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Trees with Smaller Harmonic Indices

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Abstract. The harmonic index $H(G)$ of a graph G is defined as the sum of the weights $\frac{2}{d_u+d_v}$ of all edges uv of G, where d_u denotes the degree of a vertex u in G. In this paper, we determine (i) the trees of order n and m pendant vertices with the second smallest harmonic index, (ii) the trees of order n and diameter r with the smallest and the second smallest harmonic indices, and (iii) the trees of order n with the second, the third and the fourth smallest harmonic index, respectively.

1. Introduction

In this work, we consider the harmonic index. For a simple graph (or a molecular graph) $G = (V, E)$, the harmonic index $H(G)$ is defined in [7] as $H(G) = \sum_{uv\in E(G)} \frac{2}{d_u+d_v}$, where d_u denotes the degree of a vertex u in G.

For a graph G and $u \in V(G)$, we denote $N_G(u)$ the set of all neighbors of u in G and by $n(G)$ the number of vertices of G. We denote respectively by S_n and P_n the star and the path with n vertices. By $P_{n,m}$, we denote the graph obtained from S_{n+1} and P_m by identifying the center of S_{n+1} with a vertex of degree 1 of P_m. By $S_{n,m}$, we denote the graph obtained from S_{n+2} and S_{m+1} by identifying a vertex of degree 1 of S_{n+2} with the center of S_{m+1}. We denote by $D(G)$ the diameter of G, which is defined as $D(G) = max\{d(u, v) : u, v \in V(G)\}$ where $d(u, v)$ denotes the distance between the vertices u and v in G. We denote by $\mathcal{T}(n, r)$ the set of all trees T with n vertices and $D(T) = r$.

In [8], the authors considered the relation between the harmonic index and the eigenvalues of graphs. Zhong in [17] presented the minimum and maximum values of harmonic index on simple connected graphs and trees, and characterized the corresponding extremal graphs. Deng et al. in [2] considered the relation relating the harmonic index $H(G)$ and the chromatic number $\chi(G)$ and proved that $\chi(G) \le 2H(G)$ by using the effect of removal of a minimum degree vertex on the harmonic index. It strengthens a result relating the Randić index and the chromatic number conjectured by the system AutoGraphiX and proved by Hansen et al. in [9]. Deng et al. [15] gave a best possible lower bound for the harmonic index of a graph (a triangle-free graph, respectively) with minimum degree at least two and characterize the extremal graphs. Deng et al. [3] considered the harmonic index $H(G)$ and the radius $r(G)$ and strengthened some results relating the Randić index and the radius in [1] [13] [16]. Deng et al. [4] obtained the following result on the tree of order n with m pendant vertices and with the smallest harmonic index.

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Theorem 1.1. *[4] Let T be a tree of order $n \geq 3$, with m $(1 < m < n-1)$ pendant vertices. Then*

$$H(T) \geq \frac{2(m-1)}{m+1} + \frac{2}{m+2} + \frac{2(n-m-2)}{4} + \frac{2}{3}$$

with equality if and only if T is the comet $T_{n,m}$, where $T_{n,m} \cong P_{m-1,n-m+1}$.

Other related results see [5, 6, 11, 12, 14, 18, 19]. In [10], Li and Zhao determined the trees of order n with m pendant vertices and the second smallest Randić index, the trees of order n with diameter r and the first and the second smallest Randić indices, and the trees of order n with, respectively, the second, the third and the fourth smallest Randić index. Here, we determine all trees of order n with m pendant vertices and the second smallest harmonic index, all trees of order n with diameter r and the first and the second smallest harmonic indices, and the trees of order n with, respectively, the second, the third and the fourth smallest harmonic index.

2. Main Results

In this section, we first give some basic lemmas, and then determine (i) the trees of order n with m pendant vertices and the second smallest harmonic index, (ii) the trees of order n with diameter r and the the smallest and the second smallest harmonic indices, and (iii) the trees of order n with, respectively, the second, the third and the fourth smallest harmonic index.

Lemma 2.1. *Let T be a tree with a vertex u such that $d_T(u) = k$. Suppose that $N_T(u) = \{1, 2, 3, \cdots, k\}$ and $v \notin V(T)$. Then*

$$H(T+uv) - H(T) = \frac{2}{k+2} - 2\sum_{i \in N_T(u)} \frac{1}{[k+1+d_T(i)][k+d_T(i)]}$$

Proof. Suppose that $Q = \{ui : i \in N_T(u)\}$ and $\Omega = \sum_{xy \in E(T)-Q} \frac{2}{d_T(x)+d_T(y)}$. Then we have

$$H(T) = \sum_{xy \in E(T)} \frac{2}{d_T(x)+d_T(y)} = \Omega + \sum_{i \in N_T(u)} \frac{2}{k+d_T(i)}$$

and

$$\begin{aligned} H(T+uv) &= \sum_{xy \in E(T+uv)} \frac{2}{d_{T+uv}(x)+d_{T+uv}(y)} \\ &= \Omega + \sum_{i \in N_T(u)} \frac{2}{k+1+d_T(i)} + \frac{2}{k+2} \end{aligned}$$

$$\begin{aligned} H(T+uv) - H(T) &= \frac{2}{k+2} + \sum_{i \in N_T(u)} \left[\frac{2}{k+1+d_T(i)} - \frac{2}{k+d_T(i)}\right] \\ &= \frac{2}{k+2} - 2\sum_{i \in N_T(u)} \frac{1}{[k+1+d_T(i)][k+d_T(i)]} \end{aligned}$$

□

Let u be a vertex of T with $d_T(u) = k$. One can see that there is a vertex $w \in N_T(u)$ such that $d_T(w) \geq 2$ except if u is the center of a star. So, we have

$$-2\sum_{i \in N_T(u)} \frac{1}{[k+1+d_T(i)][k+d_T(i)]} \geq \frac{-2(k-1)}{(k+1)(k+2)} - \frac{2}{(k+2)(k+3)} \tag{1}$$

Denote Q_{n_1,n_2} and P_{n_1,n_2,n_3} be the two graphs shown in Figure 1 and Figure 2, where G is a connected graph. Specially, $P_{m-1,n-m+1} = P_{m-1,n-m+1,0} = P_{m-1,n-m,1}$.

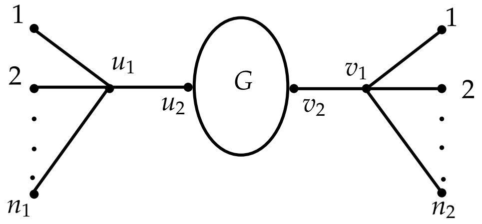

Figure 1: Graph Q_{n_1,n_2}

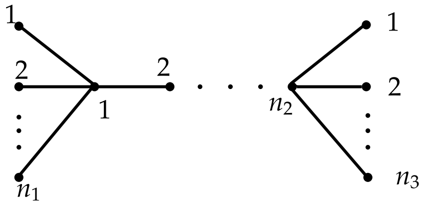

Figure 2: Graph P_{n_1,n_2,n_3}

Lemma 2.2. *Let $n_1 \geq n_3 + 2$. Then $H(P_{n_1,n_2,n_3}) < H(P_{n_1-1,n_2,n_3+1})$.*

Proof. If $n_2 \geq 3$, then

$$\begin{aligned}
&H(P_{n_1-1,n_2,n_3+1}) - H(P_{n_1,n_2,n_3})\\
&= \frac{2(n_1-1)}{n_1+1} + \frac{2}{n_1+2} + \frac{2}{n_3+4} + \frac{2(n_3+1)}{n_3+3} - \frac{2n_1}{n_1+2} - \frac{2}{n_1+3} - \frac{2}{n_3+3} - \frac{2n_3}{n_3+2}\\
&= \frac{2(n_1-n_3-1)(84+42n_1+6n_1^2+40n_3+13n_1n_3+n_1^2n_3+5n_3^2+n_1n_3^2)}{(n_1+1)(n_1+2)(n_1+3)(n_3+2)(n_3+3)(n_3+4)}
\end{aligned}$$

If $n_2 = 2$, then

$$\begin{aligned}
&H(P_{n_1-1,n_2,n_3+1}) - H(P_{n_1,n_2,n_3})\\
&= \frac{2(n_1-1)}{n_1+1} + \frac{2}{n_1+n_3+2} + \frac{2(n_3+1)}{n_3+3} - \frac{2n_1}{n_1+2} - \frac{2}{n_1+n_3+2} - \frac{2n_3}{n_3+2}\\
&= \frac{4(n_1-n_3-1)(n_1+n_3+4)}{(n_1+1)(n_1+2)(n_3+2)(n_3+3)}
\end{aligned}$$

Since $n_1 \geq n_3 + 2$, $H(P_{n_1,n_2,n_3}) < H(P_{n_1-1,n_2,n_3+1})$.

Lemma 2.3. *Let $n_1 \geq n_2 \geq 2$ and G be a tree. If Q_{n_1,n_2} has n vertices and m pendant vertices, then $H(Q_{n_1,n_2}) \geq H(P_{m-2,n-m,2})$*

Proof. By induction on m. Clearly, $m \geq n_1 + n_2 \geq 4$. When $m = 4$, $Q_{n_1,n_2} \cong P_{2,n-4,2}$. So, the lemma is true for $m = 4$ and all $n \geq m + 2$. Suppose that $m \geq 5$ and the lemma holds for every Q_{s_1,s_2} of order n with $m - 1$ pendant vertices, where $s_1 \geq s_2 \geq 2$. Now, let Q_{n_1,n_2} have n vertices and m pendant vertices, where $n_1 \geq n_2 \geq 2$. We distinguish the following cases:

Case 1. $n_2 = 2$. Let $T' = Q_{n_1,1}$. By Lemma 2.1, we have

$$H(Q_{n_1,n_2}) = H\left(T'\right) + \frac{1}{2} - \frac{2}{(2+1+1)(2+1)} - \frac{2}{(2+1+d_{T'}(v_2))(2+d_{T'}(v_2))}$$
$$H(Q_{n_1,n_2}) = H\left(T'\right) + \frac{1}{2} - \frac{1}{6} - \frac{2}{(3+d_{T'}(v_2))(2+d_{T'}(v_2))}$$

and

$$H(P_{m-2,n-m,2}) = H(P_{m-2,n-m+1}) + \frac{1}{2} - \frac{1}{6} - \frac{1}{10}$$

Note that T' has $n-1$ vertices and $m-1$ pendant vertices. From Theorem 1.1, we have that $H\left(T'\right) \geq H(P_{m-2,n-m+1})$ and the equality holds if and only if $T' \cong P_{m-2,n-m+1}$. So, we have that $H(Q_{n_1,n_2}) \geq H(P_{m-2,n-m,2})$ and the equality holds if and only if $Q_{n_1,n_2} \cong P_{m-2,n-m,2}$.

Case 2. $n_2 \geq 3$.

Let $T' = Q_{n_1,n_2-1}$. By Lemma 2.1, we have

$$H(Q_{n_1,n_2}) = H\left(T'\right) + \frac{2}{n_2+2} - \frac{2(n_2-1)}{(n_2+1)(n_2+2)} - \frac{2}{(n_2+1+d_{T'}(v_2))(n_2+d_{T'}(v_2))} \tag{2}$$

$$H(P_{m-2,n-m,2}) = H(P_{m-3,n-m,2}) + \frac{2}{m} - \frac{2(m-3)}{m(m-1)} - \frac{2}{m(m+1)} \tag{3}$$

Since $T' = Q_{n_1,n_2-1}$ and T' has $m-1$ pendant vertices, by the induction hypothesis, $H(P_{m-3,n-m,2}) \leq H\left(T'\right)$. Note that $n_1 \leq m - n_2 \leq m-3$ and Q_{n_1,n_2} is not a star. Thus, we have $H(Q_{n_1,n_2}) > H(P_{m-2,n-m,2})$ from (2) and (3). □

Let $v_1v_2v_3\cdots v_k$ be a path P_k and $T_{k,v_i,m}$ be a graph shown in Figure 3, where $k \geq 5$ and $m \geq 1$.

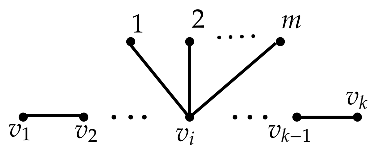

Figure 3: Graph $T_{k,v_i,m}$

Lemma 2.4. *If $r \geq 4$ and $n \geq r+3$, then $H(P_{n-r-1,r-1,2}) \geq H(T_{r+1,v_3,n-r-1})$.*

Proof. By the definition of harmonic index, we have

$$H(P_{n-r-1,r-1,2}) = \frac{2(n-r-1)}{n-r+1} + \frac{r-4}{2} + \frac{2}{n-r+2} + \frac{7}{5}$$

and

$$H(T_{r+1,v_3,n-r-1}) = \frac{2(n-r-1)}{n-r+2} + \frac{4}{n-r+3} + \frac{r-4}{2} + \frac{4}{3}.$$

Let $x = n - r$. Obviously, x is an integer and $x \geq 3$. So, we get that

$$H(P_{n-r-1,r-1,2}) - H(T_{r+1,v_3,n-r-1}) = \phi(x), \tag{4}$$

where

$$\phi(x) = \left(\frac{2(x-1)}{x+1} + \frac{r-4}{2} + \frac{2}{x+2} + \frac{7}{5}\right) - \left(\frac{2(x-1)}{x+2} + \frac{4}{x+3} + \frac{r-4}{2} + \frac{4}{3}\right)$$
$$= \frac{(x-3)(x^2+9x+38)}{15(x+1)(x+2)(x+3)}$$

And $\phi(x) = 0$ for $x = 3$ and $\phi(x) > 0$ for $x \geq 4$. So, $H(P_{n-r-1,r-1,2}) \geq H(T_{r+1,v_3,n-r-1})$. □

Let $\mathcal{T}(n,r)$ be the set of trees with n vertices and diameter r.

Lemma 2.5. *If* $T \in \mathcal{T}(n,4) - \{P_{n-4,4}\}$, *then* $H(T) \geq \frac{2(n-5)}{n-2} + \frac{4}{n-1} + \frac{4}{3}$ *and the equality holds if and only if* $T \cong T_{5,v_3,n-5}$.

Proof. By induction on n. When $n = 6$, $T \cong T(5, v_3, n-5)$. So, the lemma is true for $n = 6$.

Suppose that the lemma is true for $n-1$, where $n \geq 7$. Clearly, T has at most $n-3$ pendant vertices if $T \in \mathcal{T}(n,4) - \{P_{n-4,4}\}$. We have the following cases:

Case 1. There is a path $u_1u_2u_3u_4u_5$ in T such that $d(u_2) \geq 3$ and $d(u_4) \geq 3$. By Lemma 2.3 and Lemma 2.4, $H(T) \geq H(P_{n-5,3,2}) \geq H(T_{5,v_3,n-5})$.

Case 2. For each path $u_1u_2u_3u_4u_5$ in T, we must have $d(u_2) = 2$ or $d(u_4) = 2$. Recalling that the diameter $D(T) = 4$, one can see that T must be the graph $U_k(n_1,t)$ shown in Figure 4, where $k \geq 0$, $n_1 \geq 1$, $t \geq 2$ and $n_1 + 2t + k = n$.

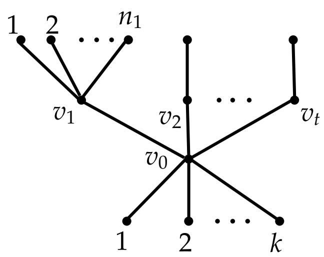

Figure 4: Graph $U_k(n_1,t)$

By Lemma 2.1, we have that

$$\begin{aligned} H(T_{5,v_3,n-5}) &= H(T_{5,v_3,n-6}) + \frac{2}{n-2} - \frac{2(n-6)}{(n-2)(n-3)} - \frac{4}{(n-1)(n-2)} \\ &= H(T_{5,v_3,n-6}) + \frac{2}{n-2}[1 - \frac{n-6}{n-3} - \frac{2}{n-1}] \\ &= H(T_{5,v_3,n-6}) + \frac{2(n+3)}{(n-1)(n-2)(n-3)} \end{aligned} \quad (5)$$

Subcase 2.1. $k \geq 1$ in $U_k(n_1,t)$.

By Lemma 2.1, we have

$$
\begin{aligned}
H(U_k(n_1,t)) &= \frac{2}{k+t+1} - \frac{2(k-1)}{(k+t)(k+t+1)} + \frac{2}{n_1+1+t+k} \\
&\quad - \frac{2}{n_1+t+k} - \frac{2(t-1)}{(k+t+1)(k+t+2)} \\
&\geq H(U_{k-1}(n_1,t)) + \frac{2}{k+t+1} - \frac{2(k-1)}{(k+t)(k+t+1)} \\
&\quad - \frac{2t}{(k+t+1)(k+t+2)} \\
&= H(U_{k-1}(n_1,t)) + \frac{2}{k+t+1}[1 - \frac{k-1}{k+t} - \frac{t}{k+t+2}] \\
&= H(U_{k-1}(n_1,t)) + \frac{2(k+3t+2)}{(k+t)(k+t+1)(k+t+2)}
\end{aligned}
$$

Since $k \geq 0$, $n_1 \geq 1$, $t \geq 2$ and $n_1 + 2t + k = n$, we have $k + 3t + 2 \geq k + t + 6$ and

$$\frac{2(k+3t+2)}{(k+t)(k+t+1)(k+t+2)} \geq \frac{2(k+t+6)}{(k+t)(k+t+1)(k+t+2)} = \frac{2(x+6)}{x(x+1)(x+2)}$$

where $x = k + t$ and $2 \leq x = n - t - n_1 \leq n - 3$. Note that $f(x) = \frac{2(x+6)}{x(x+1)(x+2)}$ is a decreasing function for $2 \leq x \leq n-3$, $f(x) \geq f(n-3) = \frac{2(n+3)}{(n-1)(n-2)(n-3)}$. So,

$$H(U_k(n_1,t)) \geq H(U_{k-1}(n_1,t)) + \frac{2(n+3)}{(n-1)(n-2)(n-3)} \tag{6}$$

the equality holds if and only if $n_1 = 1$ and $t = 2$. By the induction hypothesis, $H(U_{k-1}(n_1,t)) \geq H(T_{5,v_3,n-6})$ with the equality if and only if $U_{k-1}(n_1,t) \cong T_{5,v_3,n-6}$. From (5) and (6), we have $H(U_k(n_1,t)) \geq H(T_{5,v_3,n-5})$ and the equality if and only if $U_k(n_1,t) \cong T_{5,v_3,n-5}$.

Subcase 2.2. $k = 0$ and $t \geq 3$ in $U_k(n_1,t)$.

By Lemma 2.1, we have that

$$H(U_0(n_1,t)) = H(U_1(n_1,t-1)) + \frac{2}{3} - \frac{2}{(t+1)(t+2)}$$

and

$$
\begin{aligned}
&H(U_1(n_1+1,t-1)) = H(U_1(n_1,t-1)) + \frac{2}{n_1+3} \\
&- \frac{2n_1}{(n_1+2)(n_1+3)} - \frac{2}{(n_1+t+1)(n_1+t+2)}
\end{aligned}
$$

Clearly, $n_1 + 3 > 3$. So $H(U_0(n_1,t)) > H(U_1(n_1+1,t-1))$. From the subcase 2.1, we have $H(U_0(n_1,t)) > H(U_1(n_1+1,t-1)) \geq H(T_{5,v_3,n-5})$.

Subcase 2.3. $k = 0$ and $t = 2$ in $U_k(n_1,t)$. Then $U_0(n_1,2) \cong P_{n-4,4}$, which contradicts to the condition $T \in \mathcal{T}(n,4) - \{P_{n-4,4}\}$.

By calculation, we have

$$H(T_{5,v_3,n-5}) = \frac{2(n-5)}{n-2} + \frac{4}{n-1} + \frac{4}{3}.$$

This completes the proof. □

2.1. Trees with m pendant vertices and the second smallest harmonic indices

Let T be a tree of order $n \geq 3$ with m pendant vertices. Obviously, $m \leq n-1$ and the equality holds if and only if $T = S_n$. When $m = n-2$, one can see that $T \in \{S_{n_1,n_2} : n_1 + n_2 = n-2, n_1 \geq n_2\}$. By Lemma 2.2, we have $H(S_{n-3,1}) < H(S_{n-4,2}) < H(S_{n-t,t-2})$ for $5 \leq t \leq \frac{n}{2} + 1$. So, $S_{n-4,2}$ has the second smallest harmonic index among all trees of order n with $n-2$ pendant vertices.

For $m < n-2$, we have

Theorem 2.6. *Let T be a tree of order $n \geq 3$ with m pendant vertices. If $3 \leq m \leq n-3$ and $T \ncong P_{m-1,n-m+1}$, then*

$$H(T) \geq \frac{2(m-2)}{m+1} + \frac{n-m-3}{2} + \frac{4}{m+2} + \frac{4}{3}$$

and the equality holds if and only if $T \in \{T_{n-m+2,v_i,m-2} : 3 \leq i \leq n-m\}$.

Proof. Let T be a tree of order $n \geq 3$ with m pendant vertices, $3 \leq m \leq n-3$. By calculation, it is not difficult to obtain that for $3 \leq i \leq n-m$,

$$H(T_{n-m+2,v_3,m-2}) = H(T_{n-m+2,v_i,m-2}) = \frac{2(n-m-3)}{4} + \frac{2(m-2)}{m+1} + \frac{4}{m+2} + \frac{4}{3}.$$

So, we only need to prove that $H(T) \geq H(T_{n-m+2,v_3,m-2})$ by induction on n. One can see that the diameter $D(T) = 4$ if $n = m+3$. By Lemma 2.5, the theorem holds for $n = m+3$.

Suppose that $n \geq m+4$ and the theorem is true for all trees of order $n-1$ with m pendant vertices. Now, let T be a tree of order n with m pendant vertices, we consider the following cases:

Case 1. T is a tree of form Q_{n_1,n_2} with $n_1 \geq n_2 \geq 2$. Then, from Lemma 2.3 and Lemma 2.4, it follows that $H(T) \geq H(P_{m-2,n-m,2}) > H(T_{n-m+2,v_3,m-2})$.

Case 2. There is a path $u_1u_2u_3$ in T such that $d(u_1) = 1$, $d(u_2) = 2$ and $d(u_3) \geq 2$.

Let $T' = T - u_1$. By Lemma 2.1, we have that

$$H(T) = H\left(T'\right) + \frac{2}{3} - \frac{2}{(1+d(u_3))(2+d(u_3))} \tag{7}$$

and

$$H(T_{n-m+2,v_3,m-2}) = H(T_{n-m+1,v_3,m-2}) + \frac{1}{2} \tag{8}$$

Clearly, T' has $n-1$ vertices and m pendant vertices. Since $T \ncong P_{m-1,n-m+1}$, we have $T \cong T_{n-m+2,v_3,m-2}$ if $T' \cong P_{m-1,n-m}$. For $T' \ncong P_{m-1,n-m}$, by the induction hypothesis, we have $H\left(T'\right) > H(T_{n-m+1,v_3,m-2})$. From (7) and (8), $H(T) \geq H(T_{n-m+2,v_3,m-2})$ and the equality holds if and only if $T' \in \{T_{n-m+1,v_i,m-2} : 3 \leq i \leq n-m-1\}$ and $d(u_3) = 2$, i.e., the equality holds if and only if $T \in \{T_{n-m+2,v_i,m-2} : 3 \leq i \leq n-m\}$. □

2.2. Trees with the diameter r and the first two smallest harmonic indices

In the following, using Theorem 1.1 and Theorem 2.6, we find the smallest value of the harmonic index of trees in $\mathcal{T}(n,r)$ and determine the corresponding trees, where $\mathcal{T}(n,r)$ is the set of trees with n vertices and diameter r.

Let $T \in \mathcal{T}(n,r)$ and $r \geq 3$. Then, there is a path $u_1u_2\cdots u_{r+1}$ in T such that $d(u_1) = d(u_{r+1}) = 1$ and $d(u_i) \geq 2$ for all $2 \leq i \leq r$. So, T has at most $n-r+1$ pendant vertices. By Theorem 1.1, it is not difficult to see that $H(T) \geq H(P_{m-1,n-m+1})$ if T has m pendant vertices. By Lemma 2.2, for $m \geq 3$ we have $H(P_{m-2,n-m+1,1}) > H(P_{m-1,n-m+1,0})$, that is,

$$H(P_{m-2,n-m+2}) > H(P_{m-1,n-m+1}). \tag{9}$$

Thus, we have $H(T) \geq H(P_{n-r,r})$ and the equality if and only if $T \cong P_{n-r,r}$, i.e., $P_{n-r,r}$ is the tree with the smallest harmonic index in $\mathcal{T}(n,r)$.

For $r = 3$, $P_{n-3,3} = S_{n-3,1}$ is the tree with the smallest harmonic index in $\mathcal{T}(n,3)$, and by Lemma 2.2, we have that $S_{n-4,2}$ is the tree with the second smallest harmonic index in $\mathcal{T}(n,3)$.

For $r \geq 4$, if $T \in \mathcal{T}(n,r)$ and $T \ncong P_{n-r,r}$, let m be the number of pendant vertices in T, then by Theorem 2.6 and (9), $H(T) \geq H(T_{r+1,v_3,n-r-1})$ for $m = n-r+1$, and $H(T) \geq H(P_{m-1,n-m+1}) \geq H(P_{n-r-1,r+1})$ for $m \leq n-r$. By calculation, we have

$$H\left(T_{r+1,v_3,n-r-1}\right) = \frac{2\left(n-r-1\right)}{n-r+2} + \frac{4}{n-r+3} + \frac{r-4}{2} + \frac{4}{3}. \tag{10}$$

and

$$H\left(P_{n-r-1,r+1}\right) = \frac{2\left(n-r-1\right)}{n-r+1} + \frac{2}{n-r+2} + \frac{r-2}{2} + \frac{2}{3}. \tag{11}$$

Let $x = n-r$ and $\psi(x) = H(P_{n-r-1,r+1}) - H(T_{r+1,v_3,n-r-1})$. From (10) and (11), we have

$$\begin{aligned}\psi\left(x\right) &= \frac{2\left(x-1\right)}{x+1} + \frac{2}{x+2} + \frac{r-2}{2} + \frac{2}{3} - \frac{2\left(x-1\right)}{x+2} - \frac{4}{x+3} - \frac{r-4}{2} - \frac{4}{3}\\ &= \frac{2\left(x-1\right)}{x+1} - \frac{2\left(x-1\right)}{x+2} + \frac{2}{x+2} - \frac{4}{x+3} + \frac{1}{3}\\ &= \frac{(x-1)(x^2+7x+18)}{3(x+1)(x+2)(x+3)} > 0\end{aligned}$$

for $x \geq 2$. So, $T_{r+1,v_3,n-r-1}$ is the tree with the second smallest harmonic index in $\mathcal{T}(n,r)$ for $r \geq 4$.

Theorem 2.7. *(i) For $T \in \mathcal{T}\left(n,r\right)$ and $r \geq 3$, we have*

$$H\left(T\right) \geq \frac{2\left(n-r\right)}{n-r+2} + \frac{2}{n-r+3} + \frac{r-3}{2} + \frac{2}{3}$$

and the equality holds if and only if $T \cong P_{n-r,r}$.
(ii) For $r \geq 4$ and $T \in \mathcal{T}\left(n,r\right) - \{P_{n-r,r}\}$, we have

$$H\left(T\right) \geq \frac{2\left(n-r-1\right)}{n-r+2} + \frac{4}{n-r+3} + \frac{r-4}{2} + \frac{4}{3}$$

and the equality holds if and only if $T \in \{T_{r+1,v_i,n-r-1} : 3 \leq i \leq r-1\}$.

2.3. *Trees with small harmonic indices*

In the following, we determine the unique tree of order n with, respectively, the second, the third and the fourth smallest harmonic index.

Let T be a tree of order n. For $n = 2,3$, we have $T \cong S_n$, and we can easily check that
(a) for $n = 4$, $H\left(P_4\right) > H\left(S_4\right)$;
(b) for $n = 5$, $H\left(P_5\right) > H\left(S_{2,1}\right) > H\left(S_5\right)$;
(c) for $n = 6,7$, $H\left(T\right) > H\left(P_{n-4,4}\right) > H\left(S_{n-4,2}\right) > H\left(S_{n-3,1}\right) > H\left(S_n\right)$ if $T \notin \{P_{n-4,4}, S_{n-4,2}, S_{n-3,1}, S_n\}$.
Now, we consider the case $n \geq 8$. By Lemma 2.2, we have

$$H\left(S_{n_1,n_2}\right) > H\left(S_{n_1+1,n_2-1}\right) \quad \text{for} \quad n_1 \geq n_2 \geq 2 \tag{12}$$

By (9) and Theorem 2.7, we have

$$H\left(T\right) > H\left(P_{n-4,4}\right) \quad \text{if} \quad T \in \mathcal{T}\left(n,r\right) - \{P_{n-4,4}\} \quad \text{and} \quad r \geq 4 \tag{13}$$

By calculation, we obtain the following:
(i) $H\left(S_{n-3,1}\right) = \frac{2(n-3)}{n-1} + \frac{2}{n} + \frac{2}{3}$
(ii) $H\left(S_{n-4,2}\right) = \frac{2(n-4)}{n-2} + \frac{2}{n} + 1$

(iii) $H(S_{n-5,3}) = \frac{2(n-5)}{n-3} + \frac{2}{n} + \frac{6}{5}$
(iv) $H(P_{n-4,4}) = \frac{2(n-4)}{n-2} + \frac{2}{n-1} + \frac{7}{6}$.
From (i) to (iv), $H(S_{n-5,3}) > H(S_{n-4,2}) > H(S_{n-3,1})$ and $H(P_{n-4,4}) > H(S_{n-4,2}) > H(S_{n-3,1})$ for $n \geq 8$.
On the other hand, we have

$$H(S_{n-5,3}) - H(P_{n-4,4}) = \frac{n^4 - 6n^3 - 169n^2 + 414n - 360}{30n(n-1)(n-2)(n-3)}.$$

By calculation, one obtains that $H(S_{n-5,3}) < H(P_{n-4,4})$ for $n = 8, 9, \cdots, 15$ and $H(S_{n-5,3}) > H(P_{n-4,4})$ for $n \geq 16$.
From above, we can get the following theorem.

Theorem 2.8. *Let T be a tree of order $n \geq 6$ and $T \notin \{S_{n-4,2}, S_{n-3,1}, S_n\}$. Then*
(i) $H(T) \geq H(S_{n-5,3}) > H(S_{n-4,2}) > H(S_{n-3,1}) > H(S_n)$ for $n = 8, 9, \cdots, 15$ and the equality holds if and only if $T \cong S_{n-5,3}$.
(ii) $H(T) \geq H(P_{n-4,4}) > H(S_{n-4,2}) > H(S_{n-3,1}) > H(S_n)$ for $n = 6, 7$ or $n \geq 16$ and the equality holds if and only if $T \cong P_{n-4,4}$.

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