Research Article

On Harmonic Index and Diameter of Quasi-Tree Graphs

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The harmonic index of a graph \( H(G) \) is defined as the sum of the weights \( 2/(d_u + d_v) \) for all edges \( uv \) of \( G \), where \( d_u \) is the degree of a vertex \( u \) in \( G \). In this paper, we show that \( H(G) \geq D(G) + 5/3 - (n/2) \) and \( H(G) \geq ((1/2) + (2/3(n-2)))D(G) \), where \( G \) is a quasi-tree graph of order \( n \) and diameter \( D(G) \). Indeed, we show that both lower bounds are tight and identify all quasi-tree graphs reaching these two lower bounds.

1. Introduction

Let \( G \) be a simple connected graph with vertex set \( V(G) \) and edge set \( E(G) \) of order \( n \) (\(|V(G)| = n\)). The harmonic index of \( G \), first appeared in [1], is defined as \( H(G) = \sum_{uv \in E(G)} 2/(d_u + d_v) \), where for \( v \in V(G) \), \( d_v \) is the degree of \( v \) in \( G \). For \( u, v \in V(G) \), the distance between \( u \) and \( v \) is shown by \( d(u, v) \). Also, \( D(G) = \max\{d(u, v)\}_{u, v \in V(G)} \) is the diameter of \( G \) and \( \delta(G) = \min\{d_v\}_{v \in V(G)} \).

The applications of the harmonic index in various chemical disciplines have been demonstrated in [2–4]. Also, several studies have focused on graph theoretical properties of the harmonic index, see, for example, [5–9]. For a broad overview, we refer to [10].

A connected graph \( G \) is a quasi-tree graph if \( G \) is not a tree and there exists a vertex \( v \in V(G) \) such that \( G - v \) is a tree. A graph \( G \) is called unicyclic if it contains only one cycle. Obviously, every unicyclic graph is a quasi-tree graph. Many researchers have studied topological indices of quasi-tree graphs. See, for example, [11–16].

Liu [17] found a relation between harmonic index and diameter of a graph. He proved that if \( n \geq 4 \) and \( G \) is a connected graph of order \( n \), then \( H(G) \leq D(G) + (n/2) - 1 \) and \( H(G) \leq (n/2)D(G) \). Also, a lower bound was found for trees. If \( T \) is a tree of order \( n \geq 4 \), then \( H(T) \geq D(T) + (5/6) - (n/2) \) and \( H(T) \geq ((1/2) + (1/3(n-1)))D(T) \). Thereby, Liu [17] proposed the following conjecture.

Conjecture 1. Let \( G \) be a connected graph with order \( n \geq 4 \); then,

\[
H(G) \geq D(G) + \frac{5}{6} - \frac{n}{2},
\]

and

\[
H(G) \geq \left( \frac{1}{2} + \frac{1}{3(n-1)} \right) D(G).
\]

Jerline and Michaelraj [18, 19] found a sharper bound for unicyclic graphs. They showed that if \( G \) is a unicyclic graph of order \( n \), then \( H(G) \geq D(G) + 5/3 - (n/2) \) and \( H(G) \geq ((1/2) + (2/3(n-2)))D(G) \). They introduced a family of graphs, \( U^1_{n4} \), which is a set of graphs obtained from \( C_4 \) by attaching one pendant vertex and a path of length \( n - 5 \) to two diametrically nonadjacent vertices of \( C_4 \).
(see Figure 1). Then, they proposed the following conjecture [18].

**Conjecture 2.** Let \( G \) be a simple connected graph, which is not a tree, of order \( n \geq 7 \). Then,

\[
    H(G) \geq D(G) + \frac{5n-3}{2},
\]

where equality holds if and only if \( G = U_{n,4}^{1,n-5} \).

They also show that the inequalities of the above conjecture are not true for a graph of order 6, namely, \( U_{6,4}^{1,1} \).

Suppose \( K_5^- \) is a graph of order 4 which is obtained from \( K_4 \) by deleting an edge. Also, for \( r, s \geq 0 \), let \( V_{r,s} \) be a family of graphs obtained from \( K_5^- \) by attaching two paths of lengths \( r \) and \( s \) to two nonadjacent vertices of \( K_5^- \) (see Figure 1). We will show that the inequality holds for all quasi-tree graphs except \( U_{6,4}^{1,1} \) and the graph \( U_{5,3}^{1,1} \) which is obtained by attaching two pendant vertices to two vertices of \( K_3 \). Also, the equality holds for \( V_{1,1} \).

Two main theorems of this paper are as follows.

**Theorem 1.** Let \( G \neq U_{6,4}^{1,1}, U_{5,3}^{1,1} \) be a quasi-tree graph of order \( n \geq 3 \). Then, \( H(G) \geq D(G) + 5/3 - (n/2) \). The equality holds if and only if \( G = V_{1,1} \) or \( U_{n,4}^{1,n-5} \).

**Theorem 2.** Let \( G \) be a quasi-tree graph of order \( n \geq 3 \) and \( G \neq U_{6,4}^{1,1}, U_{5,3}^{1,1} \). Then, \( H(G) \geq (1/2) + (2/3(n-2))D(G) \). The equality holds if and only if \( G = V_{1,1} \) or \( U_{n,4}^{1,n-5} \).

In Section 2, we prove the lemmas that will be used in Section 3, where we prove the main theorems.

All graphs considered in this paper are finite, undirected, connected, and simple. Let \( G \) be a graph and \( v \in V(G) \) and \( P \) a path of \( G \); then, by \( G - v \) and \( G - P \), we mean the graph obtained from \( G \) by deleting the vertex \( v \) and the vertices of \( P \), respectively. For all other notation and definitions not given here, the readers are referred to [20].

## 2. Preliminaries

**Lemma 1.** For \( x, y \geq 2 \), the two variables’ function

\[
    f(x, y) = \frac{x + 4}{x(x + 1)(2 + x)} + \frac{y + 4}{y(y + 1)(2 + y)} - \frac{2}{(x + y)(x + y - 2)},
\]

is positive.

**Proof**

\[
    f(x, y) = \frac{x + 4}{x(x + 1)(2 + x)} + \frac{y + 4}{y(y + 1)(2 + y)} - \frac{2}{(x + y)(x + y - 2)}
\]

\[
    = \frac{2}{x(x + 1)} + \frac{2}{y(y + 1)} + \frac{1}{y(y + 1)} - \frac{1}{(x + y)(x + y - 2)}
\]

\[
    = \left( \frac{1}{x(x + 1)} - \frac{1}{(x + 2)(x + 1)} \right) + \left( \frac{1}{y(y + 1)} - \frac{1}{(y + 2)(y + 1)} \right)
\]

\[
    + \left( \frac{1}{x(x + 1)} - \frac{1}{(x + y)(x + y - 2)} \right) + \left( \frac{1}{y(y + 1)} - \frac{1}{(x + y)(x + y - 2)} \right).
\]
Given \( x, y \geq 2 \), the terms inside parentheses are positive.

**Lemma 2.** \( x/(x+2) \geq 1/(5+x) + (x-1)/(2+x) \geq 11/28 \) for every \( x \geq 2 \).

**Proof.** The first inequality is valid since \( x/(x+2) = 1/(x+2) + (x-1)/(x+2) \geq 1/(5+x) + (x-1)/(2+x) \).

Let \( f(x) = 1/(5+x) + (x-1)/(2+x) \). Then, \( f'(x) = (1/(5+x)^2) + (3/(2+x)^2) > 0 \). So, \( f \) is an increasing function and \( f(x) \geq f(2) = (11/28) \) for every \( x \geq 2 \).

**3. Proof of the Main Theorems**

In this section, we will show that Conjecture 2 is true for all quasi-tree graphs. Also, in our proof, it will be shown that the equality in both inequalities hold whenever \( G \) is the graph \( V_{1,1} \).

**Lemma 3.** Let \( G \) be a quasi-tree graph of order \( n \), where \( 3 \leq n \leq 6 \), such that \( G \neq U_{6,4}^{1,1}, U_{5,3}^{1,1} \). Then,

\[
H(G) \geq D(G) + \frac{5}{3} \frac{n}{2},
\]

\[
H(G) \geq \left( \frac{1}{2} + \frac{2}{3(n-2)} \right) D(G). \tag{5}
\]

The second and third inequalities hold by Lemma 2.

If \( G - w = P_3 \), then the graph \( G \) is one of the graphs shown in Figure 4 in which their harmonic indices are calculated. Also, \( D(G) \leq 4 \), so \( D(G) + 5/3 - (n/2) \leq 2 + (2/3) and (1/2) + (2/3(n-2))D(G) \leq 2 + (2/3) \). So, for every graph both inequalities hold, except when \( G = U_{6,4}^{1,1} \). Also, the equality holds when \( G = V_{1,1} \).

If \( G - w = K_{1,3}^1 \), then the graph \( G \) is one of the graphs shown in Figure 5 in which their harmonic indices are calculated. Also, \( D(G) \leq 3 \), so \( D(G) + 5/3 - (n/2) \leq 1 + (2/3) and (1/2) + (2/3(n-2))D(G) \leq 2 \). Obviously, for every graph, both inequalities hold.

**Proof.** If \( n = 3 \), then \( G \) should be the complete graph, \( K_3 \). In this case, \( D(G) = 1 \) and, by an easy calculation, \( H(G) = (3/2) \) and both inequalities hold.

If \( n = 4 \), then, since \( K_4 \) is not a quasi-tree graph, \( D(G) > 1 \). Also, since \( G \) is not a tree, \( G \neq P_4 \) and \( D(G) = 2 \). Hence, \( D(G) + 5/3 - (n/2) = (1/2) + (2/3(n-2))D(G) = 5/3 \). So, both inequalities hold for \( n = 4 \) (see Figure 2).

Suppose \( n = 5 \) and \( w \) is the vertex that \( G - w \) is a tree. Since \( G - w \) is a tree of order 4, \( D(G - w) = 3 \) or 2. Also, since \( G \) is a quasi-tree graph, it is not a complete graph, and hence, \( D(G) = 3 \) or 2.

If \( D(G) = 3 \), then \( D(G) + 5/3 - (n/2) = (1/2) + (2/3(n-2))D(G) = 13/6 \). If \( D(G) = 2 \), then \( D(G) + 5/3 - (n/2) = (2/3(n-2))D(G) = (13/9) \). All quasi-tree graphs of order 5 and their harmonic indices are shown in Figure 3. As it is seen, all graphs hold both inequalities except when \( G = U_{5,3}^{1,1} \).

Suppose \( n = 6 \) and \( w \) is the vertex that \( G - w \) is a tree. So, \( G - w \) is one of \( P_5 \), \( K_{1,4}^1 \), or \( K_{1,3}^1 \), where \( K_{1,3}^1 \) is obtained by attaching a new pendant vertex to a pendant vertex of \( K_{1,3} \).

If \( G - w = K_{1,4}^1 \), then \( D(G - w) = 2 \). Since \( D(G) \leq D(G - w) \) and \( G \) is not \( K_6 \), so \( D(G) = 2 \), \( D(G) + 5/3 - (n/2) = (2/3) \), and \( (1/2) + (2/3(n-2))D(G) = (4/3) \). On the contrary, for every edge \( uv \) of \( G - w \), \( (2d_u + d_v) \) is at least \( (2/7) \), where \( d_u \) and \( d_v \) are the degree of \( u \) and \( v \) in \( G \), respectively. So,

\[
H(G) \geq 4 \left( \frac{2}{7} \right) + \sum_{x \in N(w)} \frac{2}{d_x + d_w} \geq \frac{8}{7} + \frac{2}{5 + d_v} + \frac{2(d_w - 1)}{2 + d_w} \geq \frac{8}{7} + \frac{11}{14} > \frac{4}{3} \tag{6}
\]

**Theorem 3.** Let \( G \neq U_{6,4}^{1,1}, U_{5,3}^{1,1} \) be a quasi-tree graph with \( n \geq 3 \) vertices. Then, \( H(G) \geq D(G) + 5/3 - (n/2) \). The equality holds if and only if \( G = V_{1,1} \) or \( G = U_{6,4}^{1,1} \).

**Proof.** By induction on \( n \), if \( n \leq 6 \), then Theorem 3 implies that the inequality is true, unless when \( G = U_{6,4}^{1,1}, U_{5,3}^{1,1} \). Also, by Theorem 3, the equality holds when \( G = V_{1,1} \).

Let \( G \) be a quasi-tree graph with \( n \geq 7 \) vertices. Suppose \( w \) is a vertex of \( G \) such that \( G - w \) is a tree. Let \( P = u_0 - u_1 - \cdots - u_q \) be the diametrical path of \( G \). There are three cases as follows.
Figure 2: Quasi-tree graphs of order 4 and their harmonic indices.

Figure 3: Quasi-tree graphs of order 5 and their harmonic indices.

Figure 4: Quasi-tree graphs of order 6 obtained from $P_5$, and their harmonic indices.

Figure 5: Quasi-tree graphs of order 6 obtained from $K_{1,3}$, and their harmonic indices.
Case 1. There exists \( t \in G - P \) such that \( d_t = 1 \). Since \( t \) is not in diametrical path of \( G \) and \( d_t = 1 \), \( D(G - t) = D(G) \) and \( G - t \) is a quasi-tree graph too. Suppose \( N(t) = \{r\} \) and \( G - t \neq U_{6,4}^{1,1} \). Then, by induction hypothesis,

\[
H(G) = H(G - t) + \frac{2}{d_r + 1} - \frac{2}{d_r + d_x - 1} + \frac{2}{d_r + d_x}
\]

\[
= H(G - t) + \frac{2}{d_t + 1} - \frac{2}{d_t(d_t + 1)} \geq H(G - t) \tag{7}
\]

If \( G - t = U_{6,4}^{1,1} \), then \( G \) is one of the graphs shown with their harmonic indices in Figure 6. In this case, \( D(G) = 4 \) and \( D(G) + 5/3 - (n/2) = (65/30) \). Hence, the inequality holds.

Case 2. Every vertex of \( G - P \) is of degree at least 2, and there exists \( t \in G - P - w \) such that \( d_t = 2 \). Similar to the previous case, \( D(G) = D(G - t) \). Suppose \( N(t) = \{r, s\} \). Note that \( d_r, d_s \geq 0 \), otherwise \( \{r, s\} \cap P = \emptyset \), and hence, \( t \in P \), a contradiction. Since \( d_t = 2 \), it is possible that \( G - t \) be a tree. There exist three subcases as follows:

Subcase 2.1. \( G - t \) is not a tree and \( r \) and \( s \) are not adjacent in \( G \). By the hypothesis, there exist at most two vertices of degree 1 in \( G \), which are \( u_0 \) and \( u_4 \). If \( u_0, u_4 \in N(r) \), then \( D(G) = 2 \), and since \( r \) and \( s \) are not adjacent, \( d(s, u_0) \geq 3 \), a contradiction. So, \( r \) has at most one neighbor of degree 1. Same argument is valid for \( s \), so

\[
H(G) = H(G - t) + \frac{2}{2 + d_r} + \frac{2}{2 + d_s} - 2 \sum_{x \in N(r)} \frac{1}{d_r - 1 + d_x} \frac{1}{d_r + d_x} \geq D(G) + \frac{5}{3} + \frac{n - 1}{2} + \frac{2}{d_r} + \frac{2}{d_s}
\]

\[
\geq D(G) + \frac{5}{3} + \frac{n}{2} \tag{8}
\]

\[
= D(G) + \frac{5}{3} + \frac{1}{2} + \frac{4(d_r - 1)}{d_r(d_r + 1)(2 + d_r)} + \frac{4(d_s - 1)}{d_r(d_s + 1)(2 + d_s)}
\]

\[
\geq D(G) + \frac{5}{3} + \frac{n}{2}
\]
If $G - t = U_{6,4}^{1,1}$, then $G$ is one of the graphs which are shown with their harmonic indices in Figure 7. In this case, $D(G) = 4$ and $D(G) + 5/3 - (n/2) = (65/30)$.

Subcase 2.2. $G - t$ is not a tree and $r$ and $s$ are adjacent in $G$. If $G - t \neq U_{6,4}^{1,1}$, then

$$\begin{align*}
H(G) & = H(G - t) + \frac{2}{d_r + 2} + \frac{2}{d_s + 2} + \frac{2}{d_r + d_s} - \frac{2}{d_r + d_s - 2} \\
& - \sum_{x \in N(r)} \frac{2}{(d_x + d_r - 1)(d_x + d_r)} - \sum_{y \in N(s)} \frac{2}{(d_y + d_s - 1)(d_y + d_s)} \\
& \geq H(G - t) + \frac{2}{d_r + 2} + \frac{2}{d_s + 2} - \frac{4}{(d_r + d_s)(d_r + d_s - 2)} - \frac{2}{d_r(d_r + 1)} - \frac{2}{d_s(d_s + 1)} \\
& \geq H(G - t) + \frac{4}{(d_r + d_s)(d_r + d_s - 2)} + \frac{2}{d_r(d_r + 1)(d_r + 2)} + \frac{2}{d_s(d_s + 1)(d_s + 2)} \\
& > D(G) + \frac{5}{3} > \frac{n}{2}
\end{align*}$$

(9)

Since $d_r, d_s \geq 2$, the last inequality is obtained from Lemma 1.

If $G - t = U_{6,4}^{1,1}$, then $G$ is the graph which is shown with its harmonic index in Figure 8. In Subcase 2.1, $D(G) + 5/3 - (n/2) = (65/30)$ and the inequality holds.

Subcase 2.3. $G - t$ is a tree. Since $G - w$ is also a tree, by counting the number of edges and vertices, it is obtained that $d_w = d_t = 2$. This means that $G$ is a unicyclic graph and as proved by Theorem 3 in [19], $H(G) \geq D(G) + 5/3 - (n/2)$, in which equality holds if $G = U_{n,4}^{1,n-5}$.

Case 3. Every vertex of $G - \{u_0, u_1, \ldots, u_d\}$ is of degree at least 2 and if $t \in V(G)$ and $d_t = 2$, then $t \notin \{u_0, u_1, \ldots, u_d\}$. Since $G - w$ is a tree, every pendant vertex of $G - w$ is in $\{u_0, u_1, \ldots, u_d\}$. So, $G - w$ is a path and $V(G) = \{u_0, u_1, \ldots, u_d\} \cup \{w\}$. Also, since $G$ is not a tree $d_w \geq 2$. If $d_w = 2$, then $G$ is a unicyclic graph and as proposed by Theorem 3 in [19], $H(G) \geq D(G) + 5/3 - (n/2)$, with equality holds if $G = U_{n,4}^{1,n-5}$. So, there exist two subcases as follows.

Subcase 3.1. $d_w = 3$. In this case, $G$ is one of the graphs in Table 1. In all cases, $H(G) \geq D(G) + 5/3 - (n/2)$. As it is shown, the equality holds when $G = V_{1,1}$.

Subcase 3.2 ($d_w > 3$). Suppose $\{u_h, u_i, u_j, u_k\} \subseteq N(w)$ such that $h < i < j < k$. If $k - h > 2$, then the diametrical path $u_1 - \cdots - u_h - \cdots - u_k - \cdots - u_d$ is longer than the path $u_1 - \cdots - u_h - w - u_k - \cdots - u_d$, a contradiction. So, $k - h \leq 2$, which is another contradiction. Hence, this case does not happen. The inequality holds in all cases and equality holds if and only if $G = V_{1,1}$ or $U_{n,4}^{1,n^5}$.

Theorem 4. Let $G \neq U_{6,4}^{1,1}, U_{5,3}^{1,1}$ be a quasi-tree graph with $n \geq 3$ vertices, then

$$H(G) \geq \left(\frac{1}{2} + \frac{2}{3(n - 2)}\right)D(G).$$

The equality holds if and only if $G = V_{1,1}$ or $U_{n,4}^{1,n^5}$.

Proof. The proof is similar to the proof of Theorem 3. By induction on $n$, if $n \leq 6$, then Theorem 3 implies that the inequality holds unless when $G = U_{6,4}^{1,1}, U_{5,3}^{1,1}$.

Let $G$ be a quasi-tree graph with $n \geq 7$ vertices. Suppose $w$ is a vertex of $G$ such that $G - w$ is a tree. Let $P = u_0 - u_1 - \cdots - u_d(\subseteq)$ be the diametrical path of $G$. Since $G - w$ is a tree, $\delta(G) \leq 2$. There exist three cases as follows.
There exists $t \in G - P$ such that $d_t = 1$. Since $t$ is not in diametrical path of $G$, $D(G) = D(G - t)$. Suppose $N(t) = r$. So, such as Case 1 in the proof of Theorem 3, if $G - t \not\in U_{k,l}^1$, then, by induction hypothesis,

$$H(G) \geq H(G - t) + \frac{2}{d_t(d_t + 1)} \left( \frac{1}{2} + \frac{2}{3(n - 3)} \right) D(G) > \left( \frac{1}{2} + \frac{2}{3(n - 2)} \right) D(G).$$

(11)

**Table 1**: All possibilities for Case 3 of Theorems 3 and 4.

<table>
<thead>
<tr>
<th>Graph</th>
<th>$H(G)$</th>
<th>$D(G) + 5/3 - (n/2)$</th>
<th>$((1/2) + (2/3(n - 2)))D(G)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_{0,0}$</td>
<td>(29/15)</td>
<td>(25/15)</td>
<td>(25/15)</td>
</tr>
<tr>
<td>$V_{0,1}$</td>
<td>(23/10)</td>
<td>(13/6)</td>
<td>(13/6)</td>
</tr>
<tr>
<td>$V_{1,1}$</td>
<td>(8/3)</td>
<td>(8/3)</td>
<td>(8/3)</td>
</tr>
<tr>
<td>$V_{0,r} r \geq 2$</td>
<td>$(D(G)/2) + (13/15)$</td>
<td>$(D(G)/2) + (2/3)$</td>
<td>$(D(G)/2) + (2/3)$</td>
</tr>
<tr>
<td>$V_{1,r} r \geq 2$</td>
<td>$(D(G)/2) + (11/15)$</td>
<td>$(D(G)/2) + (2/3)$</td>
<td>$(D(G)/2) + (2/3)$</td>
</tr>
<tr>
<td>$V_{s,r} s, r \geq 2$</td>
<td>$(D(G)/2) + (4/5)$</td>
<td>$(D(G)/2) + (2/3)$</td>
<td>$(D(G)/2) + (2/3)$</td>
</tr>
</tbody>
</table>
If $G-t = U_{6,4}^{1,1}$, then $G$ is one of the graphs which is shown with their harmonic indices in Figure 6. In this case, $D(G) = 4$ and $((1/2) + (2/3(n - 2)))D(G) = (38/15)$. Hence, the inequality holds.

Case 2. Every vertex of $G - P$ is of degree at least 2, and there exists a vertex $t \in G - P - w$ such that $d_t = 2$. From the previous case, $D(G) = D(G-t)$. Suppose $N(t) = \{r, s\}$. Since $d_t = 2$, it is possible that $G - t$ be a tree. There exist three subcases as follows.

Subcase 2.1. $G - t$ is not a tree and $r$ and $s$ are not adjacent in $G$. By the same argument as in Subcase 2.1 of Theorem 3,

$$H(G) > H(G-t) + \frac{4(d_r - 1)}{d_r(d_r + 1)(2 + d_r)} + \frac{4(d_s - 1)}{d_s(d_s + 1)(2 + d_s)} > H(G-t).$$

Subcase 2.2. $G - t$ is not a tree and $r$ and $s$ are adjacent in $G$. By Subcase 2.2 of Theorem 3,

$$H(G) \geq H(G-t) + \frac{2(d_r + 4)}{d_r(d_r + 1)(d_r + 2)} + \frac{2(d_s + 4)}{d_s(d_s + 1)(d_s + 2)} - \frac{4}{(d_r + d_s)(d_r + d_s - 2)} > H(G-t).$$

Conflicts of Interest

The authors declare that they have no conflicts of interest.

References


