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THE HARMONIC INDEX OF TWO–TREES AND QUASI–TREE GRAPHS

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Abstract. The harmonic index 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 the vertex u in G. A graph G is called quasi-tree, if there exists $u \in V(G)$ such that $G-u$ is a tree. The graphs called two-trees are defined by recursion. The smallest two-tree is the complete graph on two vertices. A two-tree on $n+1$ vertices (where $n \geqslant 2$) is obtained by adding a new vertex adjacent to the two end vertices of one edge in a two-tree on n vertices. In this work, the sharp lower and upper bounds on the harmonic index of quasi-tree graphs are presented. Furthermore, the lower bound on the harmonic index of two-trees is presented, and the two-trees with the minimum and the second minimum harmonic index, respectively, are determined.

1. Introduction

Throughout this paper we consider only simple connected graphs. Such a graph will be denoted by $G=(V(G),E(G))$, where $V(G)$ and $E(G)$ are the vertex set and edge set of G, respectively. The degree of a vertex u is denoted by $d_G(u)$ ($d(u)$ for short). Suppose $Graph$ is the collection of all graphs. A mapping $Top : Graph \rightarrow R$ is called a topological index, if $G \cong H$ implies that $Top(G) = Top(H)$. Many topological indices are closely correlated with some physicochemical characteristics of the underlying compounds. The harmonic index of G is defined in [2] as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u)+d(v)},$$

where $d(u)$ denotes the degree of the vertex u in G. As a variant of the Randić index which is the most successful molecular descriptor in structure-property and structure-activity relationships studies, the harmonic index has better correlations with physical and chemical properties comparing with the well known Randić index. The harmonic index has good correlation with some physicochemical properties of alkanes: boiling points(experimental), kova'ts index, enthalpies of formation, chromatographic retention times(for vapour pressure), surface area, solubility in water, etc.

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Let $G = (V(G), E(G))$ be a graph of order n $(n \geqslant 3)$. For a vertex v of a graph G, we denote the neighborhood of v by $N_G(v)$. The graph that arises from G by deleting the vertex $u \in V(G)$ or the edge $uv \in E(G)$ will be denoted by $G-u$ or $G-uv$, respectively. Similarly, the graph $G+uv$ arises from G by adding an edge $uv \notin E(G)$ between the endpoints $u, v \in V(G)$. A graph G is called a quasi-tree graph, if there exists a vertex $u' \in V(G)$ such that $G-u'$ is a tree. As usual, we use C_n to denote a cycle of order n. Let Y_n denote the graph arises from complete bipartite graph $K_{2,n-2}$ by joining an edge between the two non-adjacent vertices of degree $n-2$. Let Z_n denote the graph obtained from the graph Y_{n-1} by adding a new vertex and two new edges adjacent to the new vertex such that one edge is incident to a vertex of degree 2 in Y_{n-1} and the other is incident to a vertex of degree $n-2$ in Y_{n-1} (see Fig. 1.1).

The two-tree is defined as follows.

Step 1. When $t = 0$, let $T_0 = K_2$, where K_2 (an edge) is a two-tree with 2 vertices.

Step 2. Let T_t be a two-tree generated at the t-th step. Then, T_{t+1} generated at the $(t+1)$ step is the graph obtained from T_t by adding a new vertex adjacent to the two end vertices of one edge. Clearly, T_{t+1} has $t+3$ vertices.

The two-tree has a very important structure in complex networks. It is known that the small-world Farey graph [22], fractal scale-free networks [23], the pseudofractal scale-free web [24] and the generalized Farey graph [25] are some special classes of two-tree networks.

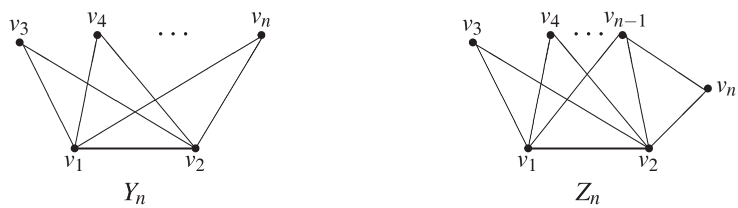

Fig. 1.1. The graphs Y_n (left) and Z_n (right)

The harmonic index was extensively studied recently. Zhong [1,4,5] determined the minimum and maximum values of the harmonic index for simple connected graphs, trees, unicyclic graphs and bicyclic graphs, respectively. Some upper and lower bounds on the harmonic index of a graph were obtained by Llić [8]. Xu [7] and Deng et al. [10] established some relationship between the harmonic index of a graph and its topological indices, such as Randić index, Atom-bond connectivity index and radius, respectively. Wu et al. [3] determined the graph with minimum harmonic index among all the graphs (or all triangle-free graphs) with minimum degree at least two. For other related results see [6,12,13,16-21]. Here we give the sharp lower and upper bounds on the harmonic index of quasi-tree graphs. We also present the lower bound on the harmonic index of two-trees, and determine the two-trees with the minimum and the second minimum harmonic index, respectively. For terminology and notations not defined here, we refer the readers to [15].

2. The harmonic index of quasi-tree graphs

2.1. Preliminaries

We begin with some useful lemmas.

LEMMA 2.1. [1] *Let G be a connected graph of order n. Then*

$$H(G) \leqslant \frac{n}{2}$$

with equality if and only if G is a regular graph.

LEMMA 2.2. *Let*

$$g(x) = \frac{1}{2} + \frac{6}{1+x} - \frac{4}{2+x} - \frac{2}{x}.$$

Then $g(x)$ is monotonous decreasing for $x \geqslant 4$.

Proof. Note that for $x \geqslant 4$

$$g'(x) = 2\left(\frac{1}{x^2} + \frac{2}{(2+x)^2} - \frac{3}{(1+x)^2}\right) = \frac{2(-2x^3+3x^2+12x+4)}{x^2(x+1)^2(x+2)^2} < 0.$$

Then $g(x)$ is monotonous decreasing for $x \geqslant 4$. □

In a similar way, we can get the following Lemma 2.3 and 2.4.

LEMMA 2.3. *Let*

$$l(x) = \frac{4}{15} + \frac{5}{x} - \frac{3}{x-1} - \frac{2}{x+1}.$$

Then $l(x)$ is monotonous increasing for $x \geqslant 6$ and $l(6) \approx 0.2143 > 0$.

LEMMA 2.4. *Let*

$$q(x) = \frac{1}{x+2} + \frac{2}{x} - \frac{3}{1+x}.$$

Then $q(x)$ is monotonous decreasing for $x \geqslant 2$.

LEMMA 2.5. *Let*

$$p(x,y) = \frac{1+x}{1+y} + \frac{y-x-1}{y+2} - \frac{x}{y} - \frac{y-x-1}{y+1},$$

where $x \geqslant 1$ and $y \geqslant 2$. Then $p(x,y)$ is monotonous decreasing in x.

Proof. Since

$$\frac{\partial p(x,y)}{\partial x}=\frac{2}{y+1}-\frac{1}{y}-\frac{1}{y+2}=\frac{-2}{y(y+1)(y+2)}<0,$$

so $p(x,y)$ is monotonous decreasing in x. □

LEMMA 2.6. *Let $G=(V,E)$ be a graph of order n with $\delta(G)=2$ and let $u,v_1,v_2\in V(G)$ with $N(u)=\{v_1,v_2\}$, $v_1v_2\in E(G)$, $d_1=d(v_1)\geqslant 3$ and $d_2=d(v_2)\geqslant 3$. Then*

$$H(G)\geqslant H(G-u)+f(d_1,d_2),$$

where $f(d_1,d_2)=2(\frac{3}{1+d_1}+\frac{3}{1+d_2}-\frac{3}{2+d_1}-\frac{3}{2+d_2}+\frac{1}{d_1+d_2}-\frac{1}{d_1+d_2-2})$, and $f(d_1,d_2)\geqslant f(n-1,n-1)=\frac{12}{n}-\frac{12}{n+1}+\frac{1}{n-1}-\frac{1}{n-2}$.

Proof. Denote $N(v_1)\backslash\{u,v_2\}=\{x_1,x_2,\cdots,x_{d_1-2}\}$, $N(v_2)\backslash\{u,v_1\}=\{y_1,y_2,\cdots,y_{d_2-2}\}$. From the definition of harmonic index and $\delta=2$, we have

$$\begin{aligned}
&H(G)-H(G-u)\\
=&\frac{2}{2+d_1}+\frac{2}{2+d_2}+\frac{2}{d_1+d_2}+\sum_{i=1}^{d_1-2}\frac{2}{d_1+d(x_i)}+\sum_{j=1}^{d_2-2}\frac{2}{d_2+d(y_j)}\\
&-\frac{2}{d_1+d_2-2}-\sum_{i=1}^{d_1-2}\frac{2}{d_1+d(x_i)-1}-\sum_{j=1}^{d_2-2}\frac{2}{d_2+d(y_j)-1}\\
=&\frac{2}{2+d_1}+\frac{2}{2+d_2}+\frac{2}{d_1+d_2}-\frac{2}{d_1+d_2-2}-\sum_{i=1}^{d_1-2}\frac{2}{(d_1+d(x_i))(d_1+d(x_i)-1)}\\
&-\sum_{j=1}^{d_2-2}\frac{2}{(d_2+d(y_j))(d_2+d(y_j)-1)}\\
\geqslant&\frac{2}{2+d_1}+\frac{2}{2+d_2}+\frac{2}{d_1+d_2}-\frac{2}{d_1+d_2-2}-\frac{2(d_1-2)}{(1+d_1)(2+d_1)}-\frac{2(d_2-2)}{(1+d_2)(2+d_2)}\\
=&2(\frac{3}{1+d_1}+\frac{3}{1+d_2}-\frac{3}{2+d_1}-\frac{3}{2+d_2}+\frac{1}{d_1+d_2}-\frac{1}{d_1+d_2-2}).
\end{aligned}$$

Now we show that for $d_1,d_2\in[3,n-1]$, $f(d_1,d_2)$ attains its minimum value for $d_1=d_2=n-1$. Note that

$$\begin{aligned}
\frac{\partial f(d_1,d_2)}{\partial d_1}&=2(\frac{3}{(2+d_1)^2}-\frac{3}{(1+d_1)^2}+\frac{1}{(d_1+d_2-2)^2}-\frac{1}{(d_1+d_2)^2}),\\
\frac{\partial^2 f(d_1,d_2)}{\partial d_1\partial d_2}&=4(\frac{1}{(d_1+d_2)^3}-\frac{1}{(d_1+d_2-2)^3})<0.
\end{aligned}$$

So

$$\frac{\partial f(d_1,d_2)}{\partial d_1}\leqslant\frac{\partial f(d_1,3)}{\partial d_1}=2(\frac{3}{(2+d_1)^2}-\frac{2}{(1+d_1)^2}-\frac{1}{(3+d_1)^2})<0.$$

By symmetry, we have $\frac{\partial f(d_1,d_2)}{\partial d_2} < 0$ for $d_1, d_2 \in [3, n-1]$. This implies that $f(d_1,d_2) \geqslant f(n-1,n-1) = \frac{12}{n} - \frac{12}{n+1} + \frac{1}{n-1} - \frac{1}{n-2}$. $\square$

Let G be a quasi-tree graph and $u' \in V(G)$ such that $G - u'$ is a tree. If $d(u') = 1$, then G is a tree and then $\frac{2(n-1)}{n} \leqslant H(G) \leqslant \frac{4}{3} + \frac{n-3}{2}$ $(n \geqslant 3)$ (see [1]). Hence, in the following, we only consider the case of $d(u') \geqslant 2$. Denote

$QT(n) = \{G | G$ is a quasi-tree graph of order n with $d(u') \geqslant 2\}$,

$$h(n) = \frac{5}{2} + \frac{4}{n+1} - \frac{6}{n},$$

and $PV = \{u_0 \in V(G) | d(u_0) = 1\}$.

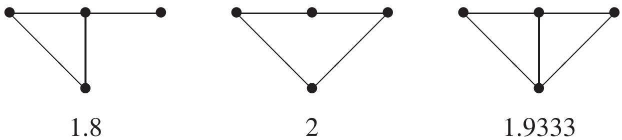

Fig. 2.1. The graphs and their harmonic indices in $QT(4)$.

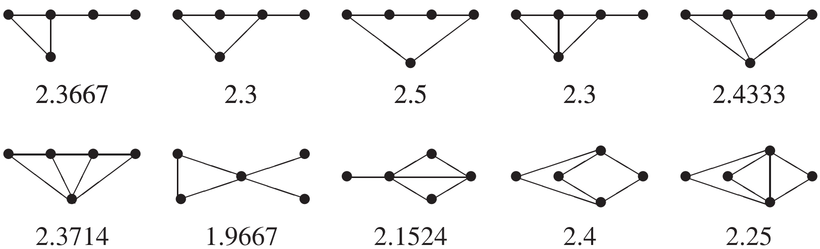

Fig. 2.2. The graphs and their harmonic indices in $QT(5)$.

LEMMA 2.7. *Let $G \in QT(n)$ with $n \geqslant 4$. If $PV = \emptyset$, then $H(G) > h(n)$.*

Proof. We prove the result by induction on n. If $n = 4$ or 5, then $h(4) = 1.8$, $h(5) = 1.9667$, and the lemma holds obviously (see Fig. 2.1 and 2.2). Since G is a quasi-tree and $PV = \emptyset$, there exists $u \in V(G)$ such that $d(u) = 2$. Let $N(u) = \{v_1, v_2\}$, $d(v_1) = d_1$ and $d(v_2) = d_2$. Now we consider the following two cases.

Case 1. $v_1 v_2 \notin E(G)$.

In this case, we have $2 \leqslant d_1, d_2 \leqslant n-2$. Since $G' = G - u + v_1 v_2 \in QT(n-1)$, by the induction hypothesis, we have

$$H(G) = H(G') + \frac{2}{2+d_1} + \frac{2}{2+d_2} - \frac{2}{d_1+d_2} \geqslant h(n-1) + \frac{2}{2+d_1} + \frac{2}{2+d_2} - \frac{2}{d_1+d_2}$$

$$
\begin{aligned}
&= h(n)+h(n-1)-h(n)+\frac{2}{2+d_1}+\frac{2}{2+d_2}-\frac{2}{d_1+d_2}\\
&= h(n)+\frac{10}{n}-\frac{6}{n-1}-\frac{4}{n+1}+\frac{2}{2+d_1}+\frac{2(d_1-2)}{(2+d_2)(d_1+d_2)}\\
&\geqslant h(n)+\frac{10}{n}-\frac{6}{n-1}-\frac{4}{n+1}+\frac{2}{n}=h(n)+\frac{2(n+2)(n-3)}{n(n-1)(n+1)}>h(n).
\end{aligned}
$$

Case 2. $v_1v_2 \in E(G)$.

Let $G' = G-u$. Then $G' \in QT(n-1)$. Denote $N(v_1)\setminus\{u,v_2\} = \{x_1,x_2,\cdots,x_{d_1-2}\}$, $N(v_2)\setminus\{u,v_1\} = \{y_1,y_2,\cdots,y_{d_2-2}\}$.

Subcase 2.1. $d_1 = 2,\ d_2 \geqslant 3$ or $d_2 = 2,\ d_1 \geqslant 3$.

Without loss of generality, we assume that $d_1 = 2,\ d_2 \geqslant 3$. Then $N(v_1\setminus\{u,v_2\}) = \emptyset$ and we have

$$
\begin{aligned}
H(G) =&H(G')+\frac{1}{2}+\frac{4}{2+d_2}+\sum_{j=1}^{d_2-2}\frac{2}{d_2+d(y_j)}-\frac{2}{d_2}-\sum_{j=1}^{d_2-2}\frac{2}{d_2+d(y_j)-1}\\
\geqslant&h(n)+\frac{10}{n}-\frac{6}{n-1}-\frac{4}{n+1}+\frac{1}{2}+\frac{4}{2+d_2}-\frac{2}{d_2}-\frac{2(d_2-2)}{(d_2+1)(d_2+2)}\\
=&h(n)+\frac{10}{n}-\frac{6}{n-1}-\frac{4}{n+1}+\frac{1}{2}+\frac{6}{1+d_2}-\frac{4}{2+d_2}-\frac{2}{d_2}. \qquad (2.1)
\end{aligned}
$$

If $d_2 = 3$, by Lemma 2.3 and (2.1), we have

$$
H(G) \geqslant h(n)+2\left(\frac{5}{n}-\frac{3}{n-1}-\frac{2}{n+1}+\frac{4}{15}\right) \geqslant h(n)+0.4286 > h(n).
$$

If $d_2 \geqslant 4$, by Lemma 2.2 and (2.1), we have

$$
\begin{aligned}
H(G) \geqslant&h(n)+\frac{10}{n}-\frac{6}{n-1}-\frac{4}{n+1}+\frac{1}{2}+\frac{6}{n}-\frac{4}{n+1}-\frac{2}{n-1}\\
\geqslant&h(n)+\frac{n^3-n-32}{2n(n-1)(n+1)} > h(n).
\end{aligned}
$$

Subcase 2.2. $d_1,d_2 \geqslant 3$.

By the induction hypothesis and Lemma 2.6, we have

$$
\begin{aligned}
H(G) \geqslant&h(n)+\frac{10}{n}-\frac{6}{n-1}-\frac{4}{n+1}+2\Big(\frac{3}{1+d_1}+\frac{3}{1+d_2}-\frac{3}{2+d_1}-\frac{3}{2+d_2}\\
&+\frac{1}{d_1+d_2}-\frac{1}{d_1+d_2-2}\Big)\\
\geqslant&h(n)+\frac{10}{n}-\frac{6}{n-1}-\frac{4}{n+1}+\frac{12}{n}-\frac{12}{n+1}+\frac{1}{n-1}-\frac{1}{n-2}\\
=&h(n)+\frac{22}{n}-\frac{5}{n-1}-\frac{16}{n+1}-\frac{1}{n-2}=h(n)+\frac{9n^2-43n+44}{n(n-1)(n+1)(n-2)}\\
>&h(n). \qquad \square
\end{aligned}
$$

LEMMA 2.8. *Let $G \in QT(n)$ with $n \geqslant 5$ and $PV \neq \emptyset$. Let $u \in PV$ and v be the neighbor of u. Denote $d(v) = d$ and $N(v) \backslash \{u\} = \{x_1, x_2, \cdots, x_{d-1}\}$. If $d(x_i) \geqslant 2$ for $i = 1, 2, \cdots, d-1$, then $H(G) > h(n)$.*

Proof. We prove the result by induction on n. If $n = 5$, then the lemma holds obviously (see Fig. 2.2). Since $u \in PV$ and v is the neighbor of u, $2 \leqslant d \leqslant n-1$. Let $G' = G - u$. Then $G' \in QT(n-1)$. By the induction hypothesis, we have

$$
\begin{aligned}
H(G) =& H(G') + \frac{2}{d+1} + \sum_{i=1}^{d-1} \left(\frac{2}{d+d(x_i)} - \frac{2}{d+d(x_i)-1} \right) \\
\geqslant& h(n) + \frac{10}{n} - \frac{6}{n-1} - \frac{4}{n+1} + \frac{2}{d+1} - \frac{2(d-1)}{(d+1)(d+2)} \\
=& h(n) + \frac{10}{n} - \frac{6}{n-1} - \frac{4}{n+1} + \frac{6}{(1+d)(2+d)} \\
\geqslant& h(n) + \frac{10}{n} - \frac{6}{n-1} - \frac{4}{n+1} + \frac{6}{n(n+1)} = h(n) + \frac{16}{n} - \frac{6}{n-1} - \frac{10}{n+1} \\
=& h(n) + \frac{4(n-4)}{n(n-1)(n+1)} > h(n). \quad \square
\end{aligned}
$$

LEMMA 2.9. *Let $G \in QT(n)$ with $n \geqslant 5$ and $PV \neq \emptyset$. Let $u \in PV$ and v be the neighbor of u. Denote $d(v) = d$ and $N(v) \backslash \{u\} = \{x_1, x_2, \cdots, x_{d-1}\}$. If $d \leqslant n-2$ and there exists some x_i, say x_1, such that $d(x_1) = 1$, then $H(G) > h(n)$.*

Proof. We prove the result by induction on n. If $n = 5$, then the lemma holds obviously (see Fig. 2.2). Let $G' = G - u$. Then $G' \in QT(n-1)$. Without loss of generality we assume that $d(x_1) = d(x_2) = \cdots = d(x_k) = 1$, where $k \geqslant 1$. By the induction hypothesis, we have

$$
\begin{aligned}
H(G) =& H(G') + \frac{2}{d+1} + \sum_{i=1}^{d-1} \left(\frac{2}{d+d(x_i)} - \frac{2}{d+d(x_i)-1} \right) \\
\geqslant& H(G') + \frac{2}{d+1} - \frac{2k}{d(d+1)} - \frac{2(d-1-k)}{(d+1)(d+2)} \\
\geqslant& h(n) + \frac{10}{n} - \frac{6}{n-1} - \frac{4}{n+1} + 2\left(\frac{1+k}{d+1} - \frac{k}{d} - \frac{d-k-1}{d+1} + \frac{d-k-1}{d+2} \right). \quad (2.2)
\end{aligned}
$$

If $d \leqslant n-3$, then $k \leqslant d-2$. For $n \geqslant 6$, by Lemma 2.4, 2.5 and (2.2), we have

$$
\begin{aligned}
H(G) \geqslant& h(n) + \frac{10}{n} - \frac{6}{n-1} - \frac{4}{n+1} + 2\left(\frac{1}{d+2} + \frac{2}{d} - \frac{3}{d+1} \right) \\
\geqslant& h(n) + \frac{10}{n} - \frac{6}{n-1} - \frac{4}{n+1} + 2\left(\frac{1}{n-1} + \frac{2}{n-3} - \frac{3}{n-2} \right) \\
=& h(n) + 2\left(\frac{5}{n} + \frac{2}{n-3} - \frac{2}{n-1} - \frac{2}{n+1} - \frac{3}{n-2} \right)
\end{aligned}
$$

$$=h(n)+\frac{4(n^2+10n-15)}{n(n-1)(n+1)(n-2)(n-3)}>h(n).$$

If $d=n-2$, since $G\in QT(n)$, then $k\leqslant n-5$. By Lemma 2.5 and (2.2), we have

$$\begin{aligned}H(G)\geqslant&h(n)+\frac{10}{n}-\frac{6}{n-1}-\frac{4}{n+1}+2(\frac{2}{n}+\frac{3}{n-2}-\frac{5}{n-1})\\=&h(n)+2(\frac{7}{n}+\frac{3}{n-2}-\frac{8}{n-1}-\frac{2}{n+1})=h(n)+\frac{4(n+7)}{n(n-1)(n+1)}>h(n).\quad\square\end{aligned}$$

2.2. Main result

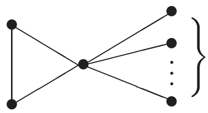

Fig. 2.3. $QT^*(n)$.

Let n be positive integer with $n\geqslant 3$. The quasi-tree graph $QT^*(n)$ with n vertices is obtained from the star graph $K_{1,n-1}$ by connecting two pendent vertices of $K_{1,n-1}$ (see Fig. 2.3). Clearly,

$$H(QT^*(n))=h(n)=\frac{5}{2}+\frac{4}{n+1}-\frac{6}{n}.$$

Let G be a quasi-tree graph and $u'\in V(G)$ such that $G-u'$ is a tree. We only consider the case of $d(u')\geqslant 2$. Now we give our main result in this section.

THEOREM 2.10. *Let $G\in QT(n)$ with $n\geqslant 3$. Then*

$$h(n)\leqslant H(G)\leqslant\frac{n}{2}.$$

The left equality holds if and only if $G\cong QT^*(n)$ and the right equality holds if and only if $G\cong C_n$.

Proof. By Lemma 2.1, we have $H(G)\leqslant\frac{n}{2}$ and the equality holds if and only if G is a regular graph. Since C_n is the only regular graph in $QT(n)$, so $H(G)=\frac{n}{2}$ if and only if G is a cycle of order n. In the following proof, we just show that $h(n)\leqslant H(G)$ and equality holds if and only if $G\cong QT^*(n)$. We prove this result by induction on n.

If $n=3$, the theorem holds clearly. If $n=4,5$, then the theorem holds obviously (see Fig. 2.1 and 2.2). Assume that $G\in QT(n)$ with $n\geqslant 6$. By Lemma 2.7, we only consider the case of $PV\neq\emptyset$. Let $u\in PV$ and v be the neighbor of u. Denote $d(v)=d$ and $N(v)\backslash\{u\}=\{x_1,x_2,\cdots,x_{d-1}\}$. Then $d\geqslant 2$. Let $G'=G-u$, then $G'\in QT(n-1)$. By Lemma 2.8 and 2.9, we suppose that there exists some i $(1\leqslant i\leqslant d-1)$ such that $d(x_i)=1$ and $d=n-1$.

Without loss of generality we assume that $d(x_1) = d(x_2) = \cdots = d(x_k) = 1$ and $d(x_i) \geqslant 2$ for $k+1 \leqslant i \leqslant d-1$, where $k \geqslant 1$. By the induction hypothesis and $d = n-1$, we have

$$\begin{aligned}
H(G) =& H(G') + \frac{2}{1+d} + \sum_{i=1}^{d-1}\left(\frac{2}{d+d(x_i)} - \frac{2}{d+d(x_i)-1}\right) \\
\geqslant& h(n-1) + \frac{2}{1+d} + \sum_{i=1}^{d-1}\left(\frac{2}{d+d(x_i)} - \frac{2}{d+d(x_i)-1}\right) \\
\geqslant& h(n) + \frac{10}{n} - \frac{6}{n-1} - \frac{4}{n+1} + 2\left(\frac{1+k}{d+1} - \frac{k}{d} - \frac{d-k-1}{d+1} + \frac{d-k-1}{d+2}\right) \\
=& h(n) + \frac{10}{n} - \frac{6}{n-1} - \frac{4}{n+1} + 2\left(\frac{3+2k}{n} - \frac{k}{n-1} - \frac{k+3}{n+1}\right) \\
=& h(n) + 2\left(\frac{8+2k}{n} - \frac{3+k}{n-1} - \frac{5+k}{n+1}\right) = h(n) + \frac{4(n-k-4)}{n(n-1)(n+1)} \geqslant h(n). \qquad (2.3)
\end{aligned}$$

Now suppose that equality holds in (2.3). Then all inequalities in the above argument must be equalities. Hence we have $H(G') = h(n-1)$ and $k = n-4$. By the induction hypothesis, $G' \in QT^*(n-1)$. Note that G' has a unique vertex of degree greater than 3, hence $G \cong QT^*(n)$. This completes the proof of Theorem 2.10. □

3. The harmonic index of two-trees

3.1. Some Lemmas

Here we give some useful lemmas in the following paper.

LEMMA 3.1. *Let*

$$f(x,d) = \frac{1}{x+d} - \frac{1}{x-1+d},$$

where $d \geqslant 2$, $x \geqslant 3$. Then $f(x,d)$ is monotonous increasing for $d \geqslant 2$.

Proof. Note that for $d \geqslant 2$,

$$\frac{\partial f(x,d)}{\partial d} = \frac{2x+2d-1}{(x+d)^2(x+d-1)^2} > 0.$$

Then $f(x,d)$ is monotonous increasing for $d \geqslant 2$. □

LEMMA 3.2. *Let*

$$g(x,y) = \frac{3}{(x+1)(x+2)} + \frac{3}{(y+1)(y+2)} + \frac{1}{x+y} - \frac{1}{x+y-2},$$

where $x \geqslant 3$ and $y \geqslant 3$. Then $g(x,y)$ is monotonous decreasing in x (resp. y).

Proof. We have

$$\begin{aligned}\frac{\partial g(x,y)}{\partial x} &= \frac{-3(2x+3)}{(x+1)^2(x+2)^2} + \frac{4(x+y-1)}{(x+y)^2(x+y-2)^2} \\ &= \frac{-(2x+3)}{(x+1)^2(x+2)^2} + \frac{-2(2x+3)}{(x+1)^2(x+2)^2} + \frac{2(2x+2y-2)}{(x+y)^2(x+y-2)^2},\end{aligned}$$

and

$$\begin{aligned}&(2x+3)(x+y)^2(x+y-2)^2 - (2x+2y-2)(x+2)^2(x+1)^2 \\ =&6x^4y - 15x^4 + 12x^3y^2 - 24x^3y - 18x^3 + 8x^2y^3 - 6x^2y^2 - 46x^2y + 14x^2 \\ &+ 2xy^4 + 4xy^3 - 28xy^2 + 16x + 3y^4 - 12y^3 + 12y^2 - 8y + 8 \\ =&(5yx^4 - 15x^4) + (8yx^3y - 24x^3y) + (2y^2x^3 - 18x^3) + (x^2yx^2 + 8y^2yx^2 \\ &- 46yx^2) + 14x^2 + (2xx^2y^2 - 6x^2y^2) + (2y^2xy^2 + 4yxy^2 - 28xy^2) \\ &+ 16x + 3y^4 - 12y^3 + 12y^2 - 8y + 8.\end{aligned}$$

Since for $x,y \geqslant 3$, $(5yx^4 - 15x^4) \geqslant 0$, $(8yx^3y - 24x^3y) \geqslant 0$, $(2y^2x^3 - 18x^3) \geqslant 0$, $(x^2yx^2 + 8y^2yx^2 - 46yx^2) > 0$, $(2xx^2y^2 - 6x^2y^2) \geqslant 0$, $(2y^2xy^2 + 4yxy^2 - 28xy^2) > 0$, $14x^2 + 16x > 0$, $3y^4 - 12y^3 + 12y^2 - 8y + 8 > 0$ (since the maximum root of $3y^4 - 12y^3 + 12y^2 - 8y + 8$ is $2.7835 < 3$, it follows that $3y^4 - 12y^3 + 12y^2 - 8y + 8 \geqslant (3y^4 - 12y^3 + 12y^2 - 8y + 8)\big|_{y=3} = 11 > 0$ for $y \geqslant 3$), then $(2x+3)(x+y)^2(x+y-2)^2 - (2x+2y-2)(x+2)^2(x+1)^2 > 0$, and $\frac{-2(2x+3)}{(x+1)^2(x+2)^2} + \frac{2(2x+2y-2)}{(x+y)^2(x+y-2)^2} < 0$. Thus, $\frac{\partial g(x,y)}{\partial x} < 0$. So $g(x,y)$ is monotonous decreasing in x. By symmetry, $g(x,y)$ is monotonous decreasing in y. □

LEMMA 3.3. *Let*

$$h(x,y) = \frac{3x+11}{(x+1)(x+2)(x+3)} + \frac{3y+11}{(y+1)(y+2)(y+3)} + \frac{1}{x+y} - \frac{1}{x+y-2},$$

where $x \geqslant 3$ and $y \geqslant 3$. Then $h(x,y)$ is monotonous decreasing in x (resp. y).

Proof. We have

$$\begin{aligned}h(x,y) =&\frac{3(x+3)+2}{(x+1)(x+2)(x+3)} + \frac{3(y+3)+2}{(y+1)(y+2)(y+3)} + \frac{1}{x+y} - \frac{1}{x+y-2} \\ =&\frac{3}{(x+1)(x+2)} + \frac{3}{(y+1)(y+2)} + \frac{1}{x+y} - \frac{1}{x+y-2} \\ &+ \frac{2}{(x+1)(x+2)(x+3)} + \frac{2}{(y+1)(y+2)(y+3)} \\ =&g(x,y) + \frac{2}{(x+1)(x+2)(x+3)} + \frac{2}{(y+1)(y+2)(y+3)}.\end{aligned}$$

By Lemma 3.2, we can get that $h(x,y)$ is monotonous decreasing in x (resp. y). □

LEMMA 3.4. *Let*

$$l(n) = \frac{12}{n+1} + \frac{8}{n-1} - \frac{18}{n} - \frac{2}{n+2} + \frac{1}{n-2} - \frac{1}{n-3} + \frac{2}{2n-5} - \frac{2}{2n-3},$$

where $n \geqslant 5$. *Then* $l(n) > 0$.

Proof. We have

$$l(n) = \frac{44n^5 - 287n^4 + 154n^3 + 2231n^2 - 5094n + 3240}{n(n-1)(n+1)(n+2)(n-2)(n-3)(2n-5)(2n-3)}.$$

Let $l_1(n) = 44n^5 - 287n^4 + 154n^3 + 2231n^2 - 5094n + 3240$. Since the maximum root of $l_1(n)$ is $4 < 5$, then $l_1(n) \geqslant l_1(5) = 10920 > 0$. Thus, $l(n) > 0$. □

3.2. Main results

In this section, the lower bound on the harmonic index of two-trees is presented, and the two-trees with the minimum and the second minimum harmonic index, respectively, are determined.

THEOREM 3.5. *Let* G *be a two-tree with* $n \geqslant 4$ *vertices. Then*

$$H(G) \geqslant 4 - \frac{12}{n+1} + \frac{1}{n-1}$$

with equality holds if and only if $G \cong Y_n$.

Proof. We prove this result by induction on n. Let G_n be a two-tree of order n.

If $n = 4$, the two-tree G_n is a unique graph obtained from the complete graph of order 4 by deleting an edge. Obviously, $H(G_4) = \frac{29}{15} = 4 - \frac{12}{5} + \frac{1}{3}$, as desired. Assume that the result holds for $n-1$. Choose one vertex of degree 2 from the graph G_n, say w. Then $G_n - w$ is a two-tree of order $n-1$. By the induction hypothesis, $H(G_n - w) \geqslant H(Y_{n-1})$ with equality holds if and only if $G_n - w \cong Y_{n-1}$. In the following we prove that $H(G_n) \geqslant H(Y_n)$.

Let u and v be two vertices adjacent to the vertex w in G_n. Let $d_{G_n}(u) = x$, $d_{G_n}(v) = y$ and $N_{G_n}(u) \setminus \{v,w\} = \{u_1, u_2, \cdots, u_{x-2}\}$, $N_{G_n}(v) \setminus \{u,w\} = \{v_1, v_2, \cdots, v_{y-2}\}$. Clearly, $3 \leqslant x, y \leqslant n-1$. By the induction hypothesis and Lemma 3.1, 3.2, we have

$$\begin{aligned} H(G_n) =& H(G_n - w) + \frac{2}{x+2} + \frac{2}{y+2} + \frac{2}{x+y} - \frac{2}{x+y-2} + \sum_{i=1}^{x-2}\Big(\frac{2}{x+d(u_i)} \\ & - \frac{2}{x+d(u_i)-1}\Big) + \sum_{j=1}^{y-2}\Big(\frac{2}{y+d(v_j)} - \frac{2}{y+d(v_j)-1}\Big) \\ \geqslant & H(Y_{n-1}) + \frac{2}{x+2} + \frac{2}{y+2} + \frac{2}{x+y} - \frac{2}{x+y-2} - \frac{2(x-2)}{(x+1)(x+2)} \end{aligned}$$

$$
\begin{aligned}
&-\frac{2(y-2)}{(y+1)(y+2)}\\
=&H(Y_{n-1})+\frac{6}{(x+1)(x+2)}+\frac{6}{(y+1)(y+2)}+\frac{2}{x+y}-\frac{2}{x+y-2}\\
\geqslant&H(Y_{n-1})+\frac{12}{n(n+1)}+\frac{1}{n-1}-\frac{1}{n-2}\\
=&H(Y_n),
\end{aligned}
$$

where the equality holds if and only if $G_n-w\cong Y_{n-1}$, $x=y=n-1$ and $d_{G_n}(u_i)=2$ ($i=1,2,\cdots,n-3$), which implies $G_n\cong Y_n$. This completes the proof. □

THEOREM 3.6. *Let G be a two-tree with $n\geqslant 5$ vertices and $G\ncong Y_n$. Then*

$$H(G)\geqslant\frac{22}{5}-\frac{6}{n+1}-\frac{8}{n}+\frac{2}{n+2}+\frac{2}{2n-3}$$

with equality holds if and only if $G\cong Z_n$.

Proof. We prove this result by induction on n. Let G_n be a two-tree of order n and $G_n\ncong Y_n$.

If $n=5$, it can be seen that $G_n\cong Y_n$ or $G_n\cong Z_n$. Since $G_n\ncong Y_n$, then $G_n\cong Z_n$. Obviously, $H(G_5)=\frac{83}{35}=\frac{22}{5}-1-\frac{8}{5}+\frac{4}{7}$, as desired. Assume that the result holds for $n-1$. It is well known that a two-tree has at least two vertices of degree 2. Furthermore, $G_n\ncong Y_n$. We choose one vertex w of degree 2 from the graph G_n such that $G_n-w\ncong Y_{n-1}$. Then G_n-w is a two-tree of order $n-1$. By the induction hypothesis, $H(G_n-w)\geqslant H(Z_{n-1})$ with equality holds if and only if $G_n-w\cong Z_{n-1}$. In the following we prove that $H(G_n)\geqslant H(Z_n)$.

Let u and v be two vertices adjacent to the vertex w in G_n. Since $n\geqslant 5$, by the definition of two-tree, there must exist a vertex p which is adjacent to u and v with $d_{G_n}(p)\geqslant 3$ (otherwise, $G_n-w\cong Y_{n-1}$). Let $d_{G_n}(u)=x$, $d_{G_n}(v)=y$, $d_{G_n}(p)=z$ and $N_{G_n}(u)\setminus\{v,w,p\}=\{u_1,u_2,\cdots,u_{x-3}\}$, $N_{G_n}(v)\setminus\{u,w,p\}=\{v_1,v_2,\cdots,v_{y-3}\}$. Then $3\leqslant x,y,z\leqslant n-1$. Without loss of generality we assume that $x\leqslant y$.

If $max\{x,y,z\}=z$. Since vertex p is not adjacent to the vertex w, then $z\leqslant n-2$. Thus $x\leqslant y\leqslant n-2$. By the induction hypothesis and Lemma 3.1, 3.3, 3.4, we have

$$
\begin{aligned}
H(G_n)=&H(G_n-w)+\frac{2}{x+2}+\frac{2}{y+2}+\frac{2}{x+y}-\frac{2}{x+y-2}+\frac{2}{x+z}\\
&-\frac{2}{x+z-1}+\frac{2}{y+z}-\frac{2}{y+z-1}+\sum_{i=1}^{x-3}\left(\frac{2}{x+d(u_i)}-\frac{2}{x+d(u_i)-1}\right)\\
&+\sum_{j=1}^{y-3}\left(\frac{2}{y+d(v_j)}-\frac{2}{y+d(v_j)-1}\right)\\
\geqslant&H(Z_{n-1})+\frac{2}{x+2}+\frac{2}{y+2}+\frac{2}{x+y}-\frac{2}{x+y-2}+\frac{2}{x+3}
\end{aligned}
$$

$$
\begin{aligned}
& -\frac{2}{x+2}+\frac{2}{y+3}-\frac{2}{y+2}-\frac{2(x-3)}{(x+1)(x+2)}-\frac{2(y-3)}{(y+1)(y+2)} \\
=& H(Z_{n-1})+2\frac{3x+11}{(x+1)(x+2)(x+3)}+2\frac{3y+11}{(y+1)(y+2)(y+3)} \\
& +\frac{2}{x+y}-\frac{2}{x+y-2} \\
=& H(Z_{n-1})+2(\frac{4}{x+1}-\frac{5}{x+2}+\frac{1}{x+3})+2(\frac{4}{y+1}-\frac{5}{y+2}+\frac{1}{y+3}) \\
& +\frac{2}{x+y}-\frac{2}{x+y-2} \\
\geqslant & H(Z_{n-1})+4(\frac{4}{n-1}-\frac{5}{n}+\frac{1}{n+1})+\frac{1}{n-2}-\frac{1}{n-3} \\
=& \frac{22}{5}-\frac{26}{n}+\frac{8}{n-1}+\frac{6}{n+1}+\frac{2}{2n-5}+\frac{1}{n-2}-\frac{1}{n-3} \\
=& H(Z_n)+\frac{12}{n+1}+\frac{8}{n-1}-\frac{18}{n}-\frac{2}{n+2}+\frac{1}{n-2}-\frac{1}{n-3} \\
& +\frac{2}{2n-5}-\frac{2}{2n-3} \\
>& H(Z_n).
\end{aligned}
$$

If $max\{x,y,z\}=y$. Then $y \leqslant n-1$ and $max\{x,z\} \leqslant n-2$ (Otherwise $G_n \cong Y_n$). By the induction hypothesis and Lemma 3.1, 3.3, we have

$$
\begin{aligned}
H(G_n) =& H(G_n-w)+\frac{2}{x+2}+\frac{2}{y+2}+\frac{2}{x+y}-\frac{2}{x+y-2}+\frac{2}{x+z} \\
& -\frac{2}{x+z-1}+\frac{2}{y+z}-\frac{2}{y+z-1}+\sum_{i=1}^{x-3}(\frac{2}{x+d(u_i)}-\frac{2}{x+d(u_i)-1}) \\
& +\sum_{j=1}^{y-3}(\frac{2}{y+d(v_j)}-\frac{2}{y+d(v_j)-1}) \\
\geqslant & H(Z_{n-1})+\frac{2}{x+2}+\frac{2}{y+2}+\frac{2}{x+y}-\frac{2}{x+y-2}+\frac{2}{x+3}-\frac{2}{x+2} \\
& +\frac{2}{y+3}-\frac{2}{y+2}-\frac{2(x-3)}{(x+1)(x+2)}-\frac{2(y-3)}{(y+1)(y+2)} \\
=& H(Z_{n-1})+2\frac{3x+11}{(x+1)(x+2)(x+3)}+2\frac{3y+11}{(y+1)(y+2)(y+3)} \\
& +\frac{2}{x+y}-\frac{2}{x+y-2} \\
=& H(Z_{n-1})+2(\frac{4}{x+1}-\frac{5}{x+2}+\frac{1}{x+3})+2(\frac{4}{y+1}-\frac{5}{y+2}+\frac{1}{y+3}) \\
& +\frac{2}{x+y}-\frac{2}{x+y-2}
\end{aligned}
$$

$$\begin{aligned}&\geqslant H(Z_{n-1})+2(\frac{4}{n-1}-\frac{5}{n}+\frac{1}{n+1})+2(\frac{4}{n}-\frac{5}{n+1}+\frac{1}{n+2})\\&\quad+\frac{2}{2n-3}-\frac{2}{2n-5}\\&=H(Z_n),\end{aligned}$$

where the equality holds if and only if $G_n - w \cong Z_{n-1}$, $x = n-2$, $y = n-1$, $z = 3$ and $d_{G_n}(u_i) = d_{G_n}(v_j) = 2$ $(i = 1,2,\cdots,n-3;\ j = 1,2,\cdots,n-2)$, which implies $G_n \cong Z_n$. This completes the proof. □

3.3. Concluding remark

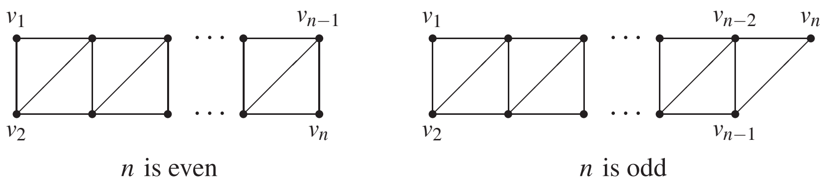

Fig. 3.1. The graphs with $H(G) = \frac{n}{2} - \frac{59}{420}$

From Theorems 3.5 and 3.6, we determine the two-trees with the first two smallest harmonic index, but the two-trees with the maximum harmonic index are still unknown, this seems to be a more difficult problem. For the maximum harmonic index, we conjecture the following result: For a two-tree G of order $n \geqslant 6$, $H(G) \leqslant \frac{n}{2} - \frac{59}{420}$. The graph attained this bound is shown in Fig. 3.1.

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