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Nordhaus–Gaddum type results for the Harary index of graphs

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ABSTRACT

The Harary index $H(G)$ of a connected graph $G$is defined as $H(G) = \sum_{u,v\in V(G)} \frac{1}{d_G(u,v)}$, where $d_G(u,v)$ is the distance between vertices u and v of G. The Steiner distance in agraph, introduced by Chartrand et al. in 1989, is a natural generalization of the concept of classical graph distance. For a connected graph G of order at least 2 and $S \subseteq V(G)$, the Steiner distance $d_G(S)$ of the vertices of S is the minimum size of a connected subgraph whose vertex set contains S. Recently, Furtula, Gutman, and Katanić introduced the concept of Steiner Harary index and gave its chemical applications. The k-center Steiner Harary index $SH_k(G)$ of G is defined by $SH_k(G) = \sum_{S\subseteq V(G),|S|=k} \frac{1}{d_G(S)}$. In this paper, we get the sharp upper and lower bounds for $SH_k(G) + SH_k(\overline{G})$ and $SH_k(G) \cdot SH_k(\overline{G})$, valid for any connected graph G whose complement $\overline{G}$ is also connected.

1. INTRODUCTION

All graphs in this paper are assumed to be undirected, finite and simple and connected. We refer to [5] for graph theoretical notation and terminology not specified here. For a graph G, let $V(G)$, $E(G)$ and $e(G) = |E(G)|$denote the set of vertices, the set of edges and the sizeof G, respectively.

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If S is a vertex-subset of a graph G, the subgraph of G induced by S is denoted by $G[S]$. We denote by $E_G[X,Y]$ the set of edges of G with one end in X and the other in Y. If $X = \{x\}$, we simply write $E_G[x,Y]$ for $E_G[\{x\},Y]$.

The connectivity of a graph G, written $\kappa(G)$, is the order of a minimum vertex-subset $S \subseteq V(G)$ such that $G - S$ is disconnected or has only one vertex. Thus, if G is connected, then $\kappa(G) \geq 1$; if G has cut vertices, then $\kappa(G) = 1$.

The introduction is divided into the three subsections, in order to state the motivations and results of this paper.

1.1 DISTANCE AND ITS GENERALIZATION

Distance is one of the basic concepts of graph theory [6]. If G is a connected graph and $u, v \in V(G)$, then the distance $d(u,v)$ between u and v is the length of a shortest path connecting u and v.

The distance between two vertices u and v in a connected graph G also equals the minimum size of a connected subgraph of G containing both u and v. This observation suggests a generalization of the distance concept. The Steiner distance of a graph, introduced by Chartrand et al. in 1989 [8], is a natural generalization of the classical graph distance. For a graph $G(V,E)$ and a set $S \subseteq V(G)$ of at least two vertices, an S-Steiner tree or a Steiner tree connecting S (or simply, an S-tree) is a subgraph $T(V',E')$ of G that is a tree with $S \subseteq V'$. Then the Steiner distance $d_G(S)$ of the vertices of S (or simply the distance of S) is the minimum size of all connected subgraphs whose vertex sets contain S. Observe that $d_G(S) = \min\{e(T)|S \subseteq V(T)\}$, where T is subtree of G. Furthermore, if $S = \{u,v\}$, then $d_G(S)$ coincides with the classical distance between u and v.

Observation 1.1 Let G be a connected graph of order n and k be an integer, $2 \leq k \leq n$. If $S \subseteq V(G)$ and $|S| = k$, then $k-1 \leq d_G(S) \leq n-1$.

The average Steiner distance $\mu_k(G)$ of a graph G, introduced by Dankelmann et al. [9, 10], is defined as the average of the Steiner distances of all k-subsets of $V(G)$, i.e.,

$$\mu_k(G) = \binom{n}{k}^{-1} \sum_{\substack{S \subseteq V(G) \\ |S|=k}} d_G(S) . \tag{1.1}$$

Let n and k be integers such that $2 \leq k \leq n$. The Steiner k-eccentricity $e_k(v)$ of a vertex v of G is defined by $e_k(v) = max\{d(S)|S \subseteq V(G), |S| = k, v \in S\}$. The Steiner k-radius of G is $srad_k(G) = \min\{e_k(v)|v \in V(G)\}$, whereas the Steiner k-diameter of G is $sdiam_k(G) = max\{e_k(v)|v \in V(G)\}$. Note that for any vertex v of any connected graph

$G, e_2(v) = e(v)$, and in addition $srad_2(G) = rad(G)$ and $sdiam_2(G) = diam(G)$. For more details on Steiner distance, we refer to [3, 7, 8, 9, 10, 17, 25, 29].

Mao [25] obtained the following results. By $\Delta(G)$ we denote the greatest degree of a vertex of G.

Lemma 1.1 [25] Let G be a connected graph with connected complement $\overline{G}$. If $sdiam_k(G) \geq 2k$, then $sdiam_k(\overline{G}) \leq k$.

Lemma 1.2 [25] Let G be a connected graph of order n. Then $sdiam_3(G) = 2$ if and only if $0 \leq \Delta(\overline{G}) \leq 1$.

Lemma 1.3 [25] Let n, k be integers such that $2 \leq k \leq n$, and let G be a connected graph of order n. If $sdiam_k(G) = k - 1$, then $0 \leq \Delta(\overline{G}) \leq k - 2$.

Lemma 1.4 [25] Let G be a connected graph of order n with connected complement. Let k be an integer such that $3 \leq k \leq n$. Let $x = 0$ if $n \geq 2k - 2$ and $x = 1$ if $n < 2k - 2$. Then

(1) $2k - 1 - x \leq sdiam_k(G) + sdiam_k(\overline{G}) \leq max\{n + k - 1, 4k - 2\}$;

(2) $(k - 1)(k - x) \leq sdiam_k(G) \cdot sdiam_k(\overline{G}) \leq max\{k(n - 1), (2k - 1)^2\}$.

Lemma 1.5 [25] Let G be a graph. Then $sdiam_{n-1}(G) = n - 2$ if and only if G is 2-connected.

The following corollary is immediate from the above lemmas.

Corollary 1.1 [28] Let G and $\overline{G}$ be connected graphs. If $sdiam_3(G) \geq 6$, then $sdiam_3(\overline{G}) = 3$.

1.2 Wiener Index and its Generalization

The *Wiener index* is defined as the sum of ordinary distances of all pairs of vertices of the underlying graph, i.e., as $W(G) = \sum_{u,v \in V(G)} d(u, v)$ and its mathematical theory is nowadays well elaborated. For details see the surveys [13, 34].

Li et al. [22] generalized the concept of Wiener index using Steiner distance, by defining the Steiner k-Wiener index $SW_k(G)$ of the connected graph G as

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

However, with regard to this definition, one should bear in mind Eq. (1.1), and the references [9, 10].

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

An application in chemistry of the Steiner Wiener index was reported in [18]. Expressions for SW_k for some special graphs were reported in [22]. Li et al. [22] also gave sharp upper and lower bounds on SW_k, and established some of its properties in the case of trees. For more details on the Steiner Wiener index, we refer to [18, 22, 23, 27].

1.3 HARARY INDEX AND ITS GENERALIZATION

The *Harary index* $H(G)$ of $G$is defined by $H(G) = \sum_{u,v \in V(G)} \frac{1}{d_G(u,v)}$. For more details on the Harary index, we refer to [4, 21, 24, 33].

Furtula et al. [15] introduced the concept of Steiner Harary index. The *Steiner Harary k-index* or *k-center Steiner Harary index* $SH_k(G)$ of G is defined as

$$SH_k(G) = \sum_{\substack{S \subseteq V(G) \\ |S|=k}} \frac{1}{d_G(S)}.$$

For $k = 2$, the above defined Steiner Harary index coincides with the ordinary Harary index. It is usual to consider SH_k for $2 \leq k \leq n-1$, but the above definition implies $SH_1(G) = 0$ and $SH_n(G) = \frac{1}{n-1}$.

The following results will be needed later.

Lemma 1.6 [26] Let T be a tree of order n, and let k be an integer such that $2 \leq k \leq n$. Then

$$n \sum_{k-1 \leq t \leq n-1} \frac{1}{t}\binom{t-1}{k-2} - \binom{n-1}{k-1} \leq SH_k(T) \leq \frac{kn-n+k}{k^2(k-1)}\binom{n-1}{k-1}.$$

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

Lemma 1.7 [26] 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

$$SH_k(P_n) = n \sum_{k-1 \le t \le n-1} \frac{1}{t}\binom{t-1}{k-2} - \binom{n-1}{k-1}.$$

2. MAIN RESULTS

Let $f(G)$ be a graph invariant and na positive integer, $n \ge 2$. The *Nordhaus–Gaddum Problem* is to determine sharp bounds for $f(G) + f(\overline{G})$ and $f(G) \cdot f(\overline{G})$, as G ranges over the class of all graphs of order n, and to characterize the extremal graphs, i.e., graphs that achieve the bounds. Nordhaus–Gaddum type relations have received wide attention; see the recent survey [2] by Aouchiche and Hansen.

Denote by $\mathcal{G}(n)$ the class of connected graphs of order n whose complements are also connected. In the studies of Nordhaus–Gaddum–type relations it must be assumed that $f(G)$ and $f(\overline{G})$ exist. Therefore, such relations are examined in the case of Wiener and Steiner Wiener indices, one must restrict the consideration to the class $\mathcal{G}(n), n \ge 2$.

Mao et al. [28] studied the Nordhaus-Gaddum type results for the Wiener index. In this paper, we investigate the analogous problem for the Steiner Harary index. Our basic idea is from [28].

2.1 RESULTS PERTAINING TO GENERAL k

For general k, we obtain the following result:

Theorem 2.1 Let $G \in \mathcal{G}(n)$ and let k be an integer such that $3 \le k \le n$. Then:

(1) $\binom{n}{k}\frac{2k-2}{max\{k(n-1),(2k-1)^2\}} \le SH_k(G) + SH_k(\overline{G}) \le \frac{(n+k-2)\binom{n}{k}}{(k-1)^2}$.

(2) $\frac{1}{max\{k(n-1),(2k-1)^2\}}\binom{n}{k}^2 \le SH_k(G) \cdot SH_k(\overline{G}) \le \frac{1}{(k-1)^2}\binom{n}{k}^2$.

Moreover, the lower bounds are sharp.

Proof. Proof of part (1):

For any $S \subseteq V(G)$ and $|S| = k$, from the definition of Steiner diameter, we have $d_G(S) + d_{\overline{G}}(S) \le \max\{n + k - 2, 2k - 2\} = n + k - 2$. Then

$$SH_k(G) + SH_k(\overline{G}) = \sum_{S\subseteq V(G)} \frac{1}{d_G(S)} + \sum_{S\subseteq V(\overline{G})} \frac{1}{d_{\overline{G}}(S)} = \sum_{S\subseteq V(G)} \frac{d_G(S)+d_{\overline{G}}(S)}{d_G(S)d_{\overline{G}}(S)}$$
$$\leq \frac{(n+k-2)\binom{n}{k}}{(k-1)^2}.$$

By the same reason, Lemma 1.4 implies

$$SH_k(G) + SH_k(\overline{G}) = \sum_{S\subseteq V(G)} \frac{d_G(S)+d_{\overline{G}}(S)}{d_G(S)d_{\overline{G}}(S)} \geq \binom{n}{k} \frac{2k-2}{max\{k(n-1),(2k-1)^2\}}.$$

Proof of part (2):

For any $S' \subseteq V(G)$, $|S'| = k$ and any $S'' \subseteq V(\bar{G})$, $|S''| = k$, from the definition of Steiner diameter and Lemma 1.4, we have $d_G(S') \cdot d_{\bar{G}}(S'') \leq \max\{k(n-1),(2k-1)^2\}$. Then

$$SH_k(G) \cdot SH_k(\overline{G}) = \sum_{S'\subseteq V(G)} \frac{1}{d_G(S')} \cdot \sum_{S''\subseteq V(\overline{G})} \frac{1}{d_{\overline{G}}(S'')} = \sum_{S'\subseteq V(G),S''\subseteq V(\overline{G})} \frac{1}{d_G(S')} \cdot \frac{1}{d_{\overline{G}}(S'')}$$
$$\geq \frac{1}{\max\{k(n-1),\ (2k-1)^2\}} \binom{n}{k}^2.$$

For any $S' \subseteq V(G)$, $|S'| = k$ and any $S'' \subseteq V(\overline{G})$, $|S''| = k$, from the definition of Steiner diameter and Lemma 1.4, we have $d_G(S') \cdot d_{\overline{G}}(S'') \geq (k-1)^2$. Then

$$SH_k(G) \cdot SH_k(\overline{G}) = \sum_{S'\subseteq V(G)} \frac{1}{d_G(S')} \cdot \sum_{S''\subseteq V(\overline{G})} \frac{1}{d_{\overline{G}}(S'')} = \sum_{S'\subseteq V(G),S''\subseteq V(\overline{G})} \frac{1}{d_G(S')} \cdot \frac{1}{d_{\overline{G}}(S'')}$$
$$\leq \frac{1}{(k-1)^2} \binom{n}{k}^2,$$

as desired.

3. FOR SOME k

For $k = n, n-1, 3$, we can improve the results in Theorem 2.1.

3.1 THE CASE $k = n, n-1$

For $k = n$, the following result is immediate.

Observation 3.1 Let $G \in \mathcal{G}(n)$. Then

(1) $SH_n(G) + SH_n(\overline{G}) = \frac{2}{n-1}$;

(2) $SH_n(G) \cdot SH_n(\overline{G}) = \frac{1}{(n-1)^2}$.

Akiyama and Harary [1] characterized the graphs for which both G and $\overline{G}$ are connected.

Lemma 3.1 [1] Let G be graph with n vertices and maximal vertex degree $\Delta(G)$. Then $\kappa(G) = \kappa(\overline{G}) = 1$ if and only if G satisfies the following conditions.

i. $\kappa(G) = 1$ and $\Delta(G) = n-2$;

ii. $\kappa(G) = 1, \Delta(G) \leq n-3$, and G has a cut vertex $v$with pendent edge uv, such that $G-u$ contains a spanning complete bipartite subgraph.

For $k = n-1$, we have the following result:

Proposition 3.1 Let G be a graph of order n $(n \geq 5)$.

1. If G and $\overline{G}$ are both 2-connected, then $SH_{n-1}(G) + SH_{n-1}(\overline{G}) = \frac{2n}{n-2}$ and $SH_{n-1}(G) \cdot SH_{n-1}(\overline{G}) = \frac{n^2}{(n-2)^2}$.

2. If $\kappa(G) = 1$ and $\overline{G}$ is 2-connected, then $SH_{n-1}(G) + SH_{n-1}(\overline{G}) = \frac{p}{n-1} + \frac{2n-p}{n-2}$ and $SH_{n-1}(G) \cdot SH_{n-1}(\overline{G}) = \frac{pn}{(n-1)(n-2)} + \frac{n(n-p)}{(n-2)^2}$, where p is the number of cut vertices in G.

3. If $\kappa(G) = \kappa(\overline{G}) = 1$, $\Delta(G) \leq n-3$, and G has a cut vertex v with pendent edge uv such that $G-u$ contains a spanning complete bipartite subgraph, and $\Delta(\overline{G}) \leq n-3$ and $\overline{G}$ has a cut vertex q with pendent edge pq such that $G-p$ contains a spanning complete bipartite subgraph, then $SH_{n-1}(G) + SH_{n-1}(\overline{G}) = \frac{2n^2-2n-2}{(n-1)(n-2)}$ and $SH_{n-1}(G) \cdot SH_{n-1}(\overline{G}) = \frac{(n^2-n-1)^2}{(n-1)^2(n-2)^2}$.

4. If $\kappa(G) = \kappa(\overline{G}) = 1$, $\Delta(\overline{G}) = n-2$, $\Delta(G) \leq n-3$ and G has a cut vertex v with pendent edge uv such that $G-u$ contains a spanning complete bipartite subgraph, then $SH_{n-1}(G) + SH_{n-1}(\overline{G}) = \frac{2n^2-2n-2}{(n-1)(n-2)}$ or $SH_{n-1}(G) +$

$SH_{n-1}(\overline{G}) = \frac{2n^2-2n-3}{(n-1)(n-2)}$ and $SH_{n-1}(G) \cdot SH_{n-1}(\overline{G}) = \frac{(n^2-n-1)^2}{(n-1)^2(n-2)^2}$ or $SH_{n-1}(G) \cdot SH_{n-1}(\overline{G}) = \frac{(n^2-n-1)(n+1)}{(n-1)^2(n-2)}$.

5. If $\kappa(G) = \kappa(\overline{G}) = 1$, $\Delta(G) = \Delta(\overline{G}) = n-2$, then $\frac{2(n+1)}{n-1} \leq SH_{n-1}(G) + SH_{n-1}(\overline{G}) \leq \frac{2n^2-2n-2}{(n-1)(n-2)}$ and $\frac{(n+1)^2}{(n-1)^2} \leq SH_{n-1}(G) \cdot SH_{n-1}(\overline{G}) \leq \frac{(n^2-n-1)^2}{(n-1)^2(n-2)^2}$.

Proof. (1): From Lemma 1.5, if G and $\overline{G}$ are both connected, then $d_G(S) = n-2$ and $d_{\overline{G}}(S) = n-2$ for any $S \subseteq V(G)$ and $|S| = n-1$. Therefore, $SH_{n-1}(G) + SH_{n-1}\overline{G} = \frac{2n}{n-2}$ and $SH_{n-1}(G) \cdot SH_{n-1}(\overline{G}) = \frac{n^2}{(n-2)^2}$.

(2): Since $\overline{G}$ is 2-connected, it follows that $d_{\overline{G}}(S) = n-2$ for any $S \subseteq V(G)$ and $|S| = n-1$, and hence $SH_{n-1}(\overline{G}) = \frac{n}{n-2}$. Note that $\kappa(G) = 1$ and there are exactly p cut vertices in G. For any $S \subseteq V(G)$ and $|S| = n-1$, if the unique vertex in $V(G) \setminus S$ is a cut vertex, then $d_G(S) = n-1$. If the unique vertex in $V(G) \setminus S$ is not a cut vertex, then $d_G(S) = n-2$. Therefore, we have $SH_{n-1}(G) = \frac{p}{n-1} + \frac{n-p}{n-2}$, and hence $SH_{n-1}(G) + SH_{n-1}(\overline{G}) = \frac{p}{n-1} + \frac{2n-p}{n-2}$ and $SH_{n-1}(G) \cdot SH_{n-1}(\overline{G}) = \frac{pn}{(n-1)(n-2)} + \frac{n(n-p)}{(n-2)^2}$, where p is the number of cut vertices in G.

(3), (4), (5): We have $\kappa(G) = \kappa(\overline{G}) = 1$. By condition (i) of Lemma 3.1, since $\Delta(G) = n-2$, there is a vertex of degree $n-2$, say x. Let the set of first neighbors of x be $N_G(x) = \{y_1, y_2, \cdots, y_{n-2}\}$. Let $V(G) \setminus (\{x\} \cup N_G(x)) = \{z\}$. Since $zx \notin E(G)$, there must exist a vertex in $N_G(x)$, say y_1, such that $zy_1 \in E(G)$, since G is connected. Since x, y_1 may be the cut vertices in G, it follows that there are one or two cut vertices in G. So

$$SH_{n-1}(G) = \frac{1}{n-1} + \frac{n-1}{n-2} = \frac{n^2-n-1}{(n-1)(n-2)} \text{ or } SH_{n-1}(G) = \frac{2}{n-1} + \frac{n-2}{n-2} = \frac{n+1}{n-1}.$$

By condition (ii) of Lemma 3.1, since $\Delta(G) \leq n-3$ and G has a cut vertex v with pendent edge uv such that $G-u$ contains a spanning complete bipartite subgraph, it follows that v is the unique cut vertex. So $SH_{n-1}(G) = \frac{1}{n-1} + \frac{n-1}{n-2} = \frac{n^2-n-1}{(n-1)(n-2)}$. From this argument, (3), (4), (5) are true.

3.2 THE CASE $k = 3$

The following lemmas and corollaries will be used later.

Lemma 3.2 [28] Let T be a tree of order n, and let k be an integer such that $3 \leq k \leq n$. Then there exist at least $(n-k+1)$ subsets of $V(T)$ for which the Steiner k-distance is equal to $k-1$.

Corollary 3.1 [28] Let G be a connected graph of order n, and let k be an integer such that $3 \leq k \leq n$. Then there exist at least $(n-k+1)$ subsets of $V(G)$ whose Steiner k-distance is $k-1$.

Lemma 3.3 [28] Let T be a tree of order n, and let k be an integer such that $3 \leq k \leq n-1$. Then there exist at least $(n-k)$ subsets of $V(T)$ whose Steiner k-distance is k.

In this section, we focus our attention on the case $k=3$. For $k=3$ and $n \geq 10$, from Theorem 2.1, we have $\binom{n}{3}\frac{4}{3(n-1)} \leq SH_3(G) + SH_3(\overline{G}) \leq \frac{(n+1)\binom{n}{3}}{4}$ and $\frac{1}{3(n-1)}\binom{n}{3}^2 \leq SH_3(G) \cdot SH_3(\overline{G}) \leq \frac{1}{4}\binom{n}{3}^2$.

We improve these bounds and prove the following result.

Theorem 3.1 Let $G \in \mathcal{G}(n)$ with $n \geq 4$. Then

1. $\frac{5}{6}\binom{n}{3} \geq SH_3(G) + SH_3(\overline{G}) \geq$
$$\begin{cases} \frac{7}{10}\binom{n}{3} + \frac{11}{60}n - \frac{1}{2} & if\ n = 6,7\ and\ sdiam_3(G) = 5 \\ & or\ n = 6,7\ and\ sdiam_3(\bar{G}) = 5 \\ \frac{1}{2}\binom{n-3}{3} - \sum_{i=2}^{n-1}\frac{n}{i} + \frac{7n^2-23n+20}{6} & otherwise. \end{cases}$$
2. $\frac{25}{144}\left[\binom{n}{3}^2\right] \geq SH_3(G) \cdot SH_3(\overline{G}) \geq \left[\frac{1}{n-1}\binom{n}{3} + \frac{(n-3)(n-2)}{2(n-1)}\right]\left[\frac{1}{2}\binom{n}{3} - \frac{(n-3)(n-2)}{2(n-1)}\right]$.

Moreover, the bounds are sharp.

We first need the following lemma.

Lemma 3.4 [28] Let G be a connected graph. If $sdiam_3(G) = 5$, then $sdiam_3(\overline{G}) \leq 4$.

Lemma 3.5 Let $G \in \mathcal{G}(n)$. Then

$$SH_3(G) + SH_3(\overline{G}) \leq \frac{5}{6}\binom{n}{3} \tag{3.1}$$

$$SH_3(G) \cdot SH_3(\overline{G}) \leq \frac{25}{144}\binom{n}{3}^2 \tag{3.2}$$

and

$$SH_3(G)\cdot SH_3(\overline{G})\geq\left[\frac{1}{n-1}\binom{n}{3}+\frac{(n-3)(n-2)}{2(n-1)}\right]\left[\frac{1}{2}\binom{n}{3}-\frac{(n-3)(n-2)}{2(n-1)}\right]. \tag{3.3}$$

Moreover, the bounds are sharp.

Proof. (1) For any $S\subseteq V(G)$ and $|S|=3$, $G[S]\cong K_3$ or $G[S]\cong P_3$ or $G[S]\cong K_2\cup K_1$ or $G[S]\cong 3K_1$. If $G[S]\cong K_3$ or $G[S]\cong P_3$, then $d_G(S)=2$. If $G[S]\cong K_2\cup K_1$ or $G[S]\cong 3K_1$, then $d_G(S)\geq 3$. Let $S_1,S_2,\cdots,S_{\binom{n}{3}}$ be all the 3-subsets of $V(G)$. Without loss of generality, let $S_1,S_2,\cdots,S_x$ be all the 3-subsets of $V(G)$ such that $G[S_i]\cong K_3$ or $G[S_i]\cong P_3$, where $1\leq i\leq x$. Therefore, $d_G(S_i)=2$ and $d_{\overline{G}}(S_i)\geq 3$ for each $i\ (1\leq i\leq x)$. Furthermore, for any S_j $(x+1\leq j\leq\binom{n}{3})$, we have

$$SH_3(G)\leq\frac{x}{2}+\frac{[\binom{n}{3}-x]}{3}=\frac{1}{3}\binom{n}{3}+\frac{x}{6}$$

$$SH_3(\overline{G})\leq\frac{x}{3}+\frac{[\binom{n}{3}-x]}{2}=\frac{1}{2}\binom{n}{3}-\frac{x}{6}$$

$$SH_3(G)\geq\frac{x}{2}+\frac{[\binom{n}{3}-x]}{n-1}=\frac{1}{n-1}\binom{n}{3}+\frac{(n-3)x}{2(n-1)}.$$

and

$$SH_3(\overline{G})\geq\frac{x}{n-1}+\frac{[\binom{n}{3}-x]}{2}=\frac{1}{2}\binom{n}{3}-\frac{(n-3)x}{2(n-1)}.$$

implying inequality (3.1).

By Corollary 3.1, there exist at least $n-2$ subsets of $V(G)$ whose Steiner 3-distances are equal to 2. The same is true for $\overline{G}$. Therefore, $n-2\leq x\leq\binom{n}{3}-n+2$, and hence

$$\begin{aligned}SH_3(G)\cdot SH_3(\overline{G})&\leq\left[\frac{1}{3}\binom{n}{3}+\frac{x}{6}\right]\left[\frac{1}{2}\binom{n}{3}-\frac{x}{6}\right]\\&=\frac{1}{6}\binom{n}{3}^2+\frac{x}{36}\binom{n}{3}-\frac{x^2}{36}\\&\leq\frac{1}{36}\left[6\binom{n}{3}^2+\frac{1}{4}\binom{n}{3}^2\right]\\&=\frac{25}{144}\left[\binom{n}{3}^2\right]\end{aligned}$$

i.e., inequality (3.2) holds.

$$\begin{aligned}\mathrm{S}H_3(G)\cdot \mathrm{S}H_3(\overline{G}) &\geq \left[\frac{1}{n-1}\binom{n}{3}+\frac{(n-3)x}{2(n-1)}\right]\left[\frac{1}{2}\binom{n}{3}-\frac{(n-3)x}{2(n-1)}\right]\\ &= \frac{1}{2(n-1)}\binom{n}{3}^2+\frac{(n-3)^2x}{4(n-1)^2}\binom{n}{3}-\frac{(n-3)^2x^2}{4(n-1)^2}\\ &\geq \left[\frac{1}{n-1}\binom{n}{3}+\frac{(n-3)(n-2)}{2(n-1)}\right]\left[\frac{1}{2}\binom{n}{3}-\frac{(n-3)(n-2)}{2(n-1)}\right]\end{aligned}$$

i.e., inequality (3.3) holds.

The sharpness of the above bounds is illustrated by the following example.

Example 3.2 Let $G \cong P_4$. Then $\overline{G} \cong P_4$. By Lemma 1.7, $SH_3(G) = SH_3(\overline{G}) = \frac{5}{3}$, and hence $\mathrm{S}H_3(G) + \mathrm{S}H_3(\overline{G}) = \frac{10}{3} = \frac{5}{6}\binom{n}{3}$ and $\mathrm{S}H_3(G)\cdot \mathrm{S}H_3(\overline{G}) = \frac{25}{9} = \frac{25}{144}\left[\binom{n}{3}^2\right] = \left[\frac{1}{n-1}\binom{n}{3}+\frac{(n-3)(n-2)}{2(n-1)}\right]\left[\frac{1}{2}\binom{n}{3}-\frac{(n-3)(n-2)}{2(n-1)}\right]$, which confirms that the lower and upper bounds are sharp.

Let S^* be a tree obtained from a star of order $n-2$ and a path of length 2 by identifying the center of the star and a vertex of degree one in the path. Then $\overline{S^*}$ is a graph obtained from a clique of order $n-1$ by deleting an edge uv and then adding an pendent edge at v.

Observation 3.2

(1) $SH_3(S^*) = \frac{13}{12}\binom{n-3}{2} + \frac{1}{3}\binom{n-3}{3} + \frac{7}{6}n - 3$;

(2) $SH_3(\overline{S^*}) = \frac{4}{3}\binom{n-3}{2} + \frac{1}{2}\binom{n-3}{3} + \frac{4}{3}n - \frac{11}{3}$.

Proof. From the structure of $S^*$and $\overline{S^*}$, we conclude

$$\begin{aligned}\mathrm{S}H_3(S^*) &= \frac{1}{4}\binom{n-3}{2}+\frac{1}{2}\left[\binom{n-3}{2}+(n-3)+1\right]\\ &+\frac{1}{3}\left[\binom{n-3}{2}+\binom{n-3}{3}+2(n-3)\right]\\ &= \frac{13}{12}\binom{n-3}{2}+\frac{1}{3}\binom{n-3}{3}+\frac{7}{6}n-3\end{aligned}$$

and

$$\mathrm{S}H_3(\overline{S^*}) = \frac{1}{2}\left[2\binom{n-3}{2} + 2(n-3) + \binom{n-3}{3}\right] + \frac{1}{3}\left[\binom{n-3}{2} + (n-2)\right]$$
$$= \frac{4}{3}\binom{n-3}{2} + \frac{1}{2}\binom{n-3}{3} + \frac{4}{3}n - \frac{11}{3}.$$

In order to show the sharpness of the above bounds, we consider the following example.

Example 3.3 Let S^* be the same tree as before. From Observation 3.2, we have

$$\mathrm{S}H_3(S^*) + \mathrm{S}H_3(\overline{S^*}) = \frac{29}{12}\binom{n-3}{2} + \frac{5}{6}\binom{n-3}{3} + \frac{15}{6}n - \frac{20}{3}$$

and

$$\mathrm{S}H_3(S^*) \cdot \mathrm{S}H_3(\overline{S^*}) = \frac{52}{36}\binom{n-3}{2}^2 + \frac{1}{6}\binom{n-3}{3}^2 + \frac{71}{72}\binom{n-3}{2}\binom{n-3}{3}$$
$$+ \left(\frac{27}{9}n - \frac{287}{36}\right)\binom{n-3}{2} + \left(\frac{37}{36}n - \frac{49}{18}\right)\binom{n-3}{3}$$
$$+ \left(\frac{4}{3}n - \frac{11}{3}\right)\left(\frac{7}{6}n - 3\right).$$

The following lemmas are preparations for deducing an upper bound on $SH_3(G) + SH_3(\overline{G})$.

Lemma 3.6 Let G be a connected graph of order n, and let T be a spanning tree of G. If $sdiam_3(\overline{G}) = 3$, then

$$\mathrm{S}H_3(T) + SH_3(\overline{T}) \leq \mathrm{S}H_3(G) + SH_3(\overline{G}).$$

Proof. Note that $\overline{G}$ is a spanning subgraph of $\overline{T}$. It suffices to prove that

$$\mathrm{S}H_3(\overline{T}) - SH_3(\overline{G}) \leq \mathrm{S}H_3(G) - SH_3(T).$$

Since $\mathrm{sdiam}_3(\overline{G}) = 3$, it follows that $d_{\overline{G}}(S) = 2$ or $d_{\overline{G}}(S) = 3$ for any $S \subseteq V(G)$ and $|S| = 3$. Since $\overline{G}$ is a spanning subgraph of $\overline{T}$ and $sdiam_3(\overline{G}) = 3$, it follows that $sdiam_3(\overline{T}) \leq 3$, and hence $d_{\overline{T}}(S) = 2$ or $d_{\overline{T}}(S) = 3$ for any $S \subseteq V(T)$ and $|S| = 3$. Then $0 \leq \frac{1}{d_{\overline{T}}(S)} - \frac{1}{d_{\overline{G}}(S)} \leq \frac{1}{6}$. We claim that $\frac{1}{d_{\overline{T}}(S)} - \frac{1}{d_{\overline{G}}(S)} \leq \frac{1}{d_G(S)} - \frac{1}{d_T(S)}$ for $S \subseteq V(T)$ and

$|S| = 3$. Because $\overline{G}$ is a spanning subgraph of $\overline{T}$, $\frac{1}{d_{\overline{G}}(S)} \leq \frac{1}{d_{\overline{T}}(S)}$ for any $S \subseteq V(T)$ and $|S| = 3$. Similarly, since T is a spanning subgraph of G, $\frac{1}{d_T(S)} \leq \frac{1}{d_G(S)}$ for any $S \subseteq V(T)$ and $|S| = 3$. If $\frac{1}{d_{\overline{T}}(S)} - \frac{1}{d_{\overline{G}}(S)} = 0$, then $\frac{1}{d_{\overline{T}}(S)} - \frac{1}{d_{\overline{G}}(S)} = 0 \leq \frac{1}{d_G(S)} - \frac{1}{d_T(S)}$, as desired. If $\frac{1}{d_{\overline{T}}(S)} - \frac{1}{d_{\overline{G}}(S)} = \frac{1}{6}$, then $d_{\overline{G}}(S) = 3$ and $d_{\overline{T}}(S) = 2$, and hence $d_G(S) = 2$ and $d_T(S) \geq 3$. Therefore, $\frac{1}{d_G(S)} - \frac{1}{d_T(S)} \geq \frac{1}{6} = \frac{1}{d_{\overline{T}}(S)} - \frac{1}{d_{\overline{G}}(S)}$, as desired. The result follows from the arbitrariness of S and the definition of Steiner Wiener index.

Lemma 3.7 Let T be a tree of order n, different from the star S_n. Let S^* be the tree same as in Observation 3.2. If $sdiam_3(\overline{G}) = 3$, then

$$SH_3(P_n) + SH_3(\overline{S^*}) \leq SH_3(T) + SH_3(\overline{T}).$$

Proof. Note first that the complements of all trees, except of the star, are connected. Therefore, $SH_3(\overline{T})$ in Lemma 3.7 is always well defined.

By Lemma 1.6 and 1.7, $SH_3(P_n) \leq SH_3(T)$. It suffices to prove $SH_3(\overline{S^*}) \leq SH_3(\overline{T})$. Since $sdiam_3(\overline{G}) \leq 3$, it follows that $sdiam_3(\overline{T}) \leq 3$. For any $S \subseteq V(T)$ and $|S| = 3$, if $T[S]$ is not connected, then $d_{\overline{T}}(S) = 2$. If $T[S]$ is connected, then $d_{\overline{T}}(S) \geq 3$. So if we want to obtain the minimum value of $SH_3(\overline{T})$ for a tree T, then we need to find as less as possible 3-subsets of $V(T)$ whose induced subgraphs in $\overline{T}$ are disconnected. Since the complement of S_n is not connected, it follows that $\overline{S^*}$ is our desired. So $SH_3(\overline{S^*}) \leq SH_3(\overline{T})$, and hence $SH_3(P_n) + SH_3(\overline{S^*}) \leq SH_3(T) + SH_3(\overline{T})$.

We are now in the position to complete the proof of Theorem 3.1. This will be achieved by combining Lemmas 3.5 and 3.8.

Let $G \in \mathcal{G}(n)$. If $n = 6, 7$ and $sdiam_3(G) = 5$, then the validity of Theorem 3.1 can be verified by direct checking.

Lemma 3.8 Let $G \in \mathcal{G}(n)$. Let $n \geq 8$, or $n \leq 5$, or $n = 6, 7$ and $sdiam_3(G) \neq 5$, or $n = 6, 7$ and $sdiam_3(\overline{G}) \neq 5$. Then the lower bounds in parts (1) and (2) of Theorem 3.1 are obeyed. Moreover, these bounds are sharp.

Proof. We need to separately examine three cases.

Case 1. $sdiam_3(G) \geq 6$ or $sdiam_3(\overline{G}) \geq 6$. Without loss of generality, let $sdiam_3(G) \geq 6$. From Corollary 1.1 it is known that $sdiam_3(\overline{G}) = 3$, and hence $SH_3(G) + SH_3(\overline{G}) \geq SH_3(P_n) + SH_3(\overline{S^*})$. By Lemma 1.7, $SH_3(P_n) = \frac{(n+1)(n-2)}{2} - \sum_{i=2}^{n-1} \frac{n}{i}$. Note that $\overline{S^*}$ is a graph obtained from a clique of order $n-1$ by deleting an edge uv and then adding a pendent edge at v. Then $SH_3(\overline{S^*}) = \frac{4}{3}\binom{n-3}{2} + \frac{1}{2}\binom{n-3}{3} + \frac{4}{3}n - \frac{11}{3}$, and hence $SH_3(G) + SH_3(\overline{G}) \geq \frac{(n+1)(n-2)}{2} - \sum_{i=2}^{n-1} \frac{n}{i} + \frac{4}{3}\binom{n-3}{2} + \frac{1}{2}\binom{n-3}{3} + \frac{4}{3}n - \frac{11}{3} = \frac{1}{2}\binom{n-3}{3} - \sum_{i=2}^{n-1} \frac{n}{i} + \frac{7n^2-23n+20}{6}$.

Case 2. $sdiam_3(G) = 5$ or $sdiam_3(\overline{G}) = 5$. In view of Lemma 3.4, we can assume that $sdiam_3(G) = 5$ and $sdiam_3(\overline{G}) \leq 4$. Let $S_1, S_2, \ldots, S_{\binom{n}{3}}$ be all the 3-subsets of $V(G)$. Without loss of generality, assume that $S_1, S_2, \ldots, S_x$ are the 3-subsets of $V(G)$ for which $G[S_i] \cong K_3$ or $G[S_i] \cong P_3$, where $1 \leq i \leq x$.

For each i $(1 \leq i \leq x)$, $d_G(S_i) = 2$. For any S_j $(x+1 \leq j \leq \binom{n}{3})$, $G[S_j] \cong K_2 \cup K_1$ or $G[S_j] \cong 3K_1$. Since G is connected, it follows that there exists a spanning tree, say T. By Lemmas 3.2 and 3.3, there exist at least $(n-3)$ subsets of $V(T)$ whose Steiner 3-distance is 3, and there exist at least $(n-2)$ subsets of $V(T)$ whose Steiner 3-distance is 2. Therefore, there exist at least $(2n-5)$ subsets of $V(G)$ whose Steiner 3-distance is at most 3. Without loss of generality, let $d_G(S_j) = 3$ for S_j $(x+1 \leq j \leq 2n-5)$. Then $d_G(S_j) \leq 5$ and $d_{\overline{G}}(S_j) = 2$ for each j $(2n-4 \leq j \leq \binom{n}{3})$. For each i $(1 \leq i \leq x)$, $d_G(S_i) = 2$. By Lemma 3.3, there exist at least $(n-3)$ subsets of $V(\overline{G})$ whose Steiner 3-distance is 3. Then there exist at most $x-(n-3)$ subsets of $V(\overline{G})$ whose Steiner 3-distance is 4. If $x \leq 2n-5$, then $SH_3(G) \geq \frac{1}{2}x + \frac{1}{3}(2n-5-x) + \frac{1}{5}\left[\binom{n}{3} - 2n + 5\right]$ and $SW_3(\overline{G}) \geq \frac{1}{3}(n-3) + \frac{1}{4}(x-n+3) + \frac{1}{2}\left[\binom{n}{3} - x\right]$, and hence $SH_3(G) + SH_3(\overline{G}) \geq \frac{7}{10}\binom{n}{3} - \frac{1}{12}x + \frac{7}{20}n - \frac{11}{12} \geq \frac{7}{10}\binom{n}{3} + \frac{11}{60}n - \frac{1}{2}$. If $x \geq 2n-5$, then $SH_3(G) \geq \frac{1}{2}x + \frac{1}{5}\left[\binom{n}{3} - x\right]$ and $SH_3(\overline{G}) \geq \frac{1}{3}(n-3) + \frac{1}{4}(x-n+3) + \frac{1}{2}\left[\binom{n}{3} - x\right]$, and hence $SH_3(G) + SH_3(\overline{G}) \geq \frac{7}{10}\binom{n}{3} + \frac{1}{20}x + \frac{1}{12}n - \frac{1}{4} \geq \frac{7}{10}\binom{n}{3} + \frac{11}{60}n - \frac{1}{2}$.

Case 3. $sdiam_3(G) \leq 4$ and $sdiam_3(\overline{G}) \leq 4$. Let $S_1, S_2, \ldots, S_{\binom{n}{3}}$ be the 3-subsets of $V(G)$. Without loss of generality, let $S_1, S_2, \ldots, S_x$ be the 3-subsets of $V(G)$ for which $G[S_i] \cong K_3$ or

$G[S_i] \cong P_3$, where $1 \le i \le x$. For each i $(1 \le i \le x)$, $d_G(S_i) = 2$. For any S_j $(x+1 \le j \le \binom{n}{3})$, $G[S_j] \cong K_2 \cup K_1$ or $G[S_j] \cong 3K_1$.Since G is connected, there exists a spanning tree, say T. By Lemmas 3.2 and 3.3, there exist at least $(n-3)$ subsets of $V(T)$ whose Steiner 3-distance is equal to 3, and there exist at least $(n-2)$ subsets of $V(T)$ whose Steiner 3-distance is 2. Therefore, there exist at least $(2n-5)$ subsets of $V(G)$ whose Steiner 3-distance is at most 3. Without loss of generality, let $d_G(S_j) = 3$ for S_j $(x+1 \le j \le 2n-5)$. Then $d_G(S_j) \le 4$ and $d_{\overline{G}}(S_j) = 2$ for each j $\left(2n-4 \le j \le \binom{n}{3}\right)$. For each i $(1 \le i \le x)$, $d_G(S_i) = 2$. By Lemma 3.3, there exist at least $(n-3)$ subsets of $V(\overline{G})$ whose Steiner 3-distance in $\overline{G}$ is 3. Then there exist at most $x-(n-3)$ subsets of $V(\overline{G})$ whose Steiner 3-distance in $\overline{G}$ is 4. If $x \le 2n-5$, then $SH_3(G) \ge \frac{1}{2}x + \frac{1}{3}(2n-5-x) + \frac{1}{4}\left[\binom{n}{3} - 2n + 5\right]$ and $SH_3(\overline{G}) \ge \frac{1}{3}(n-3) + \frac{1}{4}(x-n+3) + \frac{1}{2}\left[\binom{n}{3} - x\right]$. Thus

$$SH_3(G) + SH_3(\overline{G}) \ge \frac{3}{4}\binom{n}{3} - \frac{1}{12}x + \frac{1}{4}n - \frac{2}{3} \ge \frac{3}{4}\binom{n}{3} + \frac{1}{12}n - \frac{3}{12}.$$

If $x \ge 2n-5$, then $SH_3(G) \ge \frac{1}{2}x + \frac{1}{4}\left[\binom{n}{3} - x\right]$ and $SH_3(\overline{G}) \ge \frac{1}{3}(n-3) + \frac{1}{4}(x-n+3) + \frac{1}{2}\left[\binom{n}{3} - x\right]$. Thus $SH_3(G) + SH_3(\overline{G}) \ge \frac{3}{4}\binom{n}{3} + \frac{1}{12}n - \frac{3}{12}$.

For $n \ge 6$, one can check that $\frac{1}{2}\binom{n-3}{3} - \sum_{i=2}^{n-1}\frac{n}{i} + \frac{7n^2-23n+20}{6} \le \frac{3}{4}\binom{n}{3} + \frac{1}{12}n - \frac{3}{12}$ and $\frac{7}{10}\binom{n}{3} + \frac{11}{60}n - \frac{1}{2} \le \frac{3}{4}\binom{n}{3} + \frac{1}{12}n - \frac{3}{12}$. So we only need to consider the lower bounds in Cases 1 and 2.

From the above argument, we conclude the following:

1. For $n \ge 8$, $\frac{1}{2}\binom{n-3}{3} - \sum_{i=2}^{n-1}\frac{n}{i} + \frac{7n^2-23n+20}{6} \le \frac{7}{10}\binom{n}{3} + \frac{11}{60}n - \frac{1}{2}$ and $SH_3(G) + SH_3(\overline{G}) \ge \frac{1}{2}\binom{n-3}{3} - \sum_{i=2}^{n-1}\frac{n}{i} + \frac{7n^2-23n+20}{6}$.
2. For $n \le 5$, the lower bound in Case 2 does not exist. Then $SH_3(G) + SH_3(\overline{G}) \ge \frac{1}{2}\binom{n-3}{3} - \sum_{i=2}^{n-1}\frac{n}{i} + \frac{7n^2-23n+20}{6}$.
3. If $n = 6, 7$, $\mathrm{sdiam}_3(G) \ne 5$, and $\mathrm{sdiam}_3(\overline{G}) \ne 5$, then $SH_3(G) + SH_3(\overline{G}) \ge \frac{1}{2}\binom{n-3}{3} - \sum_{i=2}^{n-1}\frac{n}{i} + \frac{7n^2-23n+20}{6}$.

4. If $n = 6,7$ and $\mathrm{sdiam}_3(G) = 5$, or $n = 6,7$ and $\mathrm{sdiam}_3(\overline{G}) = 5$, then

$$SH_3(G) + SH_3(\overline{G}) \geq \frac{7}{10}\binom{n}{3} + \frac{11}{60}n - \frac{1}{2}.$$

This completes the proof.

In order to demonstrate the sharpness of the above bounds, we point out the following example.

Example 3.4 Let $G \cong P_4$. Then $\overline{G} \cong P_4$. By Lemma 1.1, $SH_3(G) = SH_3(\overline{G}) = \frac{5}{3}$, and hence $SH_3(G) + SH_3(\overline{G}) = \frac{10}{3} = \frac{1}{2}\binom{n-3}{3} - \sum_{i=2}^{n-1}\frac{n}{i} + \frac{7n^2-23n+20}{6}$ and $SH_3(G) \cdot SH_3(\overline{G}) = \frac{25}{9} = \left[\frac{1}{n-1}\binom{n}{3} + \frac{(n-3)(n-2)}{2(n-1)}\right]\left[\frac{1}{2}\binom{n}{3} - \frac{(n-3)(n-2)}{2(n-1)}\right]$, which implies that the upper and lower bounds are sharp.

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