On Harmonic Index and Diameter of Unicyclic Graphs

J. Amalorpava Jerline\textsuperscript{a,*}, L. Benedict Michaelraj\textsuperscript{b}

\textsuperscript{a}Department of Mathematics, Holy Cross College, Trichy 620 002, India.
\textsuperscript{b}Department of Mathematics, St. Joseph’s College, Trichy 620 002, India.

E-mail: jermaths@gmail.com
E-mail: benedict.mraj@gmail.com

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 $G$.

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1. 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
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 $H(T) - D(T) \geq \frac{5}{6} - \frac{n}{2}$ 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 $U_{x,y}^{n,l}$ 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
\[
H(G) - H(G - v) = \frac{2}{d(u) + 1} + 2 \sum_{w \in N(u) - \{v\}} \left( \frac{1}{d(u) + d(w)} - \frac{1}{d(u) + d(w) - 1} \right) \\
\geq \frac{2}{d(u) + 1} + 2(d(u) - 1) \left( \frac{1}{d(u) + 1} - \frac{1}{d(u)} \right) \text{ by lemma 1} \\
= \frac{2}{d(u)(d(u) + 1)} \\
> 0
\]
Hence $H(G) > H(G - v)$. □

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
\[
\frac{H(G)}{D(G)} = 1 \geq \frac{1}{2} + \frac{2}{3(n - 2)}. \quad \text{If } n \text{ is odd, then } D(G) = \frac{n - 1}{2}. \text{ Hence}
\]
\[
\frac{H(G)}{D(G)} = 1 + \frac{1}{n - 1} \geq \frac{1}{2} + \frac{2}{3(n - 2)}.
\]

**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, $G' \cong U^{n-1}_{n-k, n-k-1}$. 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

\[
\frac{H(G')}{D(G')} = \frac{15n - 15k - 4}{15(n - k + y - 1)}
\]

\[
= 1 - \frac{15y - 11}{15(n - k + y - 1)}
\]

\[
= 1 + \frac{15l + 7}{2 + 30(2(n - k) - l - 1)}
\]

\[
\geq \frac{1}{2} + \frac{2}{3(n - 2)}, \text{ since } n - k = l + y \text{ and } l \geq 3.
\]

**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

\[
\frac{H(G')}{D(G')} = \frac{5n - 5k - 4}{5(n - k + 2)}
\]

\[
= 1 - \frac{14}{5(n - k + 2)}
\]

\[
= 1 - \frac{14}{5(l + 4)}, \text{ since } n - k = l + 2
\]

\[
\geq \frac{1}{2} + \frac{2}{3(n - 2)}.
\]

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

\[
\frac{H(G')}{D(G')} = \frac{5n - 5k - 4}{5(n - k + 1)}
\]

\[
= 1 - \frac{9}{5(n - k + 1)}
\]

\[
= 1 - \frac{9}{5(l + 3)}, \text{ since } n - k = l + 2
\]

\[
\geq \frac{1}{2} + \frac{2}{3(n - 2)}.
\]

**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.
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 $H(G') = H(U_{n-k,l}^{x,y}) = \frac{n-k}{2} - \frac{4}{15}$ and $D(G') \leq D(U_{n-k,l}^{x,y})$. If $l$ is even, $D(G') \leq \frac{n-k+x+y}{2}$. Hence
\[
\frac{H(G')}{D(G')} \geq \frac{15n-15k-8}{15(n-k+x+y)}
= \frac{15n-15k-8}{15(2(n-k)-l)}
= \frac{1}{2} + \frac{15l-16}{30(2(n-k)-l)}
\geq \frac{1}{2} + \frac{2}{3(n-2)}.
\]

If $l$ is odd, $D(G') \leq \frac{n-k+x+y-1}{2}$. Hence
\[
\frac{H(G')}{D(G')} \geq \frac{15n-15k-8}{15(n-k+x+y-1)}
= \frac{15n-15k-8}{15(2(n-k)-l-1)}
= \frac{1}{2} + \frac{15l-1}{30(2(n-k)-l-1)}
\geq \frac{1}{2} + \frac{2}{3(n-2)}.
\]

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 $\frac{H(G)}{D(G)} = \frac{1}{2} + \frac{2}{3(n-2)}$. $U_{n,3}^{0,n-3}$, $U_{n,3}^{1,n-4}$, $U_{n,3}^{2,n-5}$, $U_{n,4}^{0,n-4}$, $U_{n,4}^{1,n-5}$ and $U_{n,4}^{2,n-6}$ are the unicyclic graphs with $D(G) = n-2$. But $U_{n,4}^{1,n-5}$ is the only graph that satisfies the equality. Hence $G \cong U_{n,4}^{1,n-5}$ and it is easy to check $\frac{H(U_{n,4}^{1,n-5})}{D(U_{n,4}^{1,n-5})} = \frac{1}{2} + \frac{2}{3(n-2)}$.

\[\square\]

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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References