, z\right)+a$, that is $d\left(u_{2}, y\right)=a-b-1+d\left(u_{2}^{\prime}, z\right)$. Then $\delta\left(w w_{1}\right)=b+2(a-b-1) \geq 2 a-b-2 \geq a-2 \geq 4$. Then consider the edge $x x_{1}$ in $\mathrm{P}(\mathrm{a})$, in this case, we have $w \in N_{x_{1}}\left(x x_{1}\right), z \in N_{x}\left(x x_{1}\right)$. If $y \in N_{0}\left(x x_{1}\right)$, by the above analysis, we have $\delta\left(x x_{1}\right) \geq 4$. So $\sum_{e \in E(G)} \delta^{2}(e) \geq a \times 4^{2}>18$. If $y \in N_{x}\left(x x_{1}\right)$, this is the Subcase 3.2.

Combining with equality (1), this completes the proof.
From Lemma 2.1, 2.2, 2.4, 2.5, 2.6 and 2.7, we have proved Theorem 1.1 ,
Remark: In fact, Theorem 1.1 can be improved to $n \geq 23$, which needs more details of the proof. But $n$ can not be decrease, because the revised Szeged index of the graph $\Theta_{4}$ with $b=c=d=e=f=1$ is less than $F_{n}$.

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