

3 THE STEINER WIENER INDEX OF A GRAPH

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20 **Abstract**

21 The Wiener index $W(G)$ of a connected graph G , introduced by Wiener
22 in 1947, is defined as $W(G) = \sum_{u,v \in V(G)} d(u,v)$ where $d_G(u,v)$ is the dis-
23 tance between vertices u and v of G . The Steiner distance in a graph, intro-
24 duced by Chartrand et al. in 1989, is a natural generalization of the concept
25 of classical graph distance. For a connected graph G of order at least 2 and
26 $S \subseteq V(G)$, the *Steiner distance* $d(S)$ of the vertices of S is the minimum
27 size of a connected subgraph whose vertex set is S . We now introduce the
28 concept of the Steiner Wiener index of a graph. The *Steiner k -Wiener index*
29 $SW_k(G)$ of G is defined by $SW_k(G) = \sum_{\substack{S \subseteq V(G) \\ |S|=k}} d(S)$. Expressions for SW_k
30 for some special graphs are obtained. We also give sharp upper and lower

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31 bounds of SW_k of a connected graph, and establish some of its properties in
 32 the case of trees. An application in chemistry of the Steiner Wiener index
 33 is reported in our another paper.

34 **Keywords:** distance; Steiner distance; Wiener index; Steiner Wiener k -
 35 index..

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 37 05C05, 05C12, 05C35.

38 1. INTRODUCTION

39 All graphs in this paper are undirected, finite, and simple. We refer to [3]
 40 for graph theoretical notation and terminology not described here. Distance
 41 is one of the basic concepts of graph theory [4]. If G is a connected graph
 42 and $u, v \in V(G)$, then the *distance* $d(u, v) = d_G(u, v)$ between u and v is the
 43 length of a shortest path connecting u and v . If v is a vertex of a connected
 44 graph G , then the *eccentricity* $\varepsilon(v)$ of v is defined by $\varepsilon(v) = \max\{d(u, v) \mid u \in$
 45 $V(G)\}$. Furthermore, the *radius* $rad(G)$ and *diameter* $diam(G)$ of G are defined
 46 by $rad(G) = \min\{\varepsilon(v) \mid v \in V(G)\}$ and $diam(G) = \max\{\varepsilon(v) \mid v \in V(G)\}$. These
 47 latter two concepts are related by the inequalities $rad(G) \leq diam(G) \leq 2rad(G)$.
 48 Goddard and Oellermann gave a survey paper on this subject [13].

The Wiener index $W(G)$ of G is defined by

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

49 The first investigations of this distance-based graph invariant were done by
 50 Harold Wiener in 1947, who realized that there exist correlations between the
 51 boiling points of paraffins and their molecular structure, see [21, 22, 23]. Mathe-
 52 maticians study the Wiener index since the 1970s [11].

53 The Wiener index obtained wide attention and numerous results have been
 54 worked out, see the surveys [10, 15, 16, 24], the recent papers [2, 7, 17, 18, 19]
 55 and the references cited therein.

56 The Steiner distance of a graph, introduced by Chartrand et al. [6] in 1989,
 57 is a natural and nice generalization of the concept of the classical graph distance.
 58 For a graph $G(V, E)$ and a set $S \subseteq V(G)$ of at least two vertices, an *S -Steiner*
 59 *tree* or a *Steiner tree connecting S* (or simply, an *S -tree*) is a such subgraph
 60 $T(V', E')$ of G that is a tree with $S \subseteq V'$. Let G be a connected graph of order
 61 at least 2 and let S be a nonempty set of vertices of G . Then the *Steiner distance*
 62 $d(S)$ among the vertices of S (or simply the distance of S) is the minimum
 63 size of a connected subgraphs whose vertex set contains S . Note that if H is

64 a connected subgraph of G such that $S \subseteq V(H)$ and $|E(H)| = d(S)$, then H
 65 is a tree. Clearly, $d(S) = \min\{|E(T)| : S \subseteq V(T)\}$, where T is subtree of G .
 66 Furthermore, if $S = \{u, v\}$, then $d(S) = d(u, v)$ is nothing new, but the classical
 67 distance between u and v . Clearly, if $|S| = k$, then $d(S) \geq k - 1$. If G is the
 68 graph depicted in Figure 1 (a) and $S = \{x, u, v\}$, then $d(S) = 4$. There could be
 several trees of size 4 containing S . One such tree is shown in Figure 1 (b).

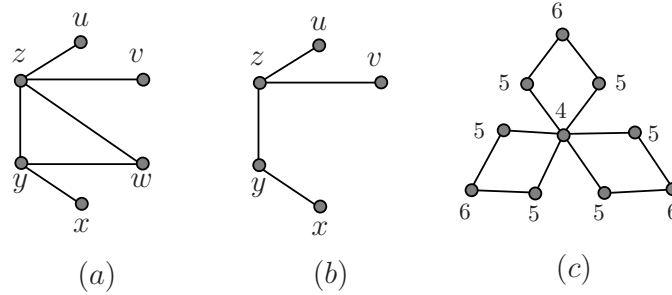


Figure 1: Graphs used to illustrate the basic definitions.

69 Let n and k be integers such that $2 \leq k \leq n$. The *Steiner k -eccentricity* $\varepsilon_k(v)$
 70 of a vertex v of G is defined by $\varepsilon_k(v) = \max\{d(S) \mid S \subseteq V(G), |S| = k, \text{ and } v \in$
 71 $S\}$. The *Steiner k -radius* of G is $srad_k(G) = \min\{\varepsilon_k(v) \mid v \in V(G)\}$, while the
 72 *Steiner k -diameter* of G is $sdiam_k(G) = \max\{\varepsilon_k(v) \mid v \in V(G)\}$. Note that for
 73 every connected graph G , $\varepsilon_2(v) = \varepsilon(v)$ for all vertices v of G , $srad_2(G) = rad(G)$
 74 and $sdiam_2(G) = diam(G)$. Each vertex of the graph G of Figure 1 (c) is labeled
 75 with its Steiner 3-eccentricity, so that $srad_3(G) = 4$ and $sdiam_3(G) = 6$. For
 76 more details on Steiner distance, we refer to [1, 5, 6, 8, 13, 20].
 77

78 The following observation is easily seen.

79 **Observation 1.1.** *Let k be an integer such that $2 \leq k \leq n$. If H is a spanning*
 80 *subgraph of G , then $sdiam_k(G) \leq sdiam_k(H)$.*

We now generalize the concept of Wiener index by Steiner distance. The *Steiner k -Wiener index* $SW_k(G)$ of G is defined by

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

81 For $k = 2$, the above defined Steiner Wiener index coincides with the ordinary
 82 Wiener index. It is usual to consider SW_k for $2 \leq k \leq n - 1$, but the above
 83 definition implies $SW_1(G) = 0$ and $SW_n(G) = n - 1$.

84 In Section 2, we obtain the exact values of the Steiner Wiener k -index of
 85 the path, star, complete graph, and complete bipartite graph. In Section 3,

86 we obtain sharp lower and upper bounds for SW_k for connected graphs and for
 87 trees. In Section 4 we establish some relations for SW_k of trees. An application
 88 in chemistry of the Steiner Wiener index is reported in our another paper [14].

89 2. RESULTS FOR SOME SPECIAL GRAPHS

90 Beginning this section, we note that the special case for $k = 2$ of all formulas
 91 derived here for the Steiner Wiener index, thus pertaining to the ordinary Wiener
 92 index, are well known and mentioned many times in the earlier literature.

Recently, we found the following concept about the Wiener distance. The
average Steiner distance $\mu_k(G)$ of a graph G is defined as the average of the
 Steiner distances of all k -subsets of $V(G)$, i.e.,

$$\mu_k(G) = \binom{n}{k}^{-1} \sum_{S \subseteq V(G), |S|=k} d_G(S),$$

93 which was introduced by Dankelmann, Oellermann and Swart in [8]. This concept
 94 is similar to our Steiner Wiener index. However, their motivation is to analyse
 95 transportation or communication networks, but ours is from chemical applications
 96 of the famous Wiener index. Therefore, fortunately most of their results are
 97 different from ours. For more details on the average Steiner distance, we refer to
 98 [8, 9].

For a connected graph G , one can easily see that

$$SW_k(G) = \mu_k(G) \binom{n}{k}, \quad (1)$$

99 Corollary 2.1 of [8] implies that $\mu_k(K_n) = (k-1)\mu_2(K_n)$. Then from Eq. (1)
 100 one can immediately get the following result.

101 **Proposition 2.1.** Let K_n be the complete graph of order n , and let k be an
 102 integer such that $2 \leq k \leq n$. Then $SW_k(K_n) = \binom{n}{k}(k-1)$.

103 For complete bipartite graphs, we have the following result.

Proposition 2.2. Let $K_{a,b}$ be the complete bipartite graph of order $a+b$ ($1 \leq a \leq b$), and let k be an integer such that $2 \leq k \leq a+b$. Then

$$SW_k(K_{a,b}) = \begin{cases} (k-1)\binom{a+b}{k} + \binom{a}{k} + \binom{b}{k}, & \text{if } 1 \leq k \leq a; \\ (k-1)\binom{a+b}{k} + \binom{b}{k}, & \text{if } a < k \leq b; \\ (k-1)\binom{a+b}{k}, & \text{if } b < k \leq a+b. \end{cases}$$

104 **Proof.** Let $G = K_{a,b}$, and let $U = \{u_1, u_2, \dots, u_a\}$ and $W = \{w_1, w_2, \dots, w_b\}$ be
105 the two parts of $G = K_{a,b}$.

106 First, we consider the case $1 \leq k \leq a$. For any $S \subseteq V(G)$ and $|S| = k$, we have
107 $S \cap U = \emptyset$, or $S \cap W = \emptyset$, or $S \cap U \neq \emptyset$ and $S \cap W \neq \emptyset$. If $S \cap U = \emptyset$, then $S \subseteq W$.
108 Without loss of generality, let $S = \{w_1, w_2, \dots, w_k\}$. Then the tree T induced by
109 the edges in $\{u_1w_1, u_1w_2, \dots, u_1w_k\}$ is a Steiner tree connecting S . This implies
110 $d(S) \leq k$. Since $G = K_{a,b}$ is a complete bipartite graph, it follows that any tree
111 connecting S must use at least k edges, and hence $d(S) \geq k$. Therefore, $d(S) = k$.
112 Similarly, if $S \cap W = \emptyset$, then $d(S) = k$. Suppose $S \cap U \neq \emptyset$ and $S \cap W \neq \emptyset$. With-
113 out loss of generality, let $S = \{u_1, u_2, \dots, u_x, w_1, w_2, \dots, w_{k-x}\}$. Then the tree T
114 induced by the edges in $\{u_1w_1, w_1u_2, w_1u_3, \dots, w_1u_x, u_1w_2, u_1w_3, \dots, u_1w_{k-x}\}$ is
115 a Steiner tree connecting S , which implies $d(S) \leq k - 1$. Since $|S| = k$, it follows
116 that any tree connecting S must use at least $k - 1$ edges, and hence $d(S) = k - 1$.
117 Thus,

$$\begin{aligned}
 SW_k(G) &= \sum_{\substack{S \subseteq V(G) \\ S \cap U = \emptyset}} d(S) + \sum_{\substack{S \subseteq V(G) \\ S \cap U = \emptyset}} d(S) + \sum_{\substack{S \subseteq V(G) \\ S \cap U \neq \emptyset, S \cap W \neq \emptyset}} d(S) \\
 &= k \binom{a}{k} + k \binom{b}{k} + (k-1) \left[\sum_{x=1}^a \binom{a}{x} \binom{b}{k-x} \right] \\
 &= k \binom{a}{k} + k \binom{b}{k} + (k-1) \left[\binom{a+b}{k} - \binom{b}{k} - \binom{a}{k} \right] \\
 &= (k-1) \binom{a+b}{k} + \binom{a}{k} + \binom{b}{k}.
 \end{aligned}$$

118 Next, we consider the case $a < k \leq b$. For any $S \subseteq V(G)$ and $|S| = k$,
119 we have $S \cap U = \emptyset$ or $S \cap U \neq \emptyset$. If $S \cap U = \emptyset$, then $S \subseteq W$. With-
120 out loss of generality, let $S = \{w_1, w_2, \dots, w_k\}$. Then the tree T induced by
121 the edges in $\{u_1w_1, u_1w_2, \dots, u_1w_k\}$ is a Steiner tree connecting S , which im-
122 plies $d(S) \leq k$. Since $G = K_{a,b}$ is a complete bipartite graph, it follows that
123 any tree connecting S must use at least k edges, and hence $d(S) \geq k$. There-
124 fore, $d(S) = k$. Suppose $S \cap U \neq \emptyset$. Without loss of generality, let $S =$
125 $\{u_1, u_2, \dots, u_x, w_1, w_2, \dots, w_{k-x}\}$ ($1 \leq x \leq a$). Then the tree T induced by the
126 edges in $\{u_1w_1, w_1u_2, w_1u_3, \dots, w_1u_x, u_1w_2, u_1w_3, \dots, u_1w_{k-x}\}$ is a Steiner tree
127 connecting S , which implies $d(S) \leq k - 1$. Since $|S| = k$, it follows that any tree

128 connecting S must use at least $k - 1$ edges, and hence $d(S) = k - 1$. Thus,

$$\begin{aligned}
SW_k(G) &= \sum_{\substack{S \subseteq V(G) \\ S \cap U = \emptyset}} d(S) + \sum_{\substack{S \subseteq V(G) \\ S \cap U \neq \emptyset}} d(S) \\
&= k \binom{b}{k} + (k-1) \left[\sum_{x=1}^a \binom{a}{x} \binom{b}{k-x} \right] \\
&= k \binom{b}{k} + (k-1) \left[\sum_{x=1}^{\infty} \binom{a}{x} \binom{b}{k-x} \right] \\
&= k \binom{b}{k} + (k-1) \left[\binom{a+b}{k} - \binom{b}{k} \right] \\
&= (k-1) \binom{a+b}{k} + \binom{b}{k}.
\end{aligned}$$

In this end, we consider the remaining case $b < k \leq a + b$. For any $S \subseteq V(G)$ and $|S| = k$, we have $S \cap U \neq \emptyset$ and $S \cap U \neq \emptyset$. Without loss of generality, let $S = \{u_1, u_2, \dots, u_x, w_1, w_2, \dots, w_{k-x}\}$. Then the tree T induced by the edges in $\{u_1 w_1, w_1 u_2, w_1 u_3, \dots, w_1 u_x, u_1 w_2, u_1 w_3, \dots, u_1 w_{k-x}\}$ is a Steiner tree connecting S , which implies $d(S) \leq k - 1$. Since $|S| = k$, it follows that any tree connecting S must use at least $k - 1$ edges, and hence $d(S) = k - 1$. Thus,

$$SW_k(G) = \sum_{\substack{S \subseteq V(G) \\ S \cap U = \emptyset}} d(S) = (k-1) \binom{a+b}{k}.$$

129 The proof is now complete. ■

130 From the above proposition, we can derive the following corollary.

Corollary 2.3. *Let S_n be the star of order n ($n \geq 3$), and let k be an integer such that $2 \leq k \leq n$. Then*

$$SW_k(S_n) = \binom{n-1}{k-1} (n-1).$$

Proof. From Proposition 2.2, we have that $SW_k(S_n) = SW_k(K_{1,n-1}) = \binom{n}{n} (n-1) = n-1$ for $k = n$ and $SW_k(S_n) = SW_k(K_{1,n-1}) = (k-1) \binom{n}{k} + \binom{n-1}{k}$ for $2 \leq k \leq n-1$. We conclude that

$$SW_k(S_n) = (k-1) \binom{n}{k} + \binom{n-1}{k} = \binom{n-1}{k-1} (n-1).$$

131 ■

132 Lemma 2.1 of [8] says that $\mu_k(P_n) = \frac{k-1}{k+1}(n+1)$. Then from Eq. (1) one can
 133 easily get the following result.

Proposition 2.4. Let P_n be the path of order n ($n \geq 3$), and let k be an integer such that $2 \leq k \leq n$. Then

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

134 3. LOWER AND UPPER BOUNDS FOR GENERAL GRAPHS

135 The following observation is immediate.

Observation 3.1. Let G be a connected graph of order n , $e \in E(G)$, and let k be an integer such that $2 \leq k \leq n$. Furthermore, let H be the graph with vertex set $V(H) = V(G)$ and edge set $E(G) \setminus e$. Then

$$SW_k(G) \leq SW_k(H).$$

136 This straightforwardly leads to the following result.

Proposition 3.2. Let G be a connected graph of order n , and T a spanning tree of G . Let k be an integer such that $2 \leq k \leq n$. Then

$$SW_k(G) \leq SW_k(T)$$

137 with equality if and only if G is a tree.

138 For a tree T , Proposition 3.1 of [8] says that $k(1 - \frac{1}{n}) \leq \mu_k(T) \leq \frac{k-1}{k+1}(n+1)$.
 139 Then from Eq. (1) one can derive lower and upper bounds for the Steiner Wiener
 140 index of a tree.

Theorem 3.3. Let T be a tree of order n , and let k be an integer such that $2 \leq k \leq n$. Then

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

141 Moreover, among all trees of order n , the star S_n minimizes the Steiner Wiener
 142 k -index whereas the path P_n maximizes the Steiner Wiener k -index.

143 We recall that Theorem 3.3 provides a generalization of the much older results
 144 known for the Wiener index [11], i.e., it yields this previous result by setting $k = 2$.

145 For a connected graph G , Theorem 2.1 of [8] says that $k-1 \leq SW_k(G) \leq$
 146 $\frac{k-1}{k+1}(n+1)$. Then from Eq. (1) one can get the following upper and lower bounds
 147 of $SW_k(G)$ for a general connected graph G .

Theorem 3.4. *Let G be a connected graph of order n , and let k be an integer such that $2 \leq k \leq n$. Then*

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

148 *Moreover, the lower bound is sharp.*

149

4. THE STEINER WIENER INDEX FOR TREES

Theorem 4.1. *Let T be a tree of order n , possessing p pendent vertices. Then*

$$SW_{n-1}(T) = n(n-1) - p, \tag{2}$$

150 *irrespective of any other structural detail of T .*

151 **Proof.** Since $k = n - 1$, the respective subsets S contain all except one vertices
152 of T . If the vertex missing from S is pendent, then the vertices contained in S
153 form a tree of order $n - 1$. Therefore $d(S) = n - 2$. There are p such subsets,
154 contributing to SW_{n-1} by $p \times (n - 2)$.

155 If the vertex of T , not present in S , is non-pendent, then the vertices con-
156 tained in S cannot form a tree, and the respective Steiner tree must contain all
157 the n vertices of T . Therefore, $d(S) = n - 1$. There are $n - p$ such subsets,
158 contributing to SW_{n-1} by $(n - p) \times (n - 1)$.

159 Thus, $SW_{n-1}(T) = p(n - 2) + (n - p)(n - 1)$, which straightforwardly leads
160 to Eq. (2). ■

161 Let G be any graph (not necessarily connected) with vertex set $V(G)$. Let e
162 be an edge of G , connecting the vertices x and y . Define the sets

$$\begin{aligned} \mathcal{N}_1(e) &= \{u \mid u \in V(G), d(u, x) < d(u, y)\} \\ \mathcal{N}_2(e) &= \{u \mid u \in V(G), d(u, x) > d(u, y)\} \end{aligned}$$

163 and let their cardinalities be $n_1(e) = |\mathcal{N}_1(e)|$ and $n_2(e) = |\mathcal{N}_2(e)|$, respectively.
164 In other words, $n_1(e)$ counts the vertices of G , lying closer to one end of the edge
165 e than to its other end, and the meaning of $n_2(e)$ is analogous.

166 In his seminal paper [23], Wiener discovered the following result:

Proposition 4.2. *If T is a tree, then for its Wiener index holds:*

$$W(T) = \sum_{e \in E(T)} n_1(e) n_2(e).$$

167 We now state the generalization of Proposition 4.2 to Steiner Wiener indices:

Theorem 4.3. *Let k be an integer such that $2 \leq k \leq n$. If T is a tree, then for its Steiner k -Wiener index holds:*

$$SW_k(T) = \sum_{e \in E(T)} \sum_{i=1}^{k-1} \binom{n_1(e)}{i} \binom{n_2(e)}{k-i}. \quad (3)$$

168 **Proof.** The Steiner k -Wiener index is equal to the sum of distances of all k -
 169 element subsets S of the vertex set of T . Each such subset determines a unique
 170 subtree of T and its contribution to SW_k is just the number edges of this subtree.
 171 Now, instead of counting these edges and adding them over all subsets S , we can
 172 count how many times a given edge, say e , is contained in the subtrees formed
 173 by all subsets S , and add this over all edges.

174 Let e be an edge of the tree T . On its two sides there are $n_1(e)$ and $n_2(e)$
 175 vertices, respectively. Choose i vertices on one side and $k - i$ vertices on the
 176 other side. Such a choice determines a k -element subset S , whose associated
 177 subtree contains the edge e . Evidently, the above described choice can be done
 178 in $\binom{n_1(e)}{i} \binom{n_2(e)}{k-i}$ different ways. If we sum these terms over all possible values of
 179 i , we obtain the total number of times the edge e is in a k -vertex Steiner tree of
 180 T . Eq. (3) thus follows. ■

181 **Corollary 4.4.** *Proposition 4.2 is obtained from Eq. (3) by setting $k = 2$.*

Corollary 4.5. *If $k = 3$, then the Steiner k -Wiener index of a tree of order n is directly related to the ordinary Wiener index as*

$$SW_3(T) = \frac{n-2}{2} W(T). \quad (4)$$

182 **Proof.** The special case of Eq. (3) for $k = 3$ reads:

$$\begin{aligned} SW_3(T) &= \sum_{e \in E(T)} \left[\binom{n_1(e)}{1} \binom{n_2(e)}{2} + \binom{n_1(e)}{2} \binom{n_2(e)}{1} \right] \\ &= \frac{1}{2} \sum_{e \in E(T)} n_1(e) n_2(e) [n_1(e) + n_2(e)] - \sum_{e \in E(T)} n_1(e) n_2(e). \end{aligned}$$

183 Eq. (4) follows now from Proposition 4.2 and the fact that for any edge of an
 184 n -vertex tree, $n_1(e) + n_2(e) = n$. ■

185 **Remark.** The Wiener index or the Steiner 2-Wiener index for any graph can be
 186 computed in polynomial time since one needs only to compute the distances of
 187 $\binom{n}{2}$ pairs of vertices in a graph of order n . However, since the problem of “Steiner

188 “Tree in Graphs” is NP-complete (see [12]), it is NP-hard to compute the Steiner
189 k -Wiener index $SW_k(G)$ for a general graph G and a general positive integer k .
190 Recall that the problem of “Steiner Tree in Graphs” is stated as follows: Given
191 a graph $G = (V, E)$, a weight $w(e)$ (a positive integer) for each $e \in E$, a subset
192 $R \subseteq V$ and a positive integer B , is there a subtree of G that includes all the
193 vertices of R and such that the sum of the weights of the edges in the subtree
194 is no more than B ? This problem remains NP-complete if all edge weights are
195 equal.

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