MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **88** (2022) 205–218
ISSN: 0340–6253
doi: 10.46793/match.88-1.205F

On the Extremal Steiner Wiener Index of Unicyclic Graphs

Yinqin Fan, Biao Zhao*

College of Mathematics and Systems Science, Xinjiang University, Urumqi, Xinjiang 830017, P. R. China

fan_yqin@163.com, zhb_xj@163.com

(Received December 29, 2021)

Abstract

The Steiner k-Wiener index $SW_k(G)$ of a connected graph G is defined as $SW_k(G) = \sum_{\substack{S \subseteq V(G) \\ |S|=k}} d(S)$, where the $d(S)$ is equal to the subtree minimum size among subtrees of G that connect S. A unicyclic graph is a connected graph with the same number of edges and vertices. In this paper, we study the lower and upper bounds of Steiner k-Wiener index of unicyclic graphs. In addition, we also obtain the second largest Steiner k-Wiener index among all trees.

1 Introduction

All graphs in this paper are assumed to be simple, finite and undirected. We refer to [1] for graph theoretical notation and terminology not explained here. For a connected graph G of order at least two, and a set $S \subseteq V(G)$ with S nonempty, a *Steiner tree connecting* S or an S-*Steiner tree* (or simply, an S-*tree*) is a subgraph T of G that is a tree with $S \subseteq V(T)$. Let G be a connected graph of order at least 2, and S be a nonempty set of vertices of G. Then the *Steiner distance* $d(S)$ is equal to

*Corresponding author.

the subtree minimum size among subtrees of G that connect S. Obviously, if $|S| = k$, $d(S) \geq k - 1$. The determination of a Steiner tree in a graph is a discrete simulation of the well-known geometric Steiner problem, and Steiner trees are also used in multiprocessor computer networks. For more details on Steiner distance, we refer to [2–5, 13].

Topological index is a kind of mathematical invariants derived from structure diagram of compounds, which is often used to describe the physical, chemical and pharmacological characteristics of organic compounds. The Steiner k-Wiener index and Wiener index are two important topological indices. They are useful tools for studying the structural relationship of organic compounds in chemical research. The *Steiner k-Wiener index* $SW_k(G)$ of a connected graph G, proposed a generalization by Li et al [8], is defined by

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

The above definition implies $SW_1(G) = 0$, and $SW_n(G) = n - 1$ for a connected graph G with n vertices. For $k = 2$, the Steiner 2-Wiener index $SW_2(G)$ coincides with the ordinary Wiener index.

In 2016, Li et al. [8] obtained the lower and upper bounds on Steiner k-Wiener index for connected graph G and tree T, that is,

$$\binom{n}{k}(k-1) \leq SW_k(G) \leq (k-1)\binom{n+1}{k+1}$$

for $2 \leq k \leq n - 1$, the equality on the right if and only if G is a path.

$$\binom{n-1}{k-1}(n-1) \leq SW_k(T) \leq (k-1)\binom{n+1}{k+1}$$

for $2 \leq k \leq n - 1$, the star S_n and the path P_n attain the lower and upper bounds, respectively. And in [11], Li et al. determined the Steiner k-Wiener indices of cycle and wheel. For more studies on Steiner k-Wiener index, we refer to reader [6] and [8–10, 12, 14, 15, 17].

Let $UC(n)$ be the family of *unicyclic graphs* (i.e., connected graphs containing exactly one cycle) with n vertices. Let G be a unicyclic graph (of order n) with its unique cycle C_t of length t, then $G - E(C_t)$ is a forest. $T_1, T_2, \cdots, T_c$ $(0 \leq c \leq t)$ are all nontrivial trees of $G - E(C_t)$, then $|V(T_i)| = t_i \geq 2$, $n = t - c + \sum_{i=1}^{c} t_i$, and the common vertex of C_t and T_i is the cut vertex of G, $i = 1, 2, \cdots, c$. Such a unicyclic graph is denoted by $C_t(T_{t_1}, T_{t_2}, \cdots, T_{t_c})$. If $c = 0$, then $G = C_n$. In particular, for unicyclic graph $C_t(S_{t_1}, S_{t_2}, \cdots, S_{t_c})$, S_{t_i} is a star with t_i vertices, and the common vertex of C_t and S_{t_i} is the centre of S_{t_i}. And for unicyclic graph $C_t(P_{t_1}, P_{t_2}, \cdots, P_{t_c})$, P_{t_i} is a path with t_i vertices, and the common vertex of C_t and P_{t_i} is a pendent vertex of P_{t_i}. When $t = 3$, $c = 1$, $C_3(S_{n-2})$ and $C_3(P_{n-2})$ are shown in Figure 1.

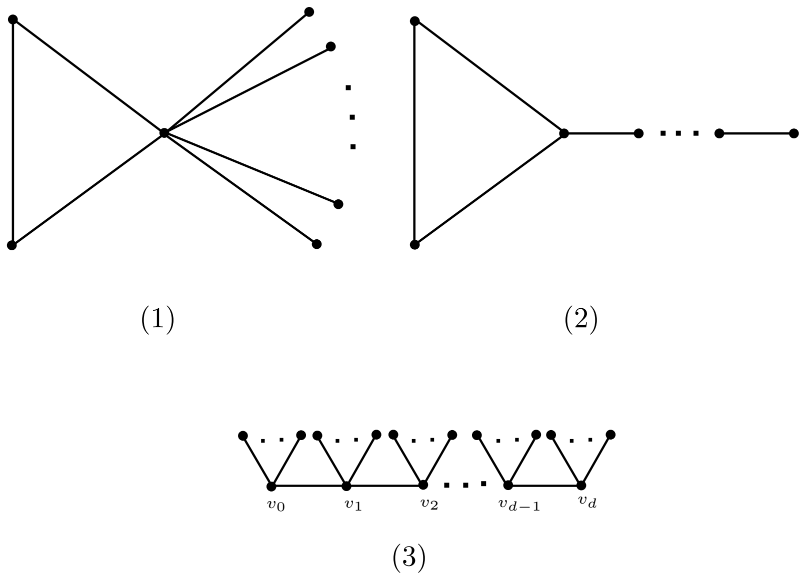

Figure 1. (1) $C_3(S_{n-2})$; (2) $C_3(P_{n-2})$; (3) $T_d^{v_0,\cdots,v_d}(m_0, \cdots, m_d)$.

The *caterpillar tree*, denoted by $T_d^{v_0,\cdots,v_d}(m_0, \cdots, m_d)$, is the tree obtained from $P_d = v_0 v_1 \cdots v_d$ by attaching $m_i \geq 0$ new vertices to v_i for $0 \leq i \leq d$ (see Figure 1). For a set $S \subseteq V(C_t(S_{t_1}, S_{t_2}, \cdots, S_{t_c}))$, the Steiner tree connecting S of $C_t(S_{t_1}, S_{t_2}, \cdots, S_{t_c})$ are caterpillar trees.

Lemma 1.1. *([16]) Let G be a unicyclic graph of order n, then*

$$SW_2(C_3(S_{n-2})) \leq SW_2(G) \leq SW_2(C_3(P_{n-2})),$$

with the equality on the left (or on the right) if and only if $G \cong C_3(S_{n-2})$ (or $G \cong C_3(P_{n-2})$).

Lemma 1.2. *([7]) Let G be a unicyclic graph of order n, and $t_i \geq 1$, then*

$$SW_{n-1}(C_n) \leq SW_{n-1}(G) \leq SW_{n-1}(C_3(P_{t_1}, P_{t_2}, P_{t_3})),$$

with the equality on the left (or on the right) if and only if $G \cong C_n$ (or $G \cong C_3(P_{t_1}, P_{t_2}, P_{t_3})$).

In above Lemmas, the lower and upper bounds of the Steiner k-Wiener index of unicyclic graphs $UC(n)$ are determined for $k = 2$ and $k = n - 1$. We consider the lower and upper bounds of the Steiner k-Wiener index of $UC(n)$ for $3 \leq k \leq n - 2$ in this paper. By a simple calculation, we can obtain the Steiner k-Wiener index of $UC(n)$ for $n \leq 5$, as shown in Table 1.

$UC(n)$	SW_2	SW_3	SW_4
C_3	6		
C_4	8	8	
$C_3(S_2)$	8	9	
C_5	15	25	15
$C_4(S_2)$	16	24	16
$C_3(S_3)$	15	24	16
$C_3(S_2, S_2)$	16	26	17
$C_3(P_3)$	17	27	17

Table 1. The Steiner k-Wiener index of $UC(n)$ for $n \leq 5$.

In this paper, we introduce some transformations for connected graphs (of order n) that do change their Steiner k-Wiener index for $3 \leq k \leq n-2$. Using these transformations, we study the lower bound of Steiner k-Wiener index of unicyclic graphs, and obtain the corresponding extremal graph as well. By studying the second largest Steiner k-Wiener index among all trees, we obtain the upper bound of Steiner k-Wiener index of unicyclic graphs. Keep in mind that we assume $n \geq 6$ for $UC(n)$.

2 The lower bound of Steiner k-Wiener index of unicyclic graphs

Let G, H be two nontrivial connected graphs with $u \in V(G)$, and $v \in V(H)$. Let GuH be the graph obtained from G and H by identifying u with v.

Lemma 2.1. *Let G be a nontrivial connected graph with $u \in V(G)$, T_m be a nontrivial tree (of order m) with $v \in V(T_m)$. Let GuS_m obtained from GuT_m by deleting the edges of T_m and connect the vertices of $T_m \backslash \{u(v)\}$ to $u(v)$. For k be an integer with $2 \leq k \leq n-1$, then*

$$SW_k(GuT_m) \geq SW_k(GuS_m),$$

with the equality if and only if $GuT_m \cong GuS_m$.

Proof. For any set $S \subseteq V(GuT_m) = V(GuS_m)$ with $|S| = k$. We consider the following.

If $S \subseteq V(G)$, then $d_{GuT_m}(S) = d_{GuS_m}(S)$.

If $S \subseteq V(T_m)$, when $k > m$, S is not exist. S contribute the same to $SW_k(T_m)$ (or $SW_k(S_m)$) and $SW_k(GuT_m)$ (or $SW_k(GuS_m)$). Since $SW_k(T_m) \geq SW_k(S_m)$ with the equality if and only if $T_m \cong S_m$, then S contribute to $SW_k(GuT_m)$ not less than $SW_k(GuS_m)$.

If $S \cap V(G\backslash\{u(v)\}) \neq \emptyset$ and $S \cap V(T_m\backslash\{u(v)\}) \neq \emptyset$. Whether $u(v)$ is contained in S or not, $u(v)$ must be contained in the Steiner trees connecting S for GuT_m and GuS_m. We divide the Steiner tree $T_{GuT_m}(S)$ into two subtrees T_G and T_{T_m}, where $V(T_{T_m}) \subseteq V(T_m)$, $V(T_G) \subseteq V(G)$, $V(T_{T_m}) \cap V(T_G) = \{u(v)\}$, $|V(T_{GuT_m}(S))| = |V(T_G)| + |V(T_{T_m})| - 1$ and $d_{GuT_m}(S) = d_{GuT_m}(V(T_{T_m})) + d_{GuT_m}(V(T_G))$. Similarly, we divide the Steiner tree $T_{GuS_m}(S)$ into two subtrees T_G and T_{S_m}. Since $d_{GuT_m}(V(T_{T_m})) \geq d_{GuS_m}(V(T_{S_m}))$, $d_{GuT_m}(V(T_G)) = d_{GuS_m}(V(T_G))$, then $d_{GuT_m}(S) \geq d_{GuS_m}(S)$.

From what has been discussed above, we can draw our conclusion. ■

By repeating the operation in Lemma 2.1, we can have the following corollary.

Corollary 2.1. *Let $G = C_t(T_{t_1}, T_{t_2}, \cdots, T_{t_c}) \neq C_n$ in $UC(n)$, and k an integer with $2 \leq k \leq n-1$, then*

$$SW_k(G) \geq SW_k\left(C_t(S_{t_1}, S_{t_2}, \cdots, S_{t_c})\right),$$

with equality if and only if $G \cong C_t(S_{t_1}, S_{t_2}, \cdots, S_{t_c})$.

Lemma 2.2. *Let $C_t(S_{t_1}, S_{t_2}, \cdots, S_{t_c}) \neq C_n$ in $UC(n)$, and k an integer with $2 \leq k \leq n-1$, then*

$$SW_k(C_t(S_{t_1}, S_{t_2}, \cdots, S_{t_c})) \geq SW_k\left(C_3(S_{n-2})\right),$$

with equality if and only if $C_t(S_{t_1}, S_{t_2}, \cdots, S_{t_c}) \cong C_3(S_{n-2})$.

Proof. Let $G = C_t(S_{t_1}, \cdots, S_{t_c})$, and let us denote vertex sets of G and $C_3(S_{n-2})$ as $V(G) = V(C_3(S_{n-2})) = \{u_0, u_1, \cdots, u_{n-1}\}$, where u_0 is a cut vertex of G and u_0 is a unique vertex of degree $n-1$ in $C_3(S_{n-2})$. For any set $S \subseteq V(G)$ with $|S| = k$, Steiner tree $T_G(S)$ is a caterpillar tree. Let $T_G(S) = T_d^{v_0,\cdots,v_d}(m_0, \cdots, m_d)$, where $v_0, v_1, \cdots, v_d \in V(C_t)$.

If $u_0 \in S$, then $d_{C_3(S_{n-2})}(S) = k-1 \leq d_G(S)$.

If $u_0 \notin S$, then $d_{C_3(S_{n-2})}(S) = k$ and $d_G(S) \geq k-1$.

When $d_G(S) = k-1 = d_{C_3(S_{n-2})}(S) - 1$, then $V(T_G(S)) = S$. Let $N(u_0)$ be the set of neighbors of u_0 in G. Define the vertex $w \in V(T_G(S))$ such that the distance between u_0 and w is the shortest in G, then $w \in V(C_t)$, and $w = v_0$ or $w = v_d$. Since u_0 is a cut vertex of G, then there is a vertex $w_0 \in N(u_0)$ such that $d_G(w_0) = 1$ and $w_0 \notin S$. Let $S' = (S \backslash \{w\}) \cup \{w_0\})$, then $d_G(S') \geq k+1 = d_{C_3(S_{n-2})}(S') + 1$. In other words, if there is an S that $d_G(S) = d_{C_3(S_{n-2})}(S) - 1$, then there must be S' such that $d_G(S') \geq d_{C_3(S_{n-2})}(S') + 1$.

Then, we have that $SW_k(G) \geq SW_k(C_3(S_{n-2}))$. ■

Observation 2.1. *Let α and k be two positive integers. If $k = 1$ or $k \geq \alpha - 1$, then $\binom{\alpha}{k} < \alpha + 1$; if $2 \leq k \leq \alpha - 2$, then $\binom{\alpha}{k} > \alpha + 1$.*

Lemma 2.3. *Let k be an integer with $3 \leq k \leq n-2$, then*

$$SW_k(C_n) > SW_k(C_3(S_{n-2})).$$

Proof. For any set $S \subseteq V(C_n)$ with $|S| = k$. If $d_{C_n}(S) = k - 1$, there are n such subsets, contributing to SW_k by $n \times (k-1)$. And if $d_{C_n}(S) \geq k$, the number of such S would be $\binom{n}{k} - n$.

For any set $S \subseteq V(C_3(S_{n-2}))$ with $|S| = k \geq 3$. If $d_{C_3(S_{n-2})}(S) = k-1$, there are $\binom{n-1}{k-1}$ such subsets, contributing to SW_k by $\binom{n-1}{k-1} \times (k-1)$. And if $d_{C_3(S_{n-2})}(S) = k$, the number of such S would be $\binom{n-1}{k}$.

It follows that

$$
\begin{aligned}
& SW_k(C_n) - SW_k(C_3(S_{n-2})) \\
&= \sum_{\substack{S \subseteq V(C_n) \\ |S|=k}} d_{C_n}(S) - \sum_{\substack{S \subseteq V(C_3(S_{n-2})) \\ |S|=k}} d_{C_3(S_{n-2})}(S) \\
&\geq \left[n(k-1) + \left(\binom{n}{k} - n \right) k \right] - \left[\binom{n-1}{k-1} (k-1) + \binom{n-1}{k} k \right] \\
&= \left[n - \binom{n-1}{k-1} \right] (k-1) + \left[\binom{n-1}{k-1} - n \right] k \\
&= \binom{n-1}{k-1} - n.
\end{aligned}
$$

By Observation 2.1, we have that $\binom{n-1}{k-1} - n > 0$ for $3 \leq k \leq n-2$.

■

Combining Corollary 2.1 and Lemma 2.2-3, we get our main result immediately.

Theorem 2.4. *For $G \in UC(n)$ $(n \geq 6)$, let k be an integer with $3 \leq k \leq n-2$, then*

$$
SW_k(G) \geq SW_k(C_3(S_{n-2})) = \binom{n-1}{k-1} (n-1),
$$

with the equality holds if and only if $G \cong C_3(S_{n-2})$.

3 The upper bound of Steiner k-Wiener index of unicyclic graphs

Let G be a unicyclic graph (of order n) with its unique cycle C_t of length t ($3 \leq t \leq n$), $T_1, T_2, \cdots, T_t$ are all spanning trees of G. For an integer k with $2 \leq k \leq n-1$, any set $S \subseteq V(G)$ with $|S| = k$, by Proposition 3.2 of [8], we have that $SW_k(G) \leq SW_k(T_i)$, $i = 1, 2, \cdots, t$. Then, $SW_k(G) \leq min\{SW_k(T_1), SW_k(T_2), \cdots, SW_k(T_t)\}$. If G is not a cycle, then G has at least one spanning tree that is not a path. When $G \in UC(n) \backslash \{C_n\}$, then $SW_k(G) < SW_k(P_n)$. It is necessary to determine the second largest Steiner k-Wiener index for trees.

Let $\mathcal{T}_l$ denote the set of trees (of order n) with l leaves. Let P_{n_1}, P_{n_2}, P_{n_3} be three paths, pairwise disjoint paths. Define three paths $P_{n_1} = x_1x_2 \cdots x_{n_1}$, $P_{n_2} = y_1y_2 \cdots y_{n_2}$ and $P_{n_3} = z_1z_2 \cdots z_{n_3}$, where $|V(P_{n_i})| = n_i \geq 2$. Let $P_{n_1}x_{n_1}P_{n_2}$ be the graph obtained from P_{n_1} and P_{n_2} by identifying x_{n_1} with y_{n_2}, and $T_3(n_1, n_2, n_3)$ be the graph obtained from $P_{n_1}x_{n_1}P_{n_2}$ and P_{n_3} by identifying x_{n_1} with z_{n_3}. Then, $T_3(n_1, n_2, n_3) \in \mathcal{T}_3$, and every graph in $\mathcal{T}_3$ can be obtained in this way.

In this section, we first prove that $SW_k(T_3(2, 2, n-2))$ reaches the second largest Steiner k-Wiener index among all trees. Then, we get the upper bound of the Steiner k-Wiener index for unicyclic graphs by computing $SW_k(T_3(2, 2, n-2)$ for $3 \leq k \leq n-2$.

Let G_0 is a connected graph with $v \in V(G_0)$, and G be the graph (of order n) obtained from G_0 and $P_{n_1}x_{n_1}P_{n_2}$ by identifying v with x_{n_1}. Then we construct a new graphs $\widetilde{G} = G - y_{n_2-1}y_{n_2} + y_{n_2-1}x_1$ from G.

Lemma 3.1. *Let G and $\widetilde{G}$ be the two graphs (of order n) above, and k an integer with $2 \leq k \leq n-1$, then*

$$SW_k(G) < SW_k(\widetilde{G}).$$

Proof. Let $T = P_{n_1}x_{n_1}P_{n_2}$, for any set $S \subseteq V(G) = V(\widetilde{G})$ with $|S| = k$.

If $S \subseteq V(G_0)$, then $d_G(S) = d_{\widetilde{G}}(S)$.

If $S \subseteq V(T)$, S contribute the same to $SW_k(G)$ and $SW_k(\widetilde{G})$ (when $k > n_1 + n_2 - 1$, S is not exist).

If $S \cap V(G_0 \backslash \{x_{n_1}\}) \neq \emptyset$ and $S \cap V(T \backslash \{x_{n_1}\}) \neq \emptyset$, then $d_G(S) \leq d_{\widetilde{G}}(S)$. Moreover, since $k \leq n-1$, there exists an $S' \subseteq V(G) = V(\widetilde{G})$ with $|S'| = k$ that contain y_1 but not x_1, then $d_G(S') < d_{\widetilde{G}}(S')$.

So, we have that $SW_k(G) < SW_k(\widetilde{G})$. ■

By repeating the operation in Lemma 3.1, we can see that the tree with the second largest Steiner k-Wiener index must be in $\mathcal{T}_3$.

Lemma 3.2. *Let p, q and k be three positive integers such that $p < q - 1$. If $2 \leq k \leq q$, then* $\binom{p}{k} + \binom{q}{k} > \binom{p+1}{k} + \binom{q-1}{k}$.
If $k \geq q + 1$, then $\binom{p}{k} + \binom{q}{k} = \binom{p+1}{k} + \binom{q-1}{k}$.

Proof. It follows that

$$\begin{aligned} &\left[\binom{p}{k} + \binom{q}{k}\right] - \left[\binom{p+1}{k} + \binom{q-1}{k}\right] \\ &= \left[\binom{q}{k} - \binom{q-1}{k}\right] - \left[\binom{p+1}{k} - \binom{p}{k}\right] \\ &= \binom{q-1}{k-1} - \binom{p}{k-1}. \end{aligned}$$

If $2 \leq k \leq q$ then $\binom{q-1}{k-1} - \binom{p}{k-1} > 0$.

If $k \geq q + 1$ then $\binom{q-1}{k-1} - \binom{p}{k-1} = 0$.

■

Let T be a tree of order n and $e = xy \in E(T)$. Denote by

$$N_x(e) = \{z \in V(T) : d(z, x) < d(z, y)\};$$

$$N_y(e) = \{z \in V(T) : d(z, x) > d(z, y)\}.$$

And denote the cardinality $|N_x(e)| = n_x(e)$, $|N_y(e)| = n_y(e)$, respectively. By the definitions, we have $n = n_x(e) + n_y(e)$. Denote by $\lambda_T(e) =$

$max\{n_x(e), n_y(e)\}$ and $\mu_T(e) = min\{n_x(e), n_y(e)\}$. There is a formula for the Steiner k-Wiener index of a tree.

Lemma 3.3. *([12]) Let T be a tree of order n, and k an integer with $2 \leq k \leq n-1$. Then*

$$SW_k(T) = (n-1)\binom{n}{k} - \sum_{e\in E(T)} \left[\binom{n_x(e)}{k} + \binom{n_y(e)}{k}\right].$$

Let $T = T_3(n_1, n_2, n_3) \in \mathcal{T}_3$, define three paths $P_{n_1} = x_1x_2\cdots x_{n_1}$, $P_{n_2} = y_1y_2\cdots y_{n_2}$ and $P_{n_3} = z_1z_2\cdots z_{n_3}$, pairwise disjoint paths, where $|V(P_i)| = n_i \geq 2$ $(i = 1, 2, 3)$, and $n_3 = max\{n_1, n_2, n_3\}$. If one of n_1 and n_2 is greater than 2, without loss of generality, suppose $n_1 > 2$ such that $\widehat{T} = T - x_1x_2 + z_1x_1$ from T.

Lemma 3.4. *Let T and $\widehat{T}$ be the two graphs (of order n) above, then $SW_k(T) < SW_k(\widehat{T})$ for $2 \leq k < n_1 + n_2$ and $SW_k(T) = SW_k(\widehat{T})$ for $n_1 + n_2 \leq k \leq n-1$.*

Proof. Let $e_i, f_j \in E(T)$ such that $e_i = x_ix_{i+1}$ and $f_j = z_jz_{j+1}$, $i = 1, 2, \cdots, n_1$, $j = 1, 2, \cdots, n_3$. For an arbitrary edge $e \in E(T)$, a feasible map from T to $\widehat{T}$ is a bijection $\varphi : E(T) \to E(\widehat{T})$ such that:

(1) $\lambda_T(e) = \lambda_{\widehat{T}}(\varphi(e))$, $e \in E(P_{n_2})$,

(2) $\lambda_T(e_i) = \lambda_{\widehat{T}}(\varphi(e_{i+1}))$, $e_i \in E(P_{n_1})(1 \leq i \leq n_1 - 2)$,

(3) $\lambda_T(f_j) = \lambda_{\widehat{T}}(\varphi(f_{j-1}))$, $f_j \in E(P_{n_3})(2 \leq j \leq n_3 - 1)$,

(4) $\lambda_T(f_1) = \lambda_{\widehat{T}}(\varphi(e_1))$.

By Lemma 3.3, we have that

$$\begin{aligned} & SW_k(\widehat{T}) - SW_k(T) \\ = & \left[(n-1)\binom{n}{k} - \sum_{e\in E(\widehat{T})} \left[\binom{\lambda_{\widehat{T}}(e)}{k} + \binom{\mu_{\widehat{T}}(e)}{k}\right]\right] \\ - & \left[(n-1)\binom{n}{k} - \sum_{e\in E(T)} \left[\binom{\lambda_T(e)}{k} + \binom{\mu_T(e)}{k}\right]\right] \end{aligned}$$

$$= \sum_{e\in E(T)} \left[\binom{\lambda_T(e)}{k} + \binom{\mu_T(e)}{k}\right] - \sum_{e\in E(\widehat{T})} \left[\binom{\lambda_{\widehat{T}}(e)}{k} + \binom{\mu_{\widehat{T}}(e)}{k}\right]$$

$$= \left[\binom{\lambda_T(e_{n_1-1})}{k} + \binom{\mu_T(e_{n_1-1})}{k}\right] - \left[\binom{\lambda_{\widehat{T}}(\varphi(f_{n_3-1}))}{k} + \binom{\mu_{\widehat{T}}(\varphi(f_{n_3-1}))}{k}\right]$$

$$= \left[\binom{n_1-1}{k} + \binom{n_2+n_3-1}{k}\right] - \left[\binom{n_3}{k} + \binom{n_1+n_2-2}{k}\right]. \qquad (3.1)$$

Since $n_1, n_2 \leq n_3$, then $n_1 - 1 < n_2 + n_3 - 2$. Let $n_3 = n_1 + \beta$, $\beta \geq 0$, by Lemma 3.2, we have that

$$\begin{aligned} \left[\binom{n_1-1}{k} + \binom{n_2+n_3-1}{k}\right] &\geq \left[\binom{n_1}{k} + \binom{n_2+n_3-2}{k}\right] \\ &\geq \cdots \\ &\geq \left[\binom{n_1+\beta}{k} + \binom{n_2+n_3-2-\beta}{k}\right] \\ &= \left[\binom{n_3}{k} + \binom{n_1+n_2-2}{k}\right]. \end{aligned}$$

Thus, we have

$$\begin{cases} SW_k(\widehat{T}) - SW_k(T) > 0 & if \quad 2 \leq k \leq n_1 + n_2 - 1; \\ SW_k(\widehat{T}) - SW_k(T) = 0 & if \quad k \geq n_1 + n_2. \end{cases}$$

■

By repeating the operation in Lemma 3.4, $SW_k(T_3(2,2,n-2))$ gets the maximum Steiner k-Wiener index for all trees in $\mathcal{T}_3$. So, $SW_k(T_3(2,2,n-2))$ is the second largest Steiner k-Wiener index among all trees. Then, we can have the following Theorem.

Theorem 3.5. *Let $T \neq P_n$ be a tree of order n, and k an integer with $2 \leq k \leq n-1$, then*

$$SW_k(T) \leq SW_k(T_3(2,2,n-2)) < SW_k(P_n),$$

where $SW_k(T_3(2,2,n-2)) = (k-1)\binom{n+1}{k+1} - \binom{n-2}{k-1} + \binom{1}{k-1}$.

Proof. Let $T = T_3(2,2,n-2)$, define three paths $P_2 = x_1x_2$, $P_2 = y_1y_2$ and $P_{n-2} = z_1z_2\cdots z_{n-2}$, pairwise disjoint paths. By the formula (3.1) in Lemma 3.4, we have that $P_n = \widehat{T} = T - x_1x_2 + z_1x_1$, and

$$\begin{aligned}
&SW_k(P_n) - SW_k(T) = SW_k(\widehat{T}) - SW_k(T)\\
&= \left[\binom{n_1-1}{k} + \binom{n_2+n_3-1}{k}\right] - \left[\binom{n_3}{k} + \binom{n_1+n_2-2}{k}\right]\\
&= \left[\binom{1}{k} + \binom{n-1}{k}\right] - \left[\binom{2}{k} + \binom{n-2}{k}\right]\\
&= \binom{n-2}{k-1} - \binom{1}{k-1}.
\end{aligned}$$

Then, $SW_k(T_3(2,2,n-2)) = SW_k(P_n) - \binom{n-2}{k-1} + \binom{1}{k-1}$.

■

If $G \in UC(n)\backslash\{C_n\}$, T_i $(i = 1,\cdots,t)$ is a spanning tree of G, then $SW_k(G) \leq min\{SW_k(T_1), SW_k(T_2),\cdots,SW_k(T_t)\} \leq SW_k(T_3(2,2,n-2))$. For any set $S \subseteq V(C_3(P_{n-2})) = V(T_3(2,2,n-2))$ with $|S| = k \geq 3$, it is easy to see that $d_{C_3(P_{n-2})}(S) = d_{T_3(2,2,n-2)}(S)$. Then $SW_k(C_3(P_{n-2})) = SW_k(T_3(2,2,n-2))$.

Now let's compare the Steiner k-Wiener indices of C_n to $C_3(P_{n-2})$.

Lemma 3.6. *Let k be an integer with $3 \leq k \leq n-2$, then*

$$SW_k(C_n) < SW_k(C_3(P_{n-2})).$$

Proof. Let $C_n = a_1a_2\cdots a_na_1$ and $V(C_3(P_{n-2})) = \{b_1, b_2,\cdots, b_n\}$, the vertex b_1 is the pendent vertex of $C_3(P_{n-2})$, and denote the path $P_{n-2} = b_1b_2\cdots b_{n-2}$. For $a_i \in V(C_n)$, a feasible map from C_n to $C_3(P_{n-2})$ is a bijection $\psi : V(C_n) \longrightarrow V(C_3(P_{n-2}))$ such that $\psi(a_i) = b_i$, $i = 1,2\cdots,n$. For any set $S \subseteq V(C_3(P_{n-2}))$ with $|S| = k$, it is easy to see that $d_{C_3(P_{n-2})}(S) \geq d_{C_n}(S)$. Moreover, since $k \leq n-2$, there must be

$S' \subseteq V(C_3(P_{n-2}))$ with $|S'| = k$ such that $d_{C_3(P_{n-2})}(S') > d_{C_n}(S')$. Then, we have that $SW_k(C_3(S_{n-2})) > SW_k(C_n)$. ■

From what has been discussed above, we obtain the upper bound of Steiner k-Wiener index of unicyclic graphs.

Theorem 3.7. *For $G \in UC(n)$ $(n \geq 6)$, let k be an integer with $3 \leq k \leq n-2$, then*

$$SW_k(G) \leq SW_k(C_3(P_{n-2})) = (k-1)\binom{n+1}{k+1} - \binom{n-2}{k-1}.$$

***Acknowledgment*:** This work is supported by the Natural Science Foundation of Xinjiang Province (No. 2021D01C069) and the National Natural Science Foundation of China (grant number 12161085).

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