On Harmonic Index and Diameter of Unicyclic Graphs

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\textbf{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 the vertex $u$ in $G$. In this work, we prove the conjecture \[ \frac{H(G)}{D(G)} \geq \frac{1}{2} + \frac{1}{3(n-1)} \] given by Jianxi Liu in 2013 when $G$ is a unicyclic graph and give a better bound \[ \frac{H(G)}{D(G)} \geq \frac{1}{2} + \frac{2}{3(n-2)} \] where $n$ is the order and $D(G)$ is the diameter of the graph $G$.

\textbf{Keywords:} Harmonic index, Diameter, Unicyclic graph.

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\section{Introduction}

Let $G = (V,E)$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex $v$ of $G$ is denoted by $d(v)$. If $u,v \in V(G)$, then the distance between $u$ and $v$ is the length of a shortest $u - v$ path in $G$. The eccentricity of a vertex $v$ is the greatest distance from $v$ to any other vertex of $G$. The diameter of a graph is the maximum over eccentricities of all vertices of the graph and it is denoted by $D(G)$. For a graph $G$, the harmonic index $H(G)$ is defined as $H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}$. As far as

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we know, this index first appeared in [4]. Zhong found the minimum and maximum values of the harmonic index for simple connected graphs, trees and unicyclic graphs and characterized the corresponding extremal graphs[8][9]. Wu et al. gave a best possible lower bound for the harmonic index of a triangle-free graph with minimum degree at least two and characterized the extremal graphs[7]. Deng et al. considered the relation connecting the harmonic index \( H(G) \) and the chromatic number \( \chi(G) \) and proved that \( \chi(G) \leq 2H(G) \) by using the effect of removal of a minimum degree vertex on the harmonic index[3]. Mehdi Sabzevari et al. gave the exact formula for Merrifield Simmons and Hosoya indices of some special graphs namely ladder graph, prism graph and book graph[6]. Zohreh Bagheria et al. computed the edge-Szeged and vertex-PI indices of some important classes of benzenoid systems[10]. Liu proved that \( \frac{H(T) - D(T)}{2} \geq \frac{5}{6} - \frac{n}{2} \) and \( \frac{H(T)}{D(T)} \geq \frac{1}{2} + \frac{1}{3(n-1)} \) for \( n \)-vertex tree \( T \) with equality for path and proposed it as a conjecture for any connected graph of order \( n \) [5]. The first part of the above conjecture was proved in [1] for unicyclic graphs. In this work, we prove the second part of the conjecture viz. \( \frac{H(G)}{D(G)} \geq \frac{1}{2} + \frac{2}{3(n-2)} \) for \( n \geq 7 \), when \( G \) is a unicyclic graph.

We conclude this section with some notations and terminology. Let \( G = (V,E) \) be a simple connected graph with vertex set \( V(G) \) and edge set \( E(G) \). If \( d(v) = 1 \), then \( v \) is said to be a pendant vertex of \( G \). The edge incident with \( v \) is referred to as pendant edge and the vertex adjacent to \( v \) is referred as the support vertex of \( v \). The set of neighbours of \( v \) is denoted by \( N(v) \). A diametrical path of a graph is a shortest path whose length is equal to the diameter of the graph. As usual, \( C_n \) and \( P_n \) denote the cycle and the path on \( n \) vertices, respectively. In a cycle \( C_n \), two vertices, say \( u \) and \( v \) are said to be diametrically opposite, if \( d(u,v) = \frac{n}{2} \), when \( n \) is even and \( d(u,v) = \frac{n-1}{2} \), when \( n \) is odd. Let \( U_{n,l}^x \) be a unicyclic graph obtained from a cycle \( C_l \) by attaching two paths \( P_x \) and \( P_y \) to two diametrically opposite vertices of \( C_l \) such that \( n = l + x + y \). For other notations in graph theory, may be consulted [2].

2. Basic Results

Lemma 1. The function \( f(x) = \frac{1}{u + x} - \frac{1}{u + x - 1} \) is an increasing function on \( x \) for \( x \geq 1 \) and \( u \geq 0 \).

Lemma 2. Let \( v \) be a pendant vertex of a connected graph \( G \). Then \( H(G) > H(G - v) \).
Proof. Let $u$ be the support vertex of $v$. Then
\[
H(G) - H(G - v) = \frac{2}{d(u) + 1} + 2 \sum_{w \in N(u) - \{v\}} \left( \frac{1}{d(u) + d(w)} - \frac{1}{d(u) + d(w) - 1} \right) \
\geq \frac{2}{d(u) + 1} + 2(d(u) - 1) \left( \frac{1}{d(u) + 1} - \frac{1}{d(u)} \right) \quad \text{by lemma 1} \
= \frac{2}{d(u)(d(u) + 1)} \
\geq 0.
\]
Hence $H(G) > H(G - v)$. \hfill \Box

Analysing the unicyclic graphs and its diametrical path, we have the following observation.

**Observation:**
If $G \not\cong C_n$ is a unicyclic graph on $n$ vertices, then at least one of the end vertices of the diametrical path of $G$ must be a pendant vertex.

3. **Main Result**

In this section, we give the sharp lower bound of the relationship involving the harmonic index and diameter of connected unicyclic graphs.

**Theorem 3.1.** Let $G$ be a unicyclic graph of order $n \geq 7$ and diameter $D(G)$. Then
\[
\frac{H(G)}{D(G)} \geq \frac{1}{2} + \frac{2}{3(n - 2)},
\]
where equality holds if and only if $G \cong U_{n,4}^{1,n-5}$.

**Proof.**

**Case 1:** Let $G \cong C_n$. Then $H(G) = \frac{n}{2}$. If $n$ is even, then $D(G) = \frac{n}{2}$. Hence
\[
\frac{H(G)}{D(G)} = 1 \geq \frac{1}{2} + \frac{2}{3(n - 2)}. \quad \text{If } n \text{ is odd, then } D(G) = \frac{n - 1}{2}. \quad \text{Hence}
\]
\[
\frac{H(G)}{D(G)} = 1 + \frac{1}{n - 1} \geq \frac{1}{2} + \frac{2}{3(n - 2)}.
\]

**Case 2:** Let $G \not\cong C_n$. Then $G$ has at least one pendant vertex. Also by the observation, at least one of the end vertices of the diametrical path of $G$ is a pendant vertex. Let $P$ be a diametrical path of $G$. Now continue to remove pendant vertices from $G$ so that $P$ remains its diametrical path. Let the resulting graph be $G'$ and $v_1, v_2, \ldots, v_k$ be the vertices in the order they were deleted. Then we have,
\[
H(G) > H(G - v_1) > \cdots > H(G - \bigcup_{i=1}^{k} v_i) = H(G')
\]
by lemma 2 and
\[
D(G) = D(G - v_1) = \cdots = D(G - \bigcup_{i=1}^{k} v_i) = D(G').
\]
Clearly $G'$ is also a unicyclic graph consisting of a cycle of length $l$ together with at most two pendant paths, say $P_x$ and $P_y$ incident with two vertices of $C_l$, say $u$ and $v$, such that $n = k + l + x + y$.

**Subcase 2.1:** Let $x = 0$ and $y = 1$. In this case, $G' \cong U^0_{n-k,n-k-1}$. Then $H(G') = \frac{n-k}{2} - \frac{1}{5}$. If $l$ is even, then $D(G') = \frac{n-k+1}{2}$. Hence

\[
\frac{H(G')}{D(G')} = \frac{5n-5k-2}{5(n-k+1)} = 1 - \frac{7}{5(n-k+1)} \\
\geq \frac{1}{2} + \frac{2}{3(n-2)}, \quad \text{since} \quad n-k \geq 5.
\]

If $l$ is odd, then $D(G') = \frac{n-k}{2}$. Hence

\[
\frac{H(G')}{D(G')} = \frac{5n-5k-2}{5(n-k)} = 1 - \frac{2}{5(n-k)} \\
\geq \frac{1}{2} + \frac{2}{3(n-2)}, \quad \text{since} \quad n-k \geq 4.
\]

**Subcase 2.2:** Let $x = 0$ and $y \geq 2$. In this case, $H(G') = \frac{n-k}{2} - \frac{2}{15}$. If $l$ is even, then $D(G') = \frac{n-k+y}{2}$. Hence

\[
\frac{H(G')}{D(G')} = \frac{15n-15k-4}{15(n-k+y)} = 1 - \frac{15y+4}{15(n-k+y)} \\
= \frac{1}{2} + \frac{15l-8}{30(2(n-k)-l)} \\
\geq \frac{1}{2} + \frac{2}{3(n-2)}, \quad \text{since} \quad n-k = l+y \quad \text{and} \quad l \geq 4.
\]
If \( l \) is odd, then \( D(G') = \frac{n - k + y - 1}{2} \). Hence

\[
\begin{align*}
\frac{H(G')}{D(G')} &= \frac{15n - 15k - 4}{15(n - k + y - 1)} \\
&= 1 - \frac{15y - 11}{15(n - k + y - 1)} \\
&= 1 + \frac{15l + 7}{2 + 30(2(n - k) - l - 1)} \\
&\geq \frac{1}{2} + \frac{2}{3(n - 2)}, \quad \text{since } n - k = l + y \text{ and } l \geq 3.
\end{align*}
\]

\textbf{Subcase 2.3:} Let \( x = 1, y = 1 \). If \( u \) and \( v \) are non adjacent, then \( G' \cong U_{n-k, l}^{1,1} \).

Clearly \( H(G') = \frac{n - k}{2} - \frac{2}{5} \). If \( l \) is even, then \( D(G') = \frac{n - k}{2} + 1 \). Hence

\[
\begin{align*}
\frac{H(G')}{D(G')} &= \frac{5n - 5k - 4}{5(n - k + 2)} \\
&= 1 - \frac{14}{5(n - k + 2)} \\
&= 1 - \frac{14}{5(l + 4)}, \quad \text{since } n - k = l + 2 \\
&\geq \frac{1}{2} + \frac{2}{3(n - 2)}.
\end{align*}
\]

If \( l \) is odd, then \( D(G') = \frac{n - k + 1}{2} \). Hence

\[
\begin{align*}
\frac{H(G')}{D(G')} &= \frac{5n - 5k - 4}{5(n - k + 1)} \\
&= 1 - \frac{9}{5(n - k + 1)} \\
&= 1 - \frac{9}{5(l + 3)}, \quad \text{since } n - k = l + 2 \\
&\geq \frac{1}{2} + \frac{2}{3(n - 2)}.
\end{align*}
\]

\textbf{Subcase 2.4:} Let \( x = 1 \) and \( y \geq 2 \). If \( u \) and \( v \) are adjacent, the only possible graph is shown in figure 1.

\begin{figure}[h]
\centering
\begin{tikzpicture}
\node (a) at (0,0) {\(G'\)};
\node (b) at (1,0) {\ldots};
\node (c) at (-1,0) {\ldots};
\draw (a) -- (b);
\end{tikzpicture}
\caption{\(G'\)}
\end{figure}
Clearly $H(G') = \frac{n - k}{2} - \frac{3}{10}$ and $D(G') = y + 2$. Hence

$$
\frac{H(G')}{D(G')} = \frac{5n - 5k - 3}{10(y + 2)}
\geq \frac{5n - 5k - 3}{10(n - 2)}
= 1 - \frac{5n + 5k - 17}{10(n - 2)}
\geq \frac{1}{2} + \frac{2}{3(n - 2)}.
$$

If $u$ and $v$ are non adjacent, then $G' \cong U_{n-k,l}^{1,y}$. Clearly $H(G') = \frac{n - k}{2} - \frac{1}{3}$. If $l$ is even, then $D(G') = \frac{n - k + y + 1}{2}$. Hence

$$
\frac{H(G')}{D(G')} = \frac{3n - 3k - 2}{3(n - k + y + 1)}
= 1 - \frac{3y + 5}{3(n - k + y + 1)}
\geq \frac{1}{2} + \frac{2}{3(n - 2)}.
$$

If $l$ is odd, then $D(G') = \frac{n - k + y}{2}$. Hence

$$
\frac{H(G')}{D(G')} = \frac{3n - 3k - 2}{3(n - k + y)}
= 1 - \frac{3y + 2}{3(n - k + y)}
\geq \frac{1}{2} + \frac{2}{3(n - 2)}.
$$

**Subcase 2.5:** Let $x \geq 2$ and $y \geq 2$. If $u$ and $v$ are adjacent, then $H(G') = \frac{n - k}{2} - \frac{7}{30}$ and $D(G') = x + y + 1 = n - k - l + 1$. Hence

$$
\frac{H(G')}{D(G')} = \frac{15n - 15k - 7}{30(n - k - l + 1)}
\geq \frac{1}{2} + \frac{2}{3(n - 2)}.
$$
If $u$ and $v$ are non adjacent, then $H(G') = H(U^{x,y}_{n-k,l}) = \frac{n-k - 4}{15}$ and $D(G') \leq D(U^{x,y}_{n-k,l})$. If $l$ is even, $D(G') \leq \frac{n-k + x + y}{2}$. Hence

\[
\frac{H(G')}{D(G')} \geq \frac{15n - 15k - 8}{15(n-k+x+y)} \geq \frac{1}{2} + \frac{15l - 16}{30(2(n-k) - l)} \geq \frac{1}{2} + \frac{2}{3(n-2)}.
\]

If $l$ is odd, $D(G') \leq \frac{n-k + x + y - 1}{2}$. Hence

\[
\frac{H(G')}{D(G')} \geq \frac{15n - 15k - 8}{15(n-k+x+y-1)} \geq \frac{1}{2} + \frac{15l - 1}{30(2(n-k) - l - 1)} \geq \frac{1}{2} + \frac{2}{3(n-2)}.
\]

For proving the equality, assume that $\frac{H(G)}{D(G)} = \frac{1}{2} + \frac{2}{3(n-2)}$. Since $D(G) \leq n-2$, $\frac{H(G)}{n-2} \leq \frac{H(G)}{D(G)}$, for all $G$. So our search is to find that $G$, for which $D(G) = n-2$ and $\frac{H(G)}{D(G)} = \frac{1}{2} + \frac{2}{3(n-2)}$. $U^{0,n-3}_{n,3}$, $U^{1,n-4}_{n,3}$, $U^{2,n-5}_{n,3}$, $U^{0,n-4}_{n,4}$, $U^{1,n-5}_{n,4}$ and $U^{2,n-6}_{n,4}$ are the unicyclic graphs with $D(G) = n-2$. But $U^{1,n-5}_{n,4}$ is the only graph that satisfies the equality. Hence $G \cong U^{1,n-5}_{n,4}$ and it is easy to check

\[
\frac{H(U^{1,n-5}_{n,4})}{D(U^{1,n-5}_{n,4})} = \frac{1}{2} + \frac{2}{3(n-2)}.
\]

\[\square\]

Remark 3.1. If $n \leq 6$, this lower bound is not true. One such graph is shown in figure 2. For this graph, $\frac{H(G)}{D(G)} = \frac{13}{20} \leq \frac{2}{3} = \frac{1}{2} + \frac{2}{3(n-2)}$.

This result seems true for any connected graph of order $n$, that is not a tree, and we propose it as a conjecture as follows.
Conjecture 1. Let $G$ be a simple connected graph, that is not a tree, of order $n \geq 7$ and diameter $D(G)$. Then $H(G) - D(G) \geq \frac{5}{3} - \frac{n}{2}$ and $\frac{H(G)}{D(G)} \geq \frac{1}{2} + \frac{2}{3(n - 2)}$, where equality holds if and only if $G \cong U_{n,4}^{1,n-5}$.

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