Tricyclic graphs with maximal revised Szeged index

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Abstract

The revised Szeged index of a graph $G$ is defined as $Sz^*(G) = \sum_{e=uv \in E} (n_u(e) + n_0(e)/2)(n_v(e) + n_0(e)/2)$, 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 $e = uv$ be an edge of $G$, and define three sets as follows:

$$N_u(e) = \{w \in V(G) : d_G(u, w) < d_G(v, w)\},$$

$$N_v(e) = \{w \in V(G) : d_G(v, w) < d_G(u, w)\},$$

$$N_0(e) = \{w \in V(G) : d_G(u, w) = d_G(v, w)\}.$$

Thus, $\{N_u(e), N_v(e), N_0(e)\}$ 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.
long time known property of the Wiener index is the formula \[W(G) = \sum_{e=uv \in E(G)} n_u(e)n_v(e),\]
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
\[Sz(G) = \sum_{e=uv \in E(G)} n_u(e)n_v(e).\]

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
\[Sz^*(G) = \sum_{e=uv \in E(G)} \left( n_u(e) + \frac{n_0(e)}{2} \right) \left( n_v(e) + \frac{n_0(e)}{2} \right).\]

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 \(\frac{n^2m}{4}\). In \[17\], Xing and Zhou determined the unicyclic graphs of order \(n\geq 5\), 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
\[Sz^*(G) \leq \begin{cases} (n^3 + 2n^2 - 16)/4, & \text{if } n \text{ is even} \\ (n^3 + 2n^2 - 18)/4, & \text{if } n \text{ is odd} \end{cases}\]
with equality if and only if \(G \cong F_n\) (see Figure [17]).

2 Main result

It is easy to check that
\[Sz^*(F_n) = \begin{cases} (n^3 + 2n^2 - 16)/4, & \text{if } n \text{ is even} \\ (n^3 + 2n^2 - 18)/4, & \text{if } n \text{ is odd} \end{cases}\]
i.e., \(F_n\) satisfies the equality of Theorem [11].

So, we are left to show that for any connected tricyclic graph \(G_n\) of order \(n \geq 29\), other than \(F_n\), \(Sz^*(G_n) < Sz^*(F_n)\). Using the fact that \(n_u(e) + n_v(e) + n_0(e) = n\) and \(m = n + 2\),
we have

\[ Sz^*(G) = \sum_{e=uv \in E(G)} \left( n_u(e) + \frac{n_0(e)}{2} \right) \left( n_v(e) + \frac{n_0(e)}{2} \right) \]

\[ = \sum_{e=uv \in E(G)} \left( \frac{n + n_u(e) - n_v(e)}{2} \right) \left( \frac{n - n_u(e) + n_v(e)}{2} \right) \]

\[ = \sum_{e=uv \in E(G)} \frac{n^2 - (n_u(e) - n_v(e))^2}{4} \]

\[ = \frac{mn^2}{4} - \frac{1}{4} \sum_{e=uv \in E(G)} (n_u(e) - n_v(e))^2. \]

\[ = \frac{n^3 + 2n^2}{4} - \frac{1}{4} \sum_{e=uv \in E(G)} (n_u(e) - n_v(e))^2 \]

For convenience, let \( \delta(e) = |n_u(e) - n_v(e)| \), where \( e = uv \). We have

\[ Sz^*(G) = \frac{n^3 + 2n^2}{4} - \frac{1}{4} \sum_{e=uv \in E(G)} \delta^2(e) \]  \hspace{1cm} (1)

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

\[ Sz^*(G_n) < Sz^*(F_n) \]
Proof. Let $e' = xy$ be a pendant edge and $d(y) = 1$. Then, for $n \geq 12$, we have

\[
\sum_{e=uv \in E} (n_u(e) - n_v(e))^2 \geq (n_x(e') - n_y(e'))^2 = (n - 1 - 1)^2 > 18.
\]

Combining with equality (1), the result follows. \qed

**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

\[
Sz^*(G) < Sz^*(F_n).
\]

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 $xy$ 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. \qed

### 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.

**Lemma 2.3** Let $G$ be a $\Theta_1$-graph composed of four paths $P_1$, $P_2$, $P_3$ and $P_4$, and $e = uv \in E(G)$. Then $|n_u(e) - n_v(e)| \leq 1$ 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 $e = uv$ belongs to $P_i$ (1 ≤ $i$ ≤ 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.
Case 1. \(x, y\) are in different sets. We claim that

\[ |n_u(e) - n_v(e)| = 2|b_i - a_i|, \]

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 \(|n_u(e) - n_v(e)| = |3(b_i - a_i) + (a_i - b_i)| = 2|b_i - a_i|\).

Case 2. \(x, y\) are in the same set. We claim that

\[ |n_u(e) - n_v(e)| = |V(G)| - g, \]

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, \(n_v(e) = \lceil \frac{a}{2} \rceil\), while \(n_u(e) = \lceil \frac{a}{2} \rceil + |V(G)| - g\). So \(|n_u(e) - n_v(e)| = |V(G)| - g\).

Case 3. One of \(x, y\) is in \(N_0(e)\). We claim that

\[ |n_u(e) - n_v(e)| \geq 2(a - 1), \]

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 $z_j \in P_j(P_j \notin C)$ be the furthest vertex from $e$ such that $z_j \in N_0(e)$. Then $|n_u(e) - n_v(e)| = \sum_j (d(x, z_j) - 1) \geq \sum_j (a + d(y, z_j) - 1) \geq 2(a - 1).

From the above, we know that $|n_u(e) - n_v(e)| \geq 2$ in Case 2. In Case 3, $|n_u(e) - n_v(e)| \leq 1$ if two paths of $P_i$ $(i = 1, 2, 3, 4)$ have length 1, which is impossible since $G$ is simple. So, $|n_u(e) - n_v(e)| \leq 1$ if and only if $x, y$ are in different sets and $|b_i - a_i| = 0$, 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 $\Theta_1$-graph of order $n \geq 12$. Then, we have

$$Sz^*(G) < Sz^*(F_n)$$

**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 $e_1 = xz$ be one of them, by Lemma 2.5 $\delta(e_1) \geq 2$. 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

$$Sz^*(G) < Sz^*(F_n)$$

**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 $xx_1, yy_1$ which belong to $P(d)$, then

$$\delta(xx_1) = \delta(yy_1) = \begin{cases} a + c + e - 2, & b \leq a + c, \\ b + e - 2, & b \geq a + c. \end{cases}$$

Therefrom, we get

$$\delta(xx_1) = \delta(yy_1) \geq a + c + e - 2.$$  

Since $c + e \geq 3, a + c + e \geq 4$. If $a + c + e \geq 6$, then $\delta(xx_1) = \delta(yy_1) \geq 4$, so $\sum_{e \in E(G)} \delta^2(e) \geq 2 \times 4^2 > 18$.

If $a = 2, c = 1, e = 2$, then $\delta(xx_1) = \delta(yy_1) \geq 3$. Now consider the edge $xx' \in P(e), \delta(xx') \geq 2$. 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 $xx' \in P(e), \delta(xx') \geq b + d - 1 \geq 8$. So $\sum_{e \in E(G)} \delta^2(e) \geq 8^2 > 18$.

If $a = 1, c = 2, e = 2$, then $\delta(xx_1) = \delta(yy_1) \geq 3$. Now consider the edge $xx' \in P(e), \delta(xx') \geq 2$. 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 $\delta(xx_1) = \delta(yy_1) \geq 4$, so $\sum_{e \in E(G)} \delta^2(e) \geq 2 \times 4^2 > 18$. If $b = 3$ or $2, \delta(xx_1) = \delta(yy_1) \geq 2, d \geq 7$. Now consider the edge $zz' \in P(c), \delta(zz') \geq 4$. 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 $xx' \in P(e), \delta(xx') \geq d \geq 9$. 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 $xx_1 \in P(c)$ and $xx_2 \in P(e)$, $\delta(xx_1) \geq d - 1 + e - 2 = b + e - 2$,

$$\delta(xx_2) = \begin{cases} d + b - 1, & c \leq a + b, \\ d - 1 + c - 1, & c \geq a + b. \end{cases}$$

Therefrom, we get $\delta(xx_2) \geq d + b - 1 = 2b$. So, $\delta^2(xx_1) + \delta^2(xx_2) = (b + e - 2)^2 + 4b^2 = 5b^2 + 2(e - 1)b + (e - 1)^2 + 3$.

If $b \geq 2$ or $e \geq 4$, $\sum_{e \in E(G)} \delta^2(e) \geq \delta^2(xx_1) + \delta^2(xx_2) > 18$.

If $b = 1$, and $e \leq 3$, Now consider the edge $xx' \in P(d), \delta(xx') \geq 4$. 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 $xx_1 \in P(c)$, since $b \geq a + c + 1, y \in N_{xx_1}$. Let $u$ be the furthest vertex in $P(d)$ such that $u \in N_{xx_1}$, $u'$ be the vertex incident with $u$ but not in $N_{xx_1}$. If the cycle $P(d) \cup P(c) \cup P(a)$ is even, then $d(u, x) = d(u', y) + a + c - 1$, that is $d(u, x) = d(u', y) = a + c - 1$. If the cycle $P(d) \cup P(c) \cup P(a)$ is odd, then $d(u, x) + 1 = d(u', y) + a + c - 1$, that is $d(u, x) = d(u', y) + 1 = a + c - 1$. So we have $\delta(xx_1) = e - 2 + a + c - 1 = a + 2c - 2$.

Then consider the edge $xx_2 \in P(e)$, since $b \geq a + c + 1, y \in N_{xx_2}$. Let $u_i (i = 1, 2)$ be the furthest vertex in $P(b)$ and $P(d)$ such that $u_i \in N_{xx_2}, u_i' (i = 1, 2)$ be the vertex incident with $u_i$ but not in $N_{xx_2}$. If the cycle $P(b) \cup P(c) \cup P(a)$ is even, then $d(u_1, x) = d(u_1', y) + a + c, d(u_2, x) + 1 = d(u_2', y) + a + c$. If the cycle $P(b) \cup P(c) \cup P(a)$ is odd, then $d(u_1, x) + 1 = d(u_1', y) + a + c, d(u_2, x) = d(u_2', y) + a + c$. So we have $\delta(xx_2) = d(u_1, x) + d(u_2, x) \geq 2a + 2c - 1$.

From above, we have

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

unless $a = c = 1$. If $a = c = 1$, now consider the edge $zz'$ belonging to $P(e), \delta(zz') \geq 3$, 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 $xx_1 \in P(e)$, then $\delta(xx_1) = d - 1 + b - 1 = 2b - 1$.

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.** $d = b + 1, e = c = 1$. 7
First, we know that $e = c \geq 2$.

**Subcase 3.1.** $a + c - 1 \geq b$.

Consider the edges $xx_1 \in P(c)$ and $xx_2 \in P(e)$, then

$$\delta(xx_1) = \delta(xx_2) \geq d - 1 + e - 1 = d + e - 2.$$  

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 $xx' \in P(d)$. If $d = 3, e = 2$, then $b = c = 2, a \geq 5, \delta(xx') \geq 3$. If $d = 2, e = 3$, then $b = 1, c = 3, a \geq 5, \delta(xx') \geq 5$. If $d = 2, e = 2$, then $b = 1, c = 2, a \geq 7, \delta(xx') \geq 4$. So $\sum_{e \in E(G)} \delta^2(e) > 18$.

**Subcase 3.2.** $b > a + c - 1$.

Consider the edge $xx_1 \in P(c)$, since $b > a + c - 1$, then $y \in N_{x_1}(xx_1)$. Let $u$ be the furthest vertex in $P(d)$ such that $z \in N_x(xx_1)$, $u'$ be the vertex incident with $u$ but not in $N_x(xx_1)$. If the cycle $P(d) \cup P(c) \cup P(a)$ is even, then $d(u, x) = d(u', y) + a + c - 1, d(u, x) - d(u', y) = a + c - 1$. If the cycle $P(b) \cup P(c) \cup P(a)$ is odd, then $d(u, x) + 1 = d(u, y) + a + c - 1, d(u, x) - (d(u', y) - 1) = a + c - 1$. So we have $\delta(xx_1) = (e - 1) + (a + c - 1) = a + 2c - 2$.

Similarly

$$\delta(xx_2) = a + 2c - 2.$$  

where $xx_2$ is the edge belonging to $P(e)$.

Since $c \geq 2, a + 2c \geq 5$.

If $a + 2c \geq 6$, then $\sum_{e \in E(G)} \delta^2(e) \geq 2 \times 4^2 > 18$.

If $a + 2c = 5$, that is $a = 1, c = e = 2$, then $b \geq 4$. Now consider $yy' \in P(d)$, then $\delta(yy') \geq 3$. 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 $xx_1 \in P(b)$, then $\delta(xx_1) = 2(e - 1)$. 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 $yy', zz'$ belonging to $P(a)$, $\delta(yy') = \delta(zz') \geq 2$, 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 $xx_1 \in P(b)$, $\delta(xx_1) = d - 1 + e - 1 = d + e - 2$. For $xx_2 \in P(d)$, we also have $\delta(xx_2) = d + e - 2$.

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 $xx' \in P(c)$, then $\delta(xx') \geq 4$. So $\sum_{e \in E(G)} \delta^2(e) > 18$.  

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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

$$Sz^*(G) < Sz^*(F_n)$$

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 $ww_1, yy_1 \in P(e)$,

$$\delta(yy_1) = \delta ww_1 = \begin{cases} a + b + d + f - 2, & c \leq a + b + d, \\ c + f - 2, & c \geq a + b + d. \end{cases}$$

Therefrom we get

$$\delta(yy_1) = \delta ww_1 \geq a + b + d + f - 2.$$ 

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 $zz' \in P(f)$ then $\delta(zz') \geq 2$, 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 $yy_1 \in P(c), yy_2 \in P(e)$, then $\delta(yy_1) = e - 2 + f - 1 = c + d - 1$,

$$\delta(yy_2) = \begin{cases} b + d + f - 1, & c \leq a + b + d, \\ c + f - 2, & c \geq a + b + d. \end{cases}$$

Therefrom, we get $\delta(yy_2) \geq b + d + f - 1 = b + 2d$.

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 $xx' \in P(f)$, we have $\delta(xx') \geq 3$, 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 $yy_1 \in P(e), xx_1 \in P(f)$, then $\delta(yy_1) = b + d + f - 2 = b + 2d - 1, \delta(xx_1) = a + c + e - 2 = a + 2c - 1$. Since $n = a + b + c + d + e + f - 2 \geq 12$, then $(a + 2c - 1) + (b + 2d - 1) \geq 10$, so $\sum_{e \in E(G)} \delta^2(e) \geq (a + 2c - 1)^2 + (b + 2d - 1)^2 > 18$.

Case 3. $e = c + 1, f = d$.

Subcase 3.1. $a + d - 1 \geq b + c$. 

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Consider the edge \( zz_1 \in P(d) \), \( \delta(zz_1) \geq e - 1 + f - 1 = c + d - 1 \). Similarly \( \delta(zz_2) \geq c + d - 1 \), where \( zz_2 \) 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 \( \delta(zz_1), \delta(zz_2) \geq 3 \). Now consider the edge \( yy' \in P(e) \), \( \delta(yy') \geq 3 \), so \( \sum_{e \in E(G)} \delta^2(e) \geq 2 \times 3^2 + 3^2 > 18 \).

If \( c = 2, d = 2 \), then \( \delta(zz_1), \delta(zz_2) \geq 3 \). Now consider the edge \( yy' \in P(e) \), \( \delta(yy') \geq 3 \), so \( \sum_{e \in E(G)} \delta^2(e) \geq 2 \times 3^2 + 3^2 > 18 \).

If \( c = 1, d = 2 \), then \( \delta(zz_1), \delta(zz_2) \geq 2 \) and \( e = f = 2 \). Now consider the edge \( yy' \in P(e) \), no matter \( b \geq 2 \) or \( b = 1 \), we both have \( \delta(yy') \geq 4 \), 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 \( ww_1 \in P(e) \), then

\[
\delta(ww_1) = \begin{cases} 
    a + d + f - 2, & c \leq a + b + d, \\
    c + f - 2, & c \geq a + b + d.
\end{cases}
\]

Therefrom, we get \( \delta(ww_1) = a + d - 1 + f - 1 = a + 2d - 2 \).

Since \( d \geq 2 \), \( a + 2d \geq 5 \).

If \( a + 2d \geq 7 \), then \( \delta(ww_1) \geq 5 \). So \( \sum_{e \in E(G)} \delta^2(e) \geq 5^2 > 18 \).

If \( a + 2d = 6 \), that is \( a = 2, d = 2 \), then \( \delta(ww_1) \geq 4 \). Now consider the edge \( yy' \in P(e) \), \( \delta(yy') \geq 2 \). So \( \sum_{e \in E(G)} \delta^2(e) \geq 4^2 + 2^2 > 18 \).

If \( a + 2d = 5 \), that is \( a = 1, d = 2 \), then \( \delta(ww_1) \geq 3 \). Now consider the edge \( yy' \in P(e) \), then we have \( \delta(yy') \geq \lceil \frac{b + c + 2}{2} \rceil - 1 \). Since \( n \geq 12 \), \( b + 2c \geq 8 \). 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 \( \delta(yy') \geq 4 \). 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 \( ww_1 \in P(e) \), \( \delta(ww_1) = f - 1 + c - 1 = c + f - 2 \). For \( ww_2 \in P(c) \), we also have \( \delta(ww_2) = c + f - 2 \).

Since \( c \geq 3 \) and \( f \geq 2 \), \( c + f \geq 5 \).

If \( c + f \geq 6 \), then \( \delta(ww_1) = \delta(ww_2) \geq 4 \), 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 \( \delta(ww_1) = \delta(ww_2) \geq 3 \). Now consider the edge \( yy' \in P(e) \), then we have \( \delta(yy') \geq 1 \). 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 \( ww_1 \in P(e), ww_2 \in P(c), \delta(ww_1) = \delta(ww_2) = f - 1 + c - 1 = 2(c - 1) \geq 4 \).

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 $ww_1 \in P(e)$, $\delta(ww_1) = 2$. Similar for $ww_2 \in P(c), xx_1 \in P(d), xx_2 \in P(f)$. Then consider the edge $yy' \in P(b)$, $\delta(yy') \geq 2$, 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 $ww_1 \in P(e)$, $\delta(ww_1) = 2$. Similar for $ww_2 \in P(c), xx_1 \in P(d), xx_2 \in P(f)$. Then consider the edge $yw_i, zz_i, (i = 1, 2)$, $\delta(yw_i) \geq 1, \delta(zz_i) \geq 1$, 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

$$Sz^*(G) < Sz^*(F_n)$$

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 $ww_1 \in P(a)$. Then $z \in N_w(ww_1)$ or $z \in N_0(ww_1)$, since $d(z, w) \leq d(z, w_1)$ by the choice of $a$. And $z \in N_0(ww_1)$ if and only if $a = c = b + d$ and $e = 1$. We can obtain the similar result for $y$. Next, let $C$ be the shortest cycle containing $ww_1$. Then $x \in N_w(ww_1)$, if $a > \frac{|C| + 1}{2}$; $x \in N_0(ww_1)$, if $a = \frac{|C| + 1}{2}$; $x \in N_w(ww_1)$, if $a < \frac{|C| + 1}{2}$.

Case 1. $a > \frac{|C| + 1}{2}$.

Since $x \in N_w(ww_1)$, we can easily get $y, z \in N_w(ww_1)$. So we have $\delta(ww_1) = n - |C|$. Similarly, $\delta(xx_1) = n - |C|$, where $xx_1 \in P(a)$.

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 $P(a)$ 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 $e + c + d \leq 4, f + b \leq 4$. 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 $\delta(e_i) = 2$. 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 $\delta(e_i) = 3$. 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, $y, z \in N_w(ww_1)$ and $b > d + c$. Let $u$ be the furthest vertex in $P(e)$ such that $u \in N_w(ww_1)$, $u'$ be the vertex incident with $u$ but not in $N_w(ww_1)$. If the cycle $P(a) \cup P(e) \cup P(d)$ is even, then $d(a, u') + a - 1 = d(u, z) + c$, that is $d(u, z) = a - c - 1 + d(x, x')$. If the cycle $P(a) \cup P(e) \cup P(d)$ is odd, then $d(x, x') + a - 1 = d(u, z) + 1 + c$, that is $d(u, z) = a - c - 2 + d(x, x')$. Then $\delta(ww_1) = b - 1 + d(u, z) \geq a + b - c - 3 \geq a - 1 \geq 5$, 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, $y \in N_w(ww_1)$ and $b \leq d + c$.

If $z \in N_0(ww_1)$, then $a = c \leq b + d$ and $e = 1$. So $\delta(ww_1) \geq c - 1 = a - 1 \geq 5$. Hence $\sum_{e \in E(G)} \delta^2(e) \geq 5^2 > 18$.

If $z \in N_w(ww_1)$, 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 $\delta(ww_1) = d - 1 + c + d(u, z) \geq a + d - 3 \geq a - 2 \geq 4$. Now consider the edge $xx_1 \in P(a)$. In this case, $w \in N_0(xx_1), y \in N_x(xx_1)$. By the above analysis, if $z \in N_0(xx_1)$, then $\delta(xx_1) \geq 5$. Hence $\sum_{e \in E(G)} \delta^2(e) \geq 5^2 > 18$. If $z \in N_x(xx_1)$, then $\delta(xx_1) \geq 4$. 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 $N_0(ww_1)$.

In this case, $a = b = c, e = f = 1$. Then $\delta(ww_1) = c - 1 = a - 1 \geq 5$. Hence $\sum_{e \in E(G)} \delta^2(e) \geq 5^2 > 18$.

Subcase 3.2. Both of $y$ and $z$ are in $N_w(ww_1)$.

In this case, we get

$$\delta(ww_1) \geq \begin{cases} a + d - 2, & d \geq |b - c|, \\ a + |b - c| - 2, & d \leq |b - c|. \end{cases}$$

Then $\delta(ww_1) \geq a + d - 2 \geq a - 1 \geq 5$. Hence $\sum_{e \in E(G)} \delta^2(e) \geq 5^2 > 18$.

Subcase 3.3. One of $y, z$ is in $N_0(ww_1)$.

We may assume that $z \in N_0(ww_1)$, then $a = c \leq b + d, e = 1$.

If $z \notin V(C)$, then $C = P(a) \cup P(f) \cup P(b)$. So $\delta(ww_1) \geq c - 1 = a - 1 \geq 5$. Hence $\sum_{e \in E(G)} \delta^2(e) \geq 5^2 > 18$. 

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If \( z \in V(C) \), for \( y \in N_w(ww_1) \), then \( C = P(a) \cup P(e) \cup P(c) \). Otherwise \( C = P(a) \cup P(f) \cup P(d) \cup P(c) \), since \( z \in N_0(ww_1) \), then \( y \in N_{w_1}(ww_1) \), a contradiction. Let \( u_1 \) be the furthest vertex in \( P(f) \) such that \( u_1 \in N_w(ww_1) \), \( u'_1 \) be the vertex incident with \( u_1 \) but not in \( N_w(ww_1) \). If the cycle \( P(a) \cup P(f) \cup P(b) \) is even, then \( d(u_1, y) + b = d(u'_1, x) + a - 1 \), that is \( d(u_1, y) - d(u'_1, x) = a - b - 1 \). If the cycle \( P(a) \cup P(f) \cup P(b) \) is odd, then \( d(u_1, y) + b + 1 = d(u'_1, x) + a - 1 \), that is \( d(u_1, y) - d(u'_1, x) - 1 = a - b - 1 \). Let \( u_2 \) be the furthest vertex in \( P(d) \) such that \( u_2 \notin N_w(ww_1) \), \( u'_2 \) be the vertex incident with \( u_2 \) but not in \( N_w(ww_1) \). If the cycle \( P(c) \cup P(e) \cup P(b) \) is even, then \( d(u_2, y) + b = d(u'_2, z) + c = d(u'_2, y) + a \), that is \( d(u_2, y) = a - b + d(u'_2, z) \). If the cycle \( P(c) \cup P(e) \cup P(b) \) is odd, then \( d(u_2, y) + b + 1 = d(u'_2, z) + a \), that is \( d(u_2, y) + b - 1 = d(u'_2, z) \). Then \( \delta(ww_1) = b + 2(a - b - 1) \geq 2a - b - 2 \geq a - 2 \geq 4 \). Then consider the edge \( xx_1 \) in \( P(a) \), in this case, we have \( w \in N_{x_1}(xx_1), z \in N_2(xx_1) \). If \( y \in N_0(xx_1) \), by the above analysis, we have \( \delta(xx_1) \geq 4 \). So \( \sum_{e \in E(G)} \delta^2(e) \geq a \times 4^2 > 18 \). If \( y \in N_2(xx_1) \), this is the Subcase 3.2.

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

From Lemma 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 \( b = e = d = e = f = 1 \) is less than \( F_n \).

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