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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.

**2000 Mathematics subject classification:** 05C07, 05C12.

### 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  $H(G) > H(G - v)$ .*

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

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

Hence  $H(G) > H(G - v)$ .  $\square$

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  $\frac{H(G)}{D(G)} = 1 \geq \frac{1}{2} + \frac{2}{3(n-2)}$ . 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  $G \not\cong C_n$ . 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  $v_1, v_2, \dots, v_k$  be the vertices in the order they were deleted. Then we have,

$$H(G) > H(G - v_1) > \dots > H(G - \bigcup_{i=1}^k v_i) = H(G')$$

by lemma 2 and

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

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,  $G' \cong U_{n-k, n-k-1}^{0,1}$ . Then

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

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

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

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

**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

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

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

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

**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

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

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

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

**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.  $G'$

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

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

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

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

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

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

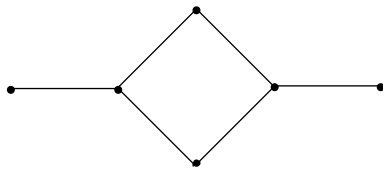
If  $l$  is odd,  $D(G') \leq \frac{n - k + x + y - 1}{2}$ . Hence

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

For proving the equality, assume that  $\frac{H(G)}{D(G)} = \frac{1}{2} + \frac{2}{3(n-2)}$ . 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  $\frac{H(U_{n,4}^{1,n-5})}{D(U_{n,4}^{1,n-5})} = \frac{1}{2} + \frac{2}{3(n-2)}$ . □

*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.

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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