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On Harmonic Index and Diameter of Unicyclic Graphs

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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 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.

Keywords: Harmonic index, Diameter, Unicyclic graph.

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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

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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 $H(T) - D(T) \geq \frac{5}{6} - \frac{n}{2}$ 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 $U_{n,l}^{x,y}$ 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* $H(G) > H(G - v)$.

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Proof. Let u be the support vertex of v. Then

$$\begin{aligned} H(G) - H(G-v) &= \frac{2}{d(u)+1} + 2\sum_{w \in N(u)-\{v\}} \left(\frac{1}{d(u)+d(w)} - \frac{1}{d(u)+d(w)-1} \right) \\ &\geq \frac{2}{d(u)+1} + 2(d(u)-1)\left(\frac{1}{d(u)+1} - \frac{1}{d(u)} \right) \quad by \quad lemma \quad 1 \\ &= \frac{2}{d(u)(d(u)+1)} \\ &> 0 \end{aligned}$$

Hence $H(G) > H(G-v)$. □

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

Observation:

If $G \ncong C_n$ 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 $\frac{H(G)}{D(G)} = 1 \geq \frac{1}{2} + \frac{2}{3(n-2)}$. If n is odd, then $D(G) = \frac{n-1}{2}$. Hence $\frac{H(G)}{D(G)} = 1 + \frac{1}{n-1} \geq \frac{1}{2} + \frac{2}{3(n-2)}$.

Case 2: Let $G \ncong C_n$. 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

$$D(G) = D(G-v_1) = \cdots = D(G - \bigcup_{i=1}^{k} v_i) = D(G').$$

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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, $G' \cong U^{0,1}_{n-k,n-k-1}$. Then $H(G') = \frac{n-k}{2} - \frac{1}{5}$. If l is even, then $D(G') = \frac{n-k+1}{2}$. Hence

$$
\begin{aligned}
\frac{H(G')}{D(G')} &= \frac{5n-5k-2}{5(n-k+1)}\\
&= 1 - \frac{7}{5(n-k+1)}\\
&\geq \frac{1}{2} + \frac{2}{3(n-2)}, \quad \textit{since} \quad n-k \geq 5.
\end{aligned}
$$

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

$$
\begin{aligned}
\frac{H(G')}{D(G')} &= \frac{5n-5k-2}{5(n-k)}\\
&= 1 - \frac{2}{5(n-k)}\\
&\geq \frac{1}{2} + \frac{2}{3(n-2)}, \quad \textit{since} \quad n-k \geq 4.
\end{aligned}
$$

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

$$
\begin{aligned}
\frac{H(G')}{D(G')} &= \frac{15n-15k-4}{15(n-k+y)}\\
&= 1 - \frac{15y+4}{15(n-k+y)}\\
&= \frac{1}{2} + \frac{15l-8}{30(2(n-k)-l)}\\
&\geq \frac{1}{2} + \frac{2}{3(n-2)}, \quad \textit{since} \quad n-k = l+y \quad \textit{and} \quad l \geq 4.
\end{aligned}
$$

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

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

Subcase 2.3: Let $x=1, y=1$. If u and v are non adjacent, then $G' \cong U^{1,1}_{n-k,l}$. Clearly $H(G') = \frac{n-k}{2} - \frac{2}{5}$. If l is even, then $D(G') = \frac{n-k}{2}+1$. Hence

$$\begin{aligned}\frac{H(G')}{D(G')} &= \frac{5n-5k-4}{5(n-k+2)}\\ &= 1-\frac{14}{5(n-k+2)}\\ &= 1-\frac{14}{5(l+4)}, \quad \textit{since} \quad n-k=l+2\\ &\geq \frac{1}{2}+\frac{2}{3(n-2)}.\end{aligned}$$

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

$$\begin{aligned}\frac{H(G')}{D(G')} &= \frac{5n-5k-4}{5(n-k+1)}\\ &= 1-\frac{9}{5(n-k+1)}\\ &= 1-\frac{9}{5(l+3)}, \quad \textit{since} \quad n-k=l+2\\ &\geq \frac{1}{2}+\frac{2}{3(n-2)}.\end{aligned}$$

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.

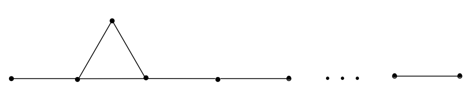

FIGURE 1. G'

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Clearly $H(G') = \frac{n-k}{2} - \frac{3}{10}$ and $D(G') = y+2$. Hence

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

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

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

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

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

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

$$\begin{aligned}\frac{H(G')}{D(G')} &= \frac{15n-15k-7}{30(n-k-l+1)}\\ &\geq \frac{1}{2} + \frac{2}{3(n-2)}.\end{aligned}$$

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

$$\begin{aligned}\frac{H(G')}{D(G')} &\geq \frac{15n-15k-8}{15(n-k+x+y)}\\ &= \frac{15n-15k-8}{15(2(n-k)-l)}\\ &= \frac{1}{2} + \frac{15l-16}{30(2(n-k)-l)}\\ &\geq \frac{1}{2} + \frac{2}{3(n-2)}.\end{aligned}$$

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

$$\begin{aligned}\frac{H(G')}{D(G')} &\geq \frac{15n-15k-8}{15(n-k+x+y-1)}\\ &= \frac{15n-15k-8}{15(2(n-k)-l-1)}\\ &= \frac{1}{2} + \frac{15l-1}{30(2(n-k)-l-1)}\\ &\geq \frac{1}{2} + \frac{2}{3(n-2)}.\end{aligned}$$

For proving the equality, assume that $\dfrac{H(G)}{D(G)} = \dfrac{1}{2} + \dfrac{2}{3(n-2)}$. Since $D(G) \leq n-2$, $\dfrac{H(G)}{n-2} \leq \dfrac{H(G)}{D(G)}$, for all G. So our search is to find that G, for which $D(G) = n-2$ and $\dfrac{H(G)}{D(G)} = \dfrac{1}{2} + \dfrac{2}{3(n-2)}$. $U^{0,n-3}_{n.3}$, $U^{1,n-4}_{n,3}$, $U^{2,n-5}_{n,3}$, $U^{0,n-4}_{n,4}$, $U^{1,n-5}_{n,4}$ *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 $\dfrac{H(U^{1,n-5}_{n,4})}{D(U^{1,n-5}_{n,4})} = \dfrac{1}{2} + \dfrac{2}{3(n-2)}$.

□

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

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.

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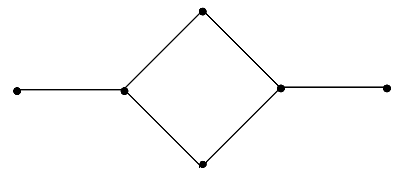

FIGURE 2. G

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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