Tricyclic graphs with maximal revised Szeged index

Lily Chen, Xueliang Li, Mengmeng Liu
Center for Combinatorics, LPMC
Nankai University, Tianjin 300071, China
Email: lily60612@126.com, lxl@nankai.edu.cn, liumm05@163.com

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 [3] 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, 9, 11, 13]. 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. A long time known property of the Wiener index is the formula [12, 23]:

$$W(G) = \sum_{e=uv\in E(G)} n_u(e)n_v(e),$$

which is applicable for trees. Motivated by the above formula, Gutman [10] introduced a graph invariant, named as the *Szeged index*, as an extension of the Wiener index and defined by

$$Sz(G) = \sum_{e=uv\in E(G)} n_u(e)n_v(e).$$

The above defined graph invariant is based on counting of vertices of the underlying graph and is sometimes referred to as the vertex Szeged index. Also the edge-variant of this invariant has been considered, called "edge Szeged index", see [7, 17] and the references cited therein. Recently, a "revised edge Szeged index" has also been considered [8].

Randić [21] 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 [2, 4, 5, 14–16, 18–20, 22]. 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 [24], 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 [18], 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 1.1).

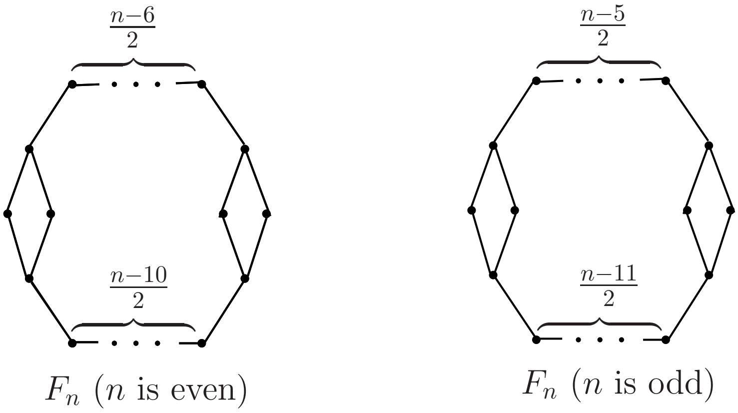

Figure 1.1: The graph for Theorem 1.1

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 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, $Sz^*(G_n) < Sz^*(F_n)$. Using the fact that $n_u(e) + n_v(e) + n_0(e) = n$ and $m = n + 2$, we have

$$\begin{aligned} Sz^*(G) &= \sum_{e=uv \in E(G)} \left(n_u(e) + \frac{n_0(e)}{2}\right)\left(n_v(e) + \frac{n_0(e)}{2}\right) \\ &= \sum_{e=uv \in E(G)} \left(\frac{n + n_u(e) - n_v(e)}{2}\right)\left(\frac{n - n_u(e) + n_v(e)}{2}\right) \\ &= \sum_{e=uv \in E(G)} \frac{n^2 - (n_u(e) - n_v(e))^2}{4} \\ &= \frac{mn^2}{4} - \frac{1}{4} \sum_{e=uv \in E(G)} (n_u(e) - n_v(e))^2. \\ &= \frac{n^3 + 2n^2}{4} - \frac{1}{4} \sum_{e=uv \in E(G)} (n_u(e) - n_v(e))^2 \end{aligned}$$

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

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

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

$$\begin{aligned} \sum_{e=uv \in E} (n_u(e) - n_v(e))^2 &\geq (n_x(e') - n_y(e'))^2 \\ &= (n - 1 - 1)^2 \\ &> 18. \end{aligned}$$

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*

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

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. ∎

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 Θ_4, respectively.

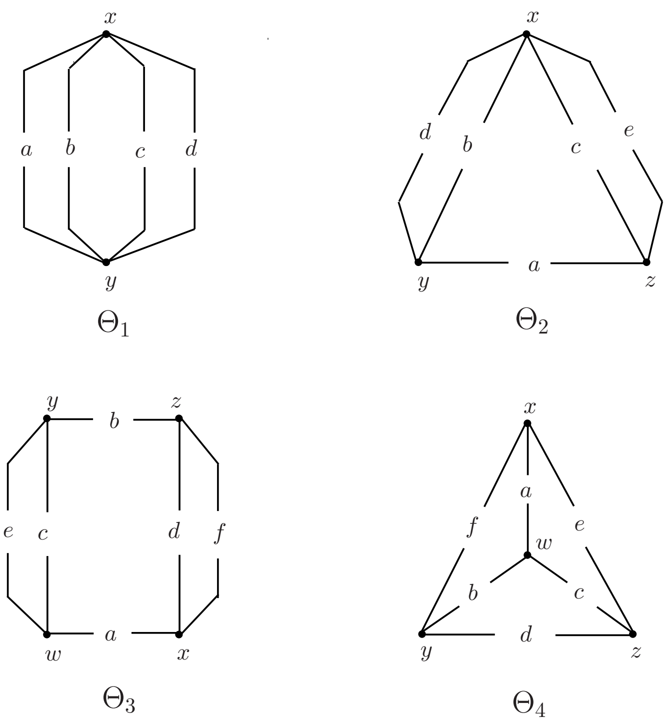

Figure 2.2: Four cases for 2-connected tricyclic graphs.

Lemma 2.3 *Let G be a Θ_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 $(1 \leq i \leq 4)$, the ith 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, $n_v(e) = \lfloor \frac{g}{2} \rfloor$, while $n_u(e) = \lfloor \frac{g}{2} \rfloor + |V(G)| - g$. 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 $z_j \in P_j (P_j \nsubseteq C)$ 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 Θ_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 2.3, $\delta(e_1) \geq 2$. 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 Θ_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 $zz' \in P(e), \delta(zz') \geq 4$. 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 $b \geq a + c + 1, y \in N_{x_1}(xx_1)$. Let u be the furthest vertex in $P(d)$ such that $u \in N_x(xx_1)$, 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 $d(u, x) = d(u', y) + a + c - 1$, 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 $b \geq a + c + 1, y \in N_{x_2}(xx_2)$. Let $u_i (i = 1, 2)$ be the furthest vertex in $P(b)$ and $P(d)$ such that $u_i \in N_x(xx_2)$, $u'_i (i = 1, 2)$ be the vertex incident with u_i but not in $N_x(xx_2)$. 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. $d = b + 1, e = c$.

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 $\sum_{e \in E(G)} \delta^2(e) > 18$.

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

Lemma 2.6 *If G is a Θ_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. $a + d - 1 \geq b + c$.

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 $\delta(yy') \geq \lceil \frac{b+c+3}{2} \rceil - 1$. 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 $yw_i, zx_i, (i=1,2)$, $\delta(yw_i)\geq 1, \delta(zx_i)\geq 1$, 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 Θ_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 $a=c\leq b+d$ 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 $a=\frac{|C|+1}{2}$; $x\in N_{w_1}(ww_1)$, 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 $e+c+d\leq 4, f+b\leq 3$. 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 $\delta(e_i)=2$. 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 $P(a)\cup P(c)\cup P(e)$ is even, then $d(x,u')+a-1=d(u,z)+c$, that is $d(u,z)=a-c-1+d(x,u')$. If the cycle $P(a)\cup P(c)\cup P(e)$ is odd, then $d(x,u')+a-1=d(u,z)+1+c$, that is $d(u,z)=a-c-2+d(x,u')$. 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 $\sum_{e\in E(G)} \delta^2(e) \geq 5^2 > 18$.

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 $u_2 \in N_w(ww_1)$, 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 $d(u_2, y) + b = d(u_2', z) + c = d(u_2', z) + a$, 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 $d(u_2, y) = a - b - 1 + d(u_2', z)$. 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 $w \in N_{x_1}(xx_1), z \in N_x(xx_1)$. 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 $y \in N_x(xx_1)$, 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 Θ_4 with $b = c = d = e = f = 1$ is no less than F_n.

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