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Steiner Wiener Index of the Square of Graphs*

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Abstract

The square of a graph G, denoted by G^2, is a graph with the same vertex set as G, in which two vertices are adjacent if and only if their distance is at most 2 in G. For $S \subseteq V(G)$, the Steiner distance $d(S)$ of S is the minimum size of a connected subgraph of G whose vertex set contains S. The kth Steiner Wiener index $SW_k(G)$ of G is defined as the sum of Steiner distances of all k-element subsets of $V(G)$. In this paper, we show that for any tree T of order n,

$$SW_3(S_n^2) \leq SW_3(T^2) \leq SW_3(P_n^2),$$

where S_n and P_n are the star and path of the order n, respectively. Let G be a connected graph of order $n \geq 5$ with connected complement $\overline{G}$. We establish the Nordahaus-Gaddum type result for a connected graph G with connected complement $\overline{G}$:

$$4\binom{n}{3} \leq SW_3(G^2) + SW_3(\overline{G}^2) \leq SW_3(P_n^2) + SW_3(\overline{P_n}^2),$$

and

$$4 \leq sdiam_3(G^2) + sdiam_3(\overline{G}^2) \leq \begin{cases} \lceil \frac{n}{2} \rceil + 2 & \text{if } n \geq 9 \\ 6 & \text{otherwise,} \end{cases}$$

where $sdiam_3(G)$ is Steiner 3-diameter of G.

1 Introduction

In this paper, we are concerned with finite undirected connected simple graphs. We refer to [2] for graph theoretical notation and terminology not specified here. The vertex

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and edge sets of G are denoted by $V(G)$ and $E(G)$, respectively. We say $|V(G)|$ the *order* of G. The *degree* and the *neighborhood* of a vertex $u \in V(G)$ are denoted by $d_G(u)$ and $N_G(u)$, respectively. The length of a path between two vertices is the number of edges on that path. The *distance* between two vertices u and v, denoted by $d_G(u, v)$, as being the length of the shortest path between them. The *square* of a graph G, denoted by G^2, is a graph with the same vertex set such that two vertices are adjacent in G^2 if and only if their distance is at most 2 in G.

As usual, we use P_n, S_n, K_n to denote the path, the star, the complete graph of order n, respectively. A tree is called a double star $S_{p,q}$ if it is obtained from S_p and S_q by connecting the center of S_p with that of S_q via an edge. The *diameter* of a graph G, denoted by $diam(G)$, is the largest distance between two vertices in G.

The Wiener index is a well-known distance-based topological index introduced as a structural descriptor for acyclic organic molecules [15]. It is defined as the sum of distance between all unordered pairs of vertices of a simple graph G, i.e.,

$$W(G) = \sum_{u,v \in V(G)} d_G(u, v).$$

For the related results and further references, we refer to a survey [6].

The Steiner distance of a graph, introduced by Chartarand, Oellermann, Tian and Zou [4] in 1989, is a natural generalization of the distance of two vertices in a graph. For a graph $G = (V, E)$ and a set $S \subseteq V$, an *S-Steiner tree* or a *Steiner tree connecting S* (or simply, an *S-tree*) is a connected subgraph $H = (V', E')$ of G with $S \subseteq V'$. Let G be a connected graph of order at least 2 and let S be a nonempty set of vertices of G. Then the *Steiner distance* $d(S)$ among the vertices of S (or simply the *distance* of S) is the minimum size of a connected subgraph H of G such that $S \subseteq V(H)$. It is clear that H must be a tree, and if $|S| = k$, then $d(S) \geq k - 1$. In particular, if $S = \{u, v\}$, then $d_G(S) = d_G(u, v)$.

Let n and k be integers such that $2 \leq k \leq n$. The *Steiner k-eccentricity* $\varepsilon_k(v)$ of a vertex v of G is defined by $\varepsilon_k(v) = \max\{d_G(S)|\ S \subseteq V(G), |S| = k, and\ v \in S\}$. The *Steiner k-radius* of G is $srad_k(G) = \min\{\varepsilon_k(v)|\ v \in V(G)\}$, while the *Steiner k-diameter* of G is $sdiam_k(G) = \max\{\varepsilon_k(v)|\ v \in V(G)\}$. Note that for every connected graph G, $srad_2(G) = rad(G)$ and $sdiam_2(G) = diam(G)$. For more results on Steiner distance, one may see [1, 3, 4, 5, 7, 14].

With respect to the concept of Steiner distance, Li, Mao, and Gutman [8] generalized the concept of Wiener index by Steiner Wiener index. For an integer k with $2 \leq k \leq n-1$, the *Steiner k-Wiener index* $SW_k(G)$ of G is the sum of Steiner k-distances of all subsets S of $V(G)$ with $|S| = k$, that is,

$$SW_k(G) = \sum_{\substack{S \subseteq V(G) \\ |S|=k}} d(S).$$

Clearly, $SW_2(G) = W(G)$, $SW_1(G) = 0$ and $SW_n(G) = n-1$ for a connected graph G of order n. For more details on Steiner Wiener index, we recommend [8, 11, 12].

The complement $\overline{G}$ of a graph G is the graph whose vertex set is $V(G)$ and whose edges are the pairs of nonadjacent vertices of G. In 1956, Nordhaus and Gaddum [13] proved that for a graph G of order n, $2\sqrt{n} \leq \chi(G) + \chi(\overline{G}) \leq n+1$, where $\chi(G)$ denotes the chromatic number of G. Since then many research devoted to the sum on various parameters of a graph and its complement in graph theory, which are known as Nordhaus-Gaddum-type results. Mao [9, 10] obtained the Nordhaus-Gaddum-type results for the parameters $sdiam_k(G)$ and the Steiner k-Wiener index of graphs.

Motivated by the above results, in this paper, we obtain similar results for $sdiam_3(G^2)$ and the Steiner Wiener index $SW_3(G^2)$ of the square of graphs.

2 The Steiner diameter

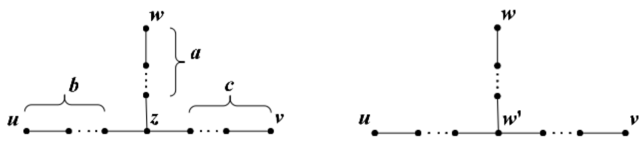
Lemma 2.1. *If $d_{G^2}(u,v) = r$ for any positive integer r, then $d_G(u,v) = 2r$ or $d_G(u,v) = 2r-1$.*

Proof. If $d_G(u,v) \geq 2r+1$, then $d_{G^2}(u,v) \geq r+1$. If $d_G(u,v) \leq 2r-2$, then $d_{G^2}(u,v) \leq r-1$. So the result follows. ■

Lemma 2.2. *Let G be a connected graph of order n ($n \geq 3$) and let $S \subseteq V$ be a set of vertices of G with $|S| = 3$. If $d_G(S) = 2$, then $d_{G^2}(S) = 2$; if $d_G(S) \geq 3$, then*

$$d_{G^2}(S) = \begin{cases} \left\lceil \dfrac{d_G(S)}{2} \right\rceil, & \text{if } d_G(S) \text{ is odd,} \\[2ex] \left\lceil \dfrac{d_G(S)}{2} \right\rceil \text{ or } \left\lceil \dfrac{d_G(S)}{2} \right\rceil + 1, & \text{if } d_G(S) \text{ is even.} \end{cases}$$

Proof. Let $S = \{u,v,w\}$. If T is a Steiner tree connecting S in G with $|E(T)| = d_G(S)$, then T must be a path or have the form $T_{a,b,c}$ as illustrated in Figure 1(a), where $T_{a,b,c}$ is a tree with a vertex z of degree 3 such that $T_{a,b,c} - z = P_a \cup P_b \cup P_c$, where $a \geq 1$, $b \geq 1$, $c \geq 1$ and $a + b + c \leq n - 1$.



(a) $T_{a,b,c}$ (b) $T_{a',b',c'}$

Figure 1. Graphs for Lemma 2.2.

If $d_G(S) = 2$, clearly $d_{G^2}(S) = 2$. Next we assume that $d_G(S) \geq 3$. The structure of Steiner tree connecting S in graph G^2 is shown in figure 1(b), denote by $T_{a',b',c'}$ and $|E(T_{a',b',c'})| = d_{G^2}(S)$. Then $d_{G^2}(S) = d_{G^2}(u, w') + d_{G^2}(w', w) + d_{G^2}(w', v)$. Without loss of generality, let $d_{G^2}(u, w') = t$, $d_{G^2}(w', w) = k$, then $d_{G^2}(w', v) = d_{G^2}(S) - t - k$, where $k \geq 0$. If $k = 0$, then $w = w'$. Clearly, $d_G(S) \leq d_G(u, w') + d_G(w', w) + d_G(w', v)$. By Lemma 2.1, $d_G(S) \leq 2t + 2k + 2(d_{G^2}(S) - t - k) = 2d_{G^2}(S)$.

Case 1. All Steiner tree T with $|E(T)| = d_G(S)$ connecting S is a path in G.

Suppose that the path T is $u \cdots w \cdots v$. We divide three subcases in terms of the parity of $d_G(u, w)$ and $d_G(w, v)$.

Case 1.1 Both $d_G(u, w)$ and $d_G(w, v)$ are even.

Let $d_G(u, w) = 2r$, $d_G(w, v) = 2p$. Thus $d_G(S) = 2r + 2p$. Then $d_{G^2}(S) \leq r + p = \lceil \frac{d_G(S)}{2} \rceil$. In this case, suppose that $d_{G^2}(S) \leq r+p-1$, then $d_G(S) \leq 2d_{G^2}(S) \leq 2r+2p-2 < 2r + 2p = d_G(S)$, a contradiction. Therefore, $d_{G^2}(S) = r + p = \lceil \frac{d_G(S)}{2} \rceil$.

Case 1.2 Both $d_G(u, w)$ and $d_G(w, v)$ are odd.

Let $d_G(u, w) = 2r + 1$, $d_G(w, v) = 2p + 1$. So, $d_G(S) = 2r + 2p + 2$. Then $d_{G^2}(S) \leq r + p + 2 = \lceil \frac{d_G(S)}{2} \rceil + 1$. In this case, suppose that $d_{G^2}(S) \leq r + p + 1$, then $d_{G^2}(w', v) \leq r + p + 1 - t - k$. By Lemma 2.1, $d_G(S) \leq 2t + 2k + 2(r + p + 1 - t - k) = 2r + 2p + 2$. If $d_G(S) = 2r + 2p + 2$, then $d_G(u, w') = 2t$, $d_G(w', w) = 2k$, $d_G(w', v) = 2(r + p + 1 - t - k)$. According to Case 1, all Steiner tree T connecting S is a path in G. Therefore, $w' = w$, then $d_G(u, w) = 2t$, contradict the fact that $d_G(u, w) = 2r+1$. Then $d_G(S) < 2r+2p+2 = d_G(S)$, a contradiction. Therefore, $d_{G^2}(S) = r + p + 2 = \lceil \frac{d_G(S)}{2} \rceil + 1$.

Case 1.3 $d_G(u, w)$ and $d_G(w, v)$ have the distinct parity.

Without loss of generality, let $d_G(u,w) = 2r+1$, $d_G(w,v) = 2p$. Thus $d_G(S) = 2r+2p+1$. Then $d_{G^2}(S) \leq r+p+1 = \lceil \frac{d_G(S)}{2} \rceil$. In this case, suppose that $d_{G^2}(S) \leq r+p$, then $d_G(S) \leq 2d_{G^2}(S) \leq 2r+2p < 2r+2p+1 = d_G(S)$, a contradiction. Therefore, $d_{G^2}(S) = r+p+1 = \lceil \frac{d_G(S)}{2} \rceil$.

Case 2. There exists a Steiner tree T with $|E(T)| = d_G(S)$ connecting S is not a path in G.

We distinguish four subcases in terms of the parity of $d_G(u,z)$, $d_G(z,v)$, $d_G(z,w)$.

Case 2.1. All of $d_G(u,z)$, $d_G(z,v)$, $d_G(z,w)$ are even.

Let $d_G(u,z) = 2r$, $d_G(z,v) = 2q$, $d_G(z,w) = 2p$. Thus $d_G(S) = 2r+2q+2p$. Then $d_{G^2}(S) \leq r+q+p = \lceil \frac{d_G(S)}{2} \rceil$. In this case, suppose that $d_{G^2}(S) \leq r+q+p-1$, then $d_G(S) \leq 2d_{G^2}(S) \leq 2r+2q+2p-2 < 2r+2q+2p = d_G(S)$, a contradiction. Therefore, $d_{G^2}(S) = r+q+p = \lceil \frac{d_G(S)}{2} \rceil$.

Case 2.2. One of $d_G(u,z)$, $d_G(z,v)$, $d_G(z,w)$ is odd, others are even.

Without loss of generality, let $d_G(u,z) = 2r+1$, $d_G(z,v) = 2q$, $d_G(z,w) = 2p$. So, $d_G(S) = 2r+2q+2p+1$. Then $d_{G^2}(S) \leq r+q+p+1 = \lceil \frac{d_G(S)}{2} \rceil$. In this case, suppose that $d_{G^2}(S) \leq r+q+p$, then $d_G(S) \leq 2d_{G^2}(S) \leq 2r+2q+2p < 2r+2q+2p+1 = d_G(S)$, a contradiction. Therefore, $d_{G^2}(S) = r+q+p+1 = \lceil \frac{d_G(S)}{2} \rceil$.

Case 2.3. One of $d_G(u,z)$, $d_G(z,v)$, $d_G(z,w)$ is even, others are odd.

Without loss of generality, let $d_G(u,z) = 2r$, $d_G(z,v) = 2q+1$, $d_G(z,w) = 2p+1$. Thus $d_G(S) = 2r+2q+2p+2$. Then $d_{G^2}(S) \leq r+q+p+2 = \lceil \frac{d_G(S)}{2} \rceil + 1$. In this case, suppose that $d_{G^2}(S) \leq r+q+p+1$, then $d_{G^2}(w',v) \leq r+q+p+1-t-k$. By Lemma 2.1, $d_G(S) \leq 2t+2k+2(r+q+p+1-t-k) = 2r+2q+2p+2$. If $d_G(S) = 2r+2q+2p+2$, then $d_G(u,w') = 2t$, $d_G(w',w) = 2k$, $d_G(w',v) = 2(r+q+p+1-t-k)$. In this case, $w' \neq z$. The Steiner tree T' with $|E(T')| = d_G(S)$ connecting S in G is mentioned in Case 2.1. If $d_G(S) < 2r+2q+2p+2$, a contradiction. Therefore, $d_{G^2}(S) = r+q+p+2 = \lceil \frac{d_G(S)}{2} \rceil + 1$.

Case 2.4. All of $d_G(u,z)$, $d_G(z,v)$, $d_G(z,w)$ are odd.

Let $d_G(u,z) = 2r+1$, $d_G(z,v) = 2q+1$, $d_G(z,w) = 2p+1$. Thus $d_G(S) = 2r+2q+2p+3$. Then $d_{G^2}(S) \leq r+q+p+2 = \lceil \frac{d_G(S)}{2} \rceil$. In this case, suppose that $d_{G^2}(S) \leq r+q+p+1$, then $d_G(S) \leq 2d_{G^2}(S) \leq 2r+2q+2p+2 < 2r+2q+2p+3 = d_G(S)$, a contradiction. Therefore, $d_{G^2}(S) = r+q+p+2 = \lceil \frac{d_G(S)}{2} \rceil$.

So the result follows. ∎

By the above lemma, we conclude that $d_{P_n^2}(S) = \lceil \frac{d_{P_n}(S)}{2} \rceil$ or $\lceil \frac{d_{P_n}(S)}{2} \rceil + 1$. Since $sdiam_3(P_n) = n-1$, we have $sdiam_3(P_n^2) = \lceil \frac{n-1}{2} \rceil$ or $\lceil \frac{n-1}{2} \rceil + 1$. By Lemma 2.2, if $n-1$ is odd, then $sdiam_3(P_n^2) = \lceil \frac{n-1}{2} \rceil$. Otherwise, $sdiam_3(P_n^2) = \lceil \frac{n-1}{2} \rceil + 1$. So $sdiam_3(P_n^2) = \lceil \frac{n}{2} \rceil$.

Lemma 2.3. *For a connected graph G of order n,*

$$2 \leq sdiam_3(G^2) \leq \left\lceil \frac{n}{2} \right\rceil.$$

Proof. The lower bound is obvious. For the upper bound, let T be a spanning tree of G, then $sdiam_3(G) \leq sdiam_3(T) \leq n-1$. Clearly, T^2 is the subgraph of G^2, thus $sdiam_3(G^2) \leq sdiam_3(T^2)$. There exists $S \subseteq V(T^2)$, such that $sdiam_3(T^2) = d_{T^2}(S) = \lceil \frac{d_T(S)}{2} \rceil$ or $\lceil \frac{d_T(S)}{2} \rceil + 1$. If $d_T(S) < n-1$, then $sdiam_3(T^2) \leq \lceil \frac{n}{2} \rceil$. From the definition of Steiner diameter and Lemma 2.2, if $d_T(S) = n-1$ and $n-1$ is odd, then $sdiam_3(T^2) = \lceil \frac{n-1}{2} \rceil = \lceil \frac{n}{2} \rceil$. Otherwise, $sdiam_3(T^2) = \lceil \frac{n-1}{2} \rceil + 1 = \lceil \frac{n}{2} \rceil$. ∎

Lemma 2.4. ([16]) *Let G be a connected graph with the connected complement. Then*

(1) if $diam(G) > 3$, then $diam(\overline{G}) = 2$,

(2) if $diam(G) = 3$, then $\overline{G}$ has a spanning subgraph which is a double star.

Theorem 2.5. *Let G be a connected graph of $n \geq 5$ with complement $\overline{G}$. Then*

$$4 \leq sdiam_3(G^2) + sdiam_3(\overline{G}^2) \leq \begin{cases} \left\lceil \frac{n}{2} \right\rceil + 2 & \text{if } n \geq 9 \\ 6 & \text{otherwise.} \end{cases}$$

Proof. The lower bound is obvious. Next, we prove that the right half of inequality holds. By Lemma 2.4, if $diam(G) > 3$, then $diam(\overline{G}) = 2$, therefore $\overline{G}^2 \cong K_n$ and $sdiam_3(\overline{G}^2) = 2$. By Lemma 2.3, we have $sdiam_3(G^2) \leq \lceil \frac{n}{2} \rceil$. Hence,

$$sdiam_3(G^2) + sdiam_3(\overline{G}^2) \leq \left\lceil \frac{n}{2} \right\rceil + 2.$$

If $diam(G) = 3$, then $diam(\overline{G}) \leq 3$, $diam(G^2) = 2$, $diam(\overline{G}^2) \leq 2$, we can obtain that $sdiam_3(G^2) \leq 3$ and $sdiam_3(\overline{G}^2) \leq 3$, therefore,

$$sdiam_3(G^2) + sdiam_3(\overline{G}^2) \leq 6.$$

If $diam(G) = 2$, then $sdiam_3(G^2) = 2$, $sdiam_3(\overline{G}^2) \leq \lceil \frac{n}{2} \rceil$.

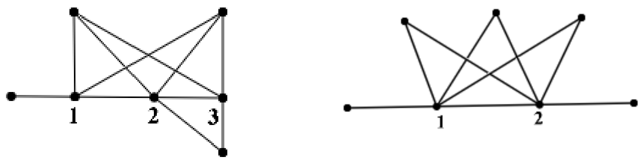
Summing up the above, we conclude that

$$4 \leq sdiam_3(G^2) + sdiam_3(\overline{G}^2) \leq \begin{cases} \left\lceil \dfrac{n}{2} \right\rceil + 2, & \text{if } n \geq 9, \\ 6, & \text{otherwise.} \end{cases}$$

■

3 Steiner Wiener index

It is natural to ask, for two graph G and G_1, whether it is true if $SW_3(G) \leq SW_3(G_1)$, $SW_3(G^2) \leq SW_3(G_1^2)$ in general. The answer is negative. For example, Let G and G_1 be two graphs of order 7 in Fig.2. Note that $SW_3(G) = 89 < SW_3(G_1) = 91$ in Fig.2, but $SW_3(G^2) = 71 > SW_3(G_1^2) = 70$. For the examples of orders greater than 7. Let G' be a graph obtained from G by adding m new vertices such that every vertex is only adjacent to 1, 2, and 3. Let G_1' be a graph obtained from G_1 by adding m new vertices such that every vertex is only adjacent to 1 and 2. By some calculation, we have $SW_3(G') < SW_3(G_1')$, but $SW_3(G'^2) = 2\binom{m+7}{3} + 1 > SW_3(G_1'^2) = 2\binom{m+7}{3}$.



(a) G (b) G_1

Figure 2. Graphs G and G_1 with $SW_3(G) < SW_3(G_1)$ and $SW_3(G^2) > SW_3(G_1^2)$.

Theorem 3.1. *For any tree T of order n, $SW_3(S_n^2) \leq SW_3(T^2) \leq SW_3(P_n^2)$.*

Proof. Since $diam(S_n) = 2$, $S_n^2 \cong K_n$. Thus $SW_3(S_n^2) = 2\binom{n}{3}$, and the left half of inequality holds and is best possible.

Let T be a tree of order n. We prove that $SW_3(T^2) \leq SW_3(P_n^2)$ by induction on the order n. It is obvious that the theorem holds when $n \leq 4$. Now let $n \geq 5$. Clearly, $d_T(u) = 1$ and $T - u$ is a tree of order $n - 1$.

By the induction hypothesis,

$$SW_3((T-u)^2) \leq SW_3((P_{n-1}^2). \tag{1}$$

Let $A = \{S : S \subseteq V(T^2), u \in S, |S| = 3\}$ and $A' = \{S' : S' \subseteq V(P_n^2), v \in S', |S'| = 3\}$. We have

$$SW_3(P_n^2) = \sum_{S' \in A'} d_{P_n^2}(S') + SW_3(P_{n-1}^2), \tag{2}$$

$$SW_3(T^2) = \sum_{S \in A} d_{T^2}(S) + SW_3((T-u)^2) \leq \sum_{S \in A} d_{T^2}(S) + SW_3(P_{n-1}^2). \tag{3}$$

So, by the above inequalities (1-3), to complete the proof of $SW_3(T^2) \leq SW_3(P_n^2)$, it remains to show that

$$\sum_{S \in A} d_{T^2}(S) \leq \sum_{S' \in A'} d_{P_n^2}(S'). \tag{4}$$

This leads us to compare the value of $d_{T^2}(S)$ and $d_{P_n^2}(S')$ in term by term. We label the vertices of P_n as $v, v_1, v_2, \ldots, v_{n-1}$, where $vv_1 \in E(P_n)$ and $v_iv_{i+1} \in E(P_n)$ for each $i \in \{1, \ldots, n-2\}$. Take a longest path of $P = uu_1u_2 \cdots u_d$ of T. Let T_i be the component of $T - u_{i-1}u_i - u_iu_{i+1}$ containing u_i for each $i \in \{1, \ldots, d-1\}$, where $u_0 = u$. We label the vertices of $V(T) \setminus V(P)$ as $u_{d+1}, u_{d+2}, \ldots, u_{n-1}$ in terms of the following rule:

(1) subscripts of labels of vertices in $V(T_i) \setminus \{u_i\}$ is less than subscripts of labels of vertices in $V(T_j) \setminus \{u_j\}$ if $i < j$;

(2) subscripts of labels of a vertex at distance smaller from u_i is less than subscripts of labels of the other one for any two vertices in $V(T_i)$ for each $i \in \{1, \ldots, d-1\}$.

We remark that if $u_k \in V(T) \backslash V(P)$, then $u_k \in V(T_l)$ for an integer $l \in \{1, \ldots, d-1\}$. It is easy to see that $d_T(u_l, u_k) \leq d_{P_n}(v_d, v_k)$. For $1 \leq i < j \leq n-1$, let $S_{i,j} = \{u, u_i, u_j\}$ and $S'_{i,j} = \{v, v_i, v_j\}$.

Claim 1. $d_T(S_{i,j}) \leq d_{P_n}(S'_{i,j})$, with equality if and only if either $1 \leq i < j \leq d$, or $i = d < j \leq n-1$ and $d_T(u_l, u_j) = j - d = d_{p_n}(v_d, v_j)$, where $u_j \in T_l$.

Proof of Claim 1: We consider the following three cases.

Case 1. $1 \leq i < j \leq d$

It is trivial to see that $d_T(S_{i,j}) = d_{P_n}(S'_{i,j})$.

Case 2. $1 \leq i \leq d < j \leq n-1$

Let $u_j \in T_l$. If $1 \leq l < i \leq d$, then $d_T(S_{i,j}) = d_T(u, u_i) + d_T(u_l, u_j)$. Clearly, $d_{P_n}(S'_{i,j}) = j = d + d_{p_n}(v_d, v_j)$, $d_{p_n}(v_d, v_j) \geq d_T(u_l, u_j)$. Then $d_T(S_{i,j}) \leq d_{P_n}(S'_{i,j})$. If

$d_T(S_{i,j}) = d_{P_n}(S'_{i,j})$, then $d_T(u,u_i) = d$, $d_T(u_l,u_j) = d_{p_n}(v_d,v_j) = j-d$. Otherwise, $d_T(S_{i,j}) < d_{P_n}(S'_{i,j})$.

If $1 \le i \le l < d$, then $d_T(S_{i,j}) = d_T(u,u_l) + d_T(u_l,u_j) < d + d_{p_n}(v_d,v_j) = d_{P_n}(S'_{i,j})$.

Case 3. $d < i < j \le n-1$

Subcase 3.1 $1 \le m < l \le d-1$.

Let $u_i \in T_m$, $u_j \in T_l$. Then $d_T(S_{i,j}) = d_T(u,u_l) + d_T(u_m,u_i) + d_T(u_l,u_j)$. Obviously, $d_{P_n}(S'_{i,j}) = j = d + d_{p_n}(v_d,v_j)$, $d_{p_n}(v_d,v_j) \ge d_T(u_m,u_i) + d_T(u_l,u_j)$. Thus $d_T(S_{i,j}) < d_{P_n}(S'_{i,j})$.

Subcase 3.2 $1 \le m = l \le d-1$

Set $u_i \in T_l$, $u_j \in T_l$, let P_1 be a shortest path of between u_l and u_j. If $u_i \in V(P_1)$, then $d_T(S_{i,j}) = d(u,u_l) + d(u_l,u_j) < d + d_{P_n}(v_d,v_j) = d_{P_n}(S'_{i,j})$.

If $u_i \in V(T_l)\backslash V(P_1)$, let the closest vertex from u_i to P_1 be u_q, then $d_T(S_{i,j}) = d_T(u,u_l) + d_T(u_l,u_j) + d_T(u_q,u_i)$. Obviously, $d_{P_n}(v_d,v_j) \ge d_T(u_l,u_j) + d_T(u_q,u_i)$. Hence, $d_T(S_{i,j}) < d_{P_n}(S'_{i,j})$.

Summing up the above, we get the conclusion, as we desired. ■

Claim 2. If $d_T(S_{i,j}) < d_{P_n}(S'_{i,j})$, then $d_{T^2}(S_{i,j}) \le d_{P_n^2}(S'_{i,j})$.

Proof: If $d_T(S_{i,j})$ is odd, then $d_{T^2}(S_{i,j}) = \lceil \frac{d_T(S_{i,j})}{2} \rceil \le \lceil \frac{d_{P_n}(S'_{i,j})}{2} \rceil \le d_{P_n^2}(S'_{i,j})$.

If $d_T(S_{i,j})$ is even, then $d_{T^2}(S_{i,j}) \le \lceil \frac{d_T(S_{i,j})}{2} \rceil + 1 \le \lceil \frac{d_{P_n}(S'_{i,j})}{2} \rceil \le d_{P_n^2}(S'_{i,j})$. ■

Claim 3. If $d_T(S_{i,j}) = d_{P_n}(S'_{i,j})$, then $d_{T^2}(S_{i,j}) \le d_{P_n^2}(S'_{i,j}) + 1$, with equality, if and only if $i = d$ and $d_T(u_l,u_j) = j-d = d_{p_n}(v_d,v_j)$, l is odd, j is even, d is even, where $u_j \in T_l$.

Proof of Claim 3: By Claim 1, we consider the following two cases.

Case 1. $1 \le i < j \le d$

It is trivial to see that $d_{T^2}(S_{i,j}) = d_{P_n^2}(S'_{i,j})$.

Case 2. $i = d < j \le n-1$ and $d_T(u_l,u_j) = j-d = d_{p_n}(v_d,v_j)$, where $u_j \in T_l$.

If $d_{T^2}(S_{d,j}) = \lceil \frac{d_T(S_{d,j})}{2} \rceil$, then $d_{T^2}(S_{d,j}) \le d_{P_n^2}(S'_{d,j})$. Since $d_T(S_{d,j}) = d_{P_n}(S'_{d,j})$, $d_{P_n^2}(S'_{d,j}) = \lceil \frac{d_{P_n}(S'_{d,j})}{2} \rceil$ or $\lceil \frac{d_{P_n}(S'_{d,j})}{2} \rceil + 1$.

If $d_{T^2}(S_{d,j}) = \lceil \frac{d_T(S_{d,j})}{2} \rceil + 1$, we divide the following three subcases by Case 2.3 in Lemma 2.2, i.e., one of $d_T(u,u_l)$, $d_T(u_l,u_d)$, $d_T(u_l,u_j)$ is even, others are odd.

Subcase 2.1 $d_T(u,u_l)$ is even

Then $d_T(u_l,u_d)$ is odd, $d_T(u_l,u_j) = j-d = d_{p_n}(v_d,v_j)$ is odd. Moreover, $d_{P_n}(S'_{d,j}) =$

$d_{P_n}(v,v_d)+d_{P_n}(v_d,v_j)=d_T(u,u_d)+d_T(u_l,u_j)$, thus $d_{P_n}(v,v_d)$ is odd and $d_{P_n}(v_d,v_j)$ is odd. By Case 1.2 in Lemma 2.2, $d_{P_n^2}(S'_{d,j})=\lceil\frac{d_{P_n}(S'_{d,j})}{2}\rceil+1$. In this case, $d_{T^2}(S_{d,j})=d_{P_n^2}(S'_{d,j})$.

Subcase 2.2 $d_T(u_l,u_d)$ is even

It is similar to Subcase 2.1, we can obtain $d_{T^2}(S_{d,j})=d_{P_n^2}(S'_{d,j})$.

Subcase 2.3 $d_T(u_l,u_j)$ is even

Then $d_{p_n}(v_d,v_j)=j-d=d_T(u_l,u_j)$ is even, $d=d_T(u,u_l)+d_T(u_l,u_d)$ is even, $d_T(S_{d,j})=d+j-d$ is even. Thus j is even. Moreover, $d_{P_n}(S'_{d,j})=d_{P_n}(v,v_d)+d_{P_n}(v_d,v_j)=d+d_T(u_l,u_j)$, thus $d_{P_n}(v,v_d)$ is even and $d_{P_n}(v_d,v_j)$ is even. By Case 1.1 in Lemma 2.2, $d_{P_n^2}(S'_{d,j})=\lceil\frac{d_{P_n}(S'_{d,j})}{2}\rceil$. In this case, $d_{T^2}(S_{d,j})=d_{P_n^2}(S'_{d,j})+1$.

Summing up the above, we get the conclusion, as we desired. ■

In view of Claim 3, let $A_1=\{(d,j):d_{T^2}(S_{d,j})=d_{P_n^2}(S'_{d,j})+1,S_{d,j}\in A\}$, and $B_1=\{(d-1,j):(d,j)\in A_1\}$. Since $d_T(u_l,u_j)$ is even, we can obtain $l\neq d-1$. Clearly, $d_T(S_{d-1,j})=d_T(u,u_l)+d_T(u_l,u_{d-1})+d_T(u_l,u_j)=d-1+j-d=j-1$ and $d_{P_n}(S'_{d-1,j})=d_{P_n}(v,v_{d-1})+d_{P_n}(v_{d-1},v_j)=j$. By Case 2.2 and Case 1.2 in Lemma 2.2, $d_{T^2}(S_{d-1,j})=\lceil\frac{d_T(S_{d-1,j})}{2}\rceil=\lceil\frac{j-1}{2}\rceil$, $d_{P_n^2}(S'_{d-1,j})=\lceil\frac{d_{P_n}(S'_{d-1,j})}{2}\rceil+1=\lceil\frac{j}{2}\rceil+1$. Since j is even, we have $d_{T^2}(S_{d-1,j})+1=d_{P_n^2}(S'_{d-1,j})$. Therefore, we have

$$\begin{aligned}
SW_3(T^2)&=\sum_{S\in A}d_{T^2}(S)+SW_3((T-u)^2)\leq\sum_{S\in A}d_{T^2}(S)+SW_3(P_{n-1}^2)\\
&=\sum_{(i,j)\in A_1\cup B_1}d_{T^2}(S_{i,j})+\left(\sum_{S\in A}d_{T^2}(S)-\sum_{(i,j)\in A_1\cup B_1}d_{T^2}(S_{i,j})\right)+SW_3(P_{n-1}^2)\\
&\leq\sum_{(i,j)\in A_1\cup B_1}d_{P_n^2}(S'_{i,j})+\left(\sum_{S'\in A'}d_{P_n^2}(S')-\sum_{(i,j)\in A_1\cup B_1}d_{P_n^2}(S'_{i,j})\right)+SW_3(P_{n-1}^2)\\
&=SW_3(P_n^2)\ .
\end{aligned}$$

■

Corollary 3.2. *For a connected graph G of order n, $SW_3(G^2)\leq SW_3(P_n^2)$.*

Proof. Let T be a spanning tree of G, then T^2 is the subgraph of G^2 with vertex set $V(T^2)=V(G^2)$. For any S, $d_{G^2}(S)\leq d_{T^2}(S)$. Thus $SW_3(G^2)\leq SW_3(T^2)$. Moreover, by Theorem 3.1, $SW_3(T^2)\leq SW_3(P_n^2)$, the result follows. ■

Note that P_4 is the unique graph of order 4 whose complement is connected. Since $\overline{P_4}\cong P_4$, we have $SW_3(P_4^2)+SW_3(\overline{P_4}^2)=2SW_3(P_4^2)=16$. Next, we calculate the value of $SW_3(P_n^2)+SW_3(\overline{P_n}^2)$ for $n\geq 5$. Let $P_n=v_1v_2\cdots v_n$, $sdiam_3(P_n^2)=\lceil\frac{n}{2}\rceil$. For any $S\subseteq V(P_n)$ with $|S|=3$, $d_{p_n^2}(S)=m$, then $2\leq m\leq\lceil\frac{n}{2}\rceil$. Hence, if n is even,

$$\begin{aligned}SW_3(P_n^2)=&\sum_{m=2}^{\frac{n}{2}-1}m[(m-1)(n-2(m-1))+2(m-1)(n-(2m-1))\\&+(m-1)(n-2m)]+\frac{n}{2}(n-2+n-2)\\=&\sum_{m=2}^{\frac{n}{2}-1}m(m-1)(4n-8m+4)+\frac{n}{2}(2n-4)\\=&\frac{2(\frac{n}{2}-1)[2n-3(\frac{n}{2}-1)]\frac{n}{2}(\frac{n}{2}-2)}{3}+\frac{n}{2}(2n-4)\\=&\frac{n^2}{6}\left(\frac{n^2}{4}-1\right)\end{aligned}$$

if n is odd,

$$\begin{aligned}SW_3(P_n^2)=&\sum_{m=2}^{\frac{n+1}{2}-1}m[(m-1)(n-2(m-1))+2(m-1)(n-(2m-1))\\&+(m-1)(n-2m)]+\frac{n+1}{2}\frac{n-1}{2}\\=&\sum_{m=2}^{\frac{n+1}{2}-1}m(m-1)(4n-8m+4)+\frac{n+1}{2}\frac{n-1}{2}\\=&\frac{2(\frac{n+1}{2}-1)[2n-3(\frac{n+1}{2}-1)]\frac{n+1}{2}(\frac{n+1}{2}-2)}{3}+\frac{n+1}{2}\frac{n-1}{2}\\=&\frac{n^4-4n^2+3}{24}\end{aligned}$$

On the other hand, for $n\geq 5$, $diam(\overline{P_n})=2$ by Lemma 2.4, $\overline{P_n}^2\cong K_n$ and we have $SW_3(\overline{P_n}^2)=2\binom{n}{3}$. Then

$$SW_3({P_n}^2)+SW_3(\overline{P_n}^2)=\begin{cases}\dfrac{n^2}{6}\left(\dfrac{n^2}{4}-1\right)+2\dbinom{n}{3}, & \text{if } n \text{ is even,}\\[2ex] \dfrac{n^4-4n^2+3}{24}+2\dbinom{n}{3}, & \text{if } n \text{ is odd.}\end{cases}$$

Corollary 3.3. *Let G be a graph of $n\geq 5$. If $diam(\overline{G})=2$ or $diam(G)=2$, then $SW_3(G^2)+SW_3(\overline{G}^2)\leq SW_3(P_n^2)+SW_3(\overline{P_n}^2)$.*

Lemma 3.4. *Let G be a connected graph of order $n \geq 5$ with connected complement $\overline{G}$. For any $S \subseteq V(G)$ with $|S| = 3$, $d_G(S) = 2$ if and only if $d_{\overline{G}}(S) > 2$.*

Proof. For any $S = \{u, v, w\} \subseteq V(G)$. If $d_G(S) = 2$, then at least two elements in $\{uv, vw, uw\}$ belong to $E(G)$, at most one element in $\{uv, vw, uw\}$ belong to $E(\overline{G})$. Thus $d_{\overline{G}}(S) > 2$.

Conversely, if $d_{\overline{G}}(S) > 2$ and uv, uw, $vw \notin E(\overline{G})$, then the tree T induced by the edges in $\{uv, uw\}$ is an S-Steiner tree in G, hence $d_G(S) = 2$. If $d_{\overline{G}}(S) > 2$ and there is an element in $\{uv, vw, uw\}$ belong to $E(\overline{G})$, without loss of generality, let $uv \in E(\overline{G})$, uw, $vw \notin E(\overline{G})$, then uw, $vw \in E(G)$, the tree T induced by the edges in $\{uw, vw\}$ is an S-Steiner tree in G, namely, $d_G(S) = 2$, as we want. ■

Theorem 3.5. *Let G be a connected graph of order $n \geq 5$ with connected complement $\overline{G}$. Then $4\binom{n}{3} \leq SW_3(G^2) + SW_3(\overline{G}^2) \leq SW_3(P_n^2) + SW_3(\overline{P_n}^2)$.*

Proof. The lower bound is obvious. For the upper bound, from Lemma 2.4(1) and Corollary 3.3, it remains to consider the case when $diam(G) = diam(\overline{G}) = 3$. Note that $diam(G^2) = diam(\overline{G}^2) = 2$. By Lemma 2.4(2), G has a spanning subgraph which is a double star. Then $2 \leq d_G(S) \leq 4$ for any $S \subseteq V(G)$ with $|S| = 3$. For $i = 2$, 3 and 4, let s_i be the number of all 3-element subsets of $V(G)$ with Steiner distance i in G and $\overline{s_i}$ be that for $\overline{G}$. By Lemma 3.4, $s_2 + \overline{s_2} = \binom{n}{3}$, $s_2 = \overline{s_3} + \overline{s_4}$ and $\overline{s_2} = s_3 + s_4$. By Lemma 2.2, if $d_G(S) = 4$, then $d_{G^2}(S) \leq 3$. If $d_G(S) \leq 3$, then $d_{G^2}(S) = 2$. Thus

$$SW_3(G^2) + SW_3(\overline{G}^2) \leq 2s_2 + 2s_3 + 3s_4 + 2\overline{s_2} + 2\overline{s_3} + 3\overline{s_4} = 4\binom{n}{3} + s_4 + \overline{s_4}.$$

By Lemma 2.4(2), let S_{p_1,q_1} be a spanning subgraph of G and S_{p_2,q_2} be that of $\overline{G}$, where $p_j + q_j = n$ for $j = 1, 2$. Hence $s_4 \leq (p_1 - 1)\binom{q_1-1}{2} + \binom{p_1-1}{2}(q_1 - 1)$ and $\overline{s_4} \leq (p_2 - 1)\binom{q_2-1}{2} + \binom{p_2-1}{2}(q_2 - 1)$. Since $p_i \cdot q_i \leq \lfloor \frac{n^2}{4} \rfloor$ for $i = 1$ and 2, $s_4 \leq \frac{\lfloor \frac{n^2}{4} \rfloor - n + 1}{2}(n - 4)$ and $\overline{s_4} \leq \frac{\lfloor \frac{n^2}{4} \rfloor - n + 1}{2}(n - 4)$. So

$$SW_3(G^2) + SW_3(\overline{G}^2) \leq 4\binom{n}{3} + \left(\left\lfloor \frac{n^2}{4} \right\rfloor - n + 1\right)(n - 4).$$

One can easily check that

$$4\binom{n}{3} + \left(\left\lfloor \frac{n^2}{4} \right\rfloor - n + 1\right)(n - 4) \leq \begin{cases} \dfrac{n^2}{6}\left(\dfrac{n^2}{4} - 1\right) + 2\dbinom{n}{3}, & \text{if } n \text{ is even,} \\ \dfrac{n^4 - 4n^2 + 3}{24} + 2\dbinom{n}{3}, & \text{if } n \text{ is odd.} \end{cases}$$

This completes the proof. ■

Note that the bounds are sharp in Theorem 2.5 and Theorem 3.5. Obviously, the upper bound can be obtained on the graph P_n. To see that the lower bound is best possible, we construct a sequence of graphs. Let G_n be a graph of order n, which is obtained from C_5 by replacing a vertex of C_5 by a complete graph of order $n-4$. It is easy to see that $diam(G_n) = diam(\overline{G_n}) = 2$, so $diam(G_n^2) = diam(\overline{G}_n^2) = 1$, $sdiam_3(G_n^2) + sdiam_3(\overline{G}_n^2) = 4$ and $SW_3(G_n^2) + SW_3(\overline{G}_n^2) = 4\binom{n}{3}$.

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