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THE FIRST TO $(k+1)$-TH SMALLEST WIENER (HYPER-WIENER) INDICES OF CONNECTED GRAPHS

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Abstract. Let n and k be two nonnegative integers with $n > 2k$, this paper presents the first to $(k+1)$-th smallest Wiener indices, and the first to $(k+1)$-th smallest hyper-Wiener indices among all connected graphs of order n, respectively.

1. INTRODUCTION

Throughout this paper, we only concern with connected, undirected simple graphs. Let $\mathcal{G}(n)$ denote the set of all connected graphs of order n. Let uv be an edge with end vertices u and v.

The *distance* $d_G(u,v)$ between the vertices u and v of the graph G is equal to the length of the shortest path that connects u and v. Let $\gamma(G,k)$ denote the number of vertex pairs of G, whose distance is equal to k. There are two important graph-based structure-descriptors, called Wiener index and hyper-Wiener index, based on distances in a graph. The *Wiener index* $W(G)$ [1] is denoted by

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v) = \sum_{k\geq 1} k\gamma(G,k),$$

and the *hyper-Wiener index* $WW(G)$ [2] is defined as

$$WW(G) = \frac{1}{2}W(G) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d_G(u,v)^2 = \frac{1}{2}\sum_{k\geq 1} k(k+1)\gamma(G,k).$$

The Wiener index was introduced long time ago [1]. Its chemical applications and mathematical properties were stated in [3-5]. However, the hyper-Wiener index is defined much later [2]. It rapidly gained popularity and numerous results on it were raised [6-10].

Up to now, lots of relations between $W(G)$ and $WW(G)$ have been discovered [11-13]. Suppose n and k are two nonnegative integers with $n > 2k$, this paper will present the first to $(k+1)$-th smallest Wiener indices, and the first to $(k+1)$-th smallest hyper-Wiener indices among all connected graphs of order n, respectively. It's surprising that the graphs which reach the i-th smallest Wiener indices even share the i-th smallest hyper-Wiener indices of $\mathcal{G}(n)$ for every $i \in \{1, 2, \ldots, k+1\}$.

2. THE FIRST TO $(k+1)$-TH SMALLEST WIENER INDICES OF $\mathcal{G}(n)$

A graph H is called a *subgraph* of G, written $H \subseteq G$, if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. If H is a connected subgraph of G with $V(H) = V(G)$ and $E(H) \neq E(G)$, then we called H a *connected spanning subgraph* of G. Suppose that V' is a nonempty subset of V. The subgraph of G whose vertex set is V' and whose edge set is the set of those edges of G that have both ends in V' is called the subgraph of G induced by V' and is denoted by $G[V']$, and we say that $G[V']$ is an *induced subgraph* of G.

Lemma 1. *If G' is a connected spanning subgraph of G, then $W(G') > W(G)$.*

Proof. Suppose $P_{u,v}$ is a shortest path in G' that connects u and v, since G' is a connected spanning subgraph of G, then $P_{u,v}$ is a path in G that connects u and v, thus $d_{G'}(u,v) \geq d_G(u,v)$. This implies that

$$W(G') = \sum_{\{u,v\} \subseteq V(G')} d_{G'}(u,v) \geq \sum_{\{u,v\} \subseteq V(G)} d_G(u,v) = W(G).$$

Moreover, since G' is a connected spanning subgraph of G, then $E(G') \subseteq E(G)$ but $E(G') \neq E(G)$. Assume $e = v_1v_2 \in E(G)$, but $e \notin E(G')$, then $d_{G'}(v_1,v_2) \geq 2 > 1 = d_G(v_1,v_2)$. Thus, $W(G') > W(G)$. □

The *join* of two vertex disjoint graphs G_1 and G_2 , denoted by $G_1 \vee G_2$, is the graph having vertex set $V(G_1 \vee G_2) = V(G_1 \cup G_2)$ and edge set $E(G_1 \vee G_2) = E(G_1) \cup E(G_2) \cup \{uv : u \in V(G_1), v \in V(G_2)\}$.

Lemma 2. *Let $G = G_1 \vee G_2$ with $|V(G)| = n$ and $|E(G)| = \binom{n}{2} - k$, where k is a nonnegative integer, then $W(G) = \binom{n}{2} + k$.*

Proof. Since $G = G_1 \vee G_2$, then $d_G(u,v) \leq 2$ holds for each vertex pair $\{u,v\} \subseteq V(G)$. Moreover, $d_G(u,v) = 1$ if and only if $uv \in E(G)$, and $d_G(u,v) = 2$ if and only if $uv \notin E(G)$. Thus, $\gamma(G,2) = k$. By the definition, we have

$$W(G) = \sum_{k \geq 1} k\gamma(G,k) = \gamma(G,1) + 2\gamma(G,2) = \binom{n}{2} - k + 2k = \binom{n}{2} + k.$$

This implies the result. □

Suppose k is a nonnegative integer, the notation $\mathcal{S}(K_n - ke)$ denotes the set of all connected graphs raised from K_n by deleting k edges. By the definition, it follows that $\mathcal{S}(K_n - 0e) = \{K_n\}$.

Lemma 3. *If $H \in \mathcal{S}(K_n - te)$ $(t \geq 1)$, then there exists $G \in \mathcal{S}(K_n - (t-1)e)$ such that H is a connected spanning subgraph of G.*

Proof. Suppose H is obtained from K_n by deleting the edges $e_1, \ldots, e_t$, then let G be the graph raised from K_n by deleting the edges $e_1, \ldots, e_{t-1}$. Since H is connected, then G is also connected. Thus, $G \in \mathcal{S}(K_n - (t-1)e)$. It is easy to see that H is a spanning connected subgraph of G. This completes the proof. □

Theorem 1. *Suppose n and k are nonnegative integers. If $n > 2k$, then the first to $(k+1)$-th smallest Wiener indices of $\mathcal{G}(n)$ is $\binom{n}{2}$, $\binom{n}{2}+1$, $\ldots$, $\binom{n}{2}+k$. Moreover, $W(G) = \binom{n}{2}+i$ if and only if $G \in \mathcal{S}(K_n - ie)$, where $0 \le i \le k$.*

Proof. Clearly, $W(K_n) = \binom{n}{2}$. If $1 \le i \le k$ and $G \in \mathcal{S}(K_n - ie)$, let $V_1 = \{v : v \in V(G) \text{ and } d(v) = n-1\}$, since $|E(G)| = \binom{n}{2} - i$ and $n > 2k \ge 2i$, then $V_1 \ne \emptyset$. Let $V_2 = V(G) \setminus V_1$, clearly $V_2 \ne \emptyset$. Set $G_1 = G[V_1]$ and $G_2 = G[V_2]$, then $G = G_1 \vee G_2$. By Lemma 2, we have $W(G) = \binom{n}{2} + i$.

Next we shall prove that if $H \in \mathcal{G}(n) \setminus \{K_n, \mathcal{S}(K_n - e), \ldots, \mathcal{S}(K_n - ke)\}$, then $W(H) > \binom{n}{2} + k$. Once this is proved, the conclusion holds. By Lemma 1, we only need to show that for each $H \in \mathcal{G}(n) \setminus \{K_n, \mathcal{S}(K_n - e), \ldots, \mathcal{S}(K_n - ke)\}$, there exists one graph $G \in \mathcal{S}(K_n - ke)$ such that H is a connected spanning subgraph of G. Now suppose $H \in \mathcal{S}(K_n - te)$, where $t > k$, by Lemma 3 there exists some graph $H_1 \in \mathcal{S}(K_n - (t-1)e)$ such that H is a connected spanning subgraph of H_1. Once again, by Lemma 3 there exists one graph $H_2 \in \mathcal{S}(K_n - (t-2)e)$ such that H_1 is a connected spanning subgraph of H_2. By the definition, H is also a connected spanning subgraph of H_2. Repeat the above process, we can conclude that there must exist one graph $G \in \mathcal{S}(K_n - ke)$ such that H is a connected spanning subgraph of G. By Lemma 1, $W(H) > W(G) = \binom{n}{2} + k$. This completes the proof. □

By Theorem 1, the next Corollary follows at once.

Corollary 1. *If $n > 18$, then the first to tenth smallest Wiener indices of $\mathcal{G}(n)$ is $\binom{n}{2}$, $\binom{n}{2}+1$, $\ldots$, $\binom{n}{2}+9$. Moreover, $W(G) = \binom{n}{2}+i$ if and only if $G \in \mathcal{S}(K_n - ie)$, where $0 \le i \le 9$.*

3. THE FIRST TO $(k+1)$-TH SMALLEST HYPER-WIENER INDICES OF $\mathcal{G}(n)$

Suppose k is a nonnegative integer. In this section, we shall list the first to $(k+1)$-th smallest hyper-Wiener indices of $\mathcal{G}(n)$ for any $n > 2k$.

Lemma 4. *If G' is a connected spanning subgraph of G, then $WW(G') > WW(G)$.*

Proof. Suppose $P_{u,v}$ is a shortest path in G' that connects u and v, since G' is a connected spanning subgraph of G, then $P_{u,v}$ is a path in G that connects u and v, thus $d_{G'}(u,v) \geq d_G(u,v)$ and $d_{G'}(u,v)^2 \geq d_G(u,v)^2$. By Lemma 1 it follows that

$$\sum_{\{u,v\}\subseteq V(G')} d_{G'}(u,v) > \sum_{\{u,v\}\subseteq V(G)} d_G(u,v),$$

and

$$\sum_{\{u,v\}\subseteq V(G')} d_{G'}(u,v)^2 \geq \sum_{\{u,v\}\subseteq V(G)} d_G(u,v)^2.$$

Thus,

$$\begin{aligned} WW(G') &= \frac{1}{2}\sum_{\{u,v\}\subseteq V(G')} d_{G'}(u,v) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G')} d_{G'}(u,v)^2 \\ &> \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d_G(u,v) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d_G(u,v)^2 \\ &= WW(G). \end{aligned}$$

This completes the proof of this lemma. □

Lemma 5. *Let $G = G_1 \vee G_2$ with $|V(G)| = n$ and $|E(G)| = \binom{n}{2} - k$, where k is a nonnegative integer, then $WW(G) = \binom{n}{2} + 2k$.*

Proof. Since $G = G_1 \vee G_2$, then $d_G(u,v) \leq 2$ holds for each vertex pair $\{u,v\} \subseteq V(G)$. Moreover, $d_G(u,v) = 1$ if and only if $uv \in E(G)$, and $d_G(u,v) = 2$ if and only if $uv \notin E(G)$, thus $\gamma(G,2) = k$. By the definition, we have

$$WW(G) = \frac{1}{2}\sum_{k\geq 1} k(k+1)\gamma(G,k) = \gamma(G,1) + 3\gamma(G,2) = \binom{n}{2} - k + 3k = \binom{n}{2} + 2k.$$

Thus, the lemma follows. □

Theorem 2. *Suppose n and k are nonnegative integers. If $n > 2k$, then the first to $(k+1)$-th smallest hyper-Wiener indices of $\mathcal{G}(n)$ is $\binom{n}{2}$, $\binom{n}{2} + 2$, …, $\binom{n}{2} + 2k$. Moreover, $WW(G) = \binom{n}{2} + 2i$ if and only if $G \in \mathcal{S}(K_n - ie)$, where $0 \leq i \leq k$.*

Proof. Clearly, $WW(K_n) = \binom{n}{2}$. If $1 \leq i \leq k$ and $G \in \mathcal{S}(K_n - ie)$, let $V_1 = \{v : v \in V(G) \text{ and } d(v) = n-1\}$, and $V_2 = V(G) \setminus V_1$. By the proof of Theorem

1, $V_1 \neq \emptyset$ and $V_2 \neq \emptyset$. Set $G_1 = G[V_1]$ and $G_2 = G[V_2]$, then $G = G_1 \vee G_2$. By Lemma 5, we have $WW(G) = \binom{n}{2} + 2i$.

Next we shall prove that if $H \in \mathcal{G}(n) \setminus \{K_n, \mathcal{S}(K_n - e), \ldots, \mathcal{S}(K_n - ke)\}$, then $WW(H) > \binom{n}{2} + 2k$. By the proof of Theorem 1, we can conclude that for each $H \in \mathcal{G}(n) \setminus \{K_n, \mathcal{S}\ (K_n - e), \ldots, \mathcal{S}(K_n - ke)\}$, there exists one graph $G \in \mathcal{S}(K_n - ke)$ such that H is a connected spanning subgraph of G. Thus, $WW(H) > WW(G) = \binom{n}{2} + 2k$ by Lemma 4. By combining the above discussion, the results follow. □

By Theorem 2, the next Corollary follows at once.

Corollary 2. *If $n > 18$, then the first to tenth smallest hyper-Wiener indices of $\mathcal{G}(n)$ is $\binom{n}{2}$, $\binom{n}{2} + 2$, $\ldots$, $\binom{n}{2} + 18$. Moreover, $W(G) = \binom{n}{2} + 2i$ if and only if $G \in \mathcal{S}(K_n - ie)$, where $0 \leq i \leq 9$.*

Remark. *Suppose n and k are two nonnegative integers with $n > 2k$. Theorem 1 and Theorem 2 imply that the graphs which reach the i-th smallest Wiener indices even share the i-th smallest hyper-Wiener indices of $\mathcal{G}(n)$ for each $i \in \{1, 2, \ldots, k+1\}$.*

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