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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 trianglefree 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  $H(T) - D(T) \ge \frac{5}{6} - \frac{n}{2}$  and  $\frac{H(T)}{D(T)} \ge \frac{1}{2} + \frac{1}{3(n-1)}$  for *n*-vertex tree Twith 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.  $\frac{H(G)}{D(G)} \ge \frac{1}{2} + \frac{2}{3(n-2)}$  for  $n \ge 7$ , 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 v vertices, respectively. In a cycle  $C_n$ , two vertices, say v and v are said to be diametrically opposite, if v if v is even and v are said to be diametrically opposite, if v if v is even and v are said to be v if v is odd. Let v if v is a unicyclic graph obtained from a cycle v is v attaching two paths v and v is two diametrically opposite vertices of v is uch that v is v if v is v in v

## 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  $x \ge 1$  and  $u \ge 0$ .

**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

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

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

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,

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

by lemma 2 and

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

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

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

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

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

**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

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

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

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

**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

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

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

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

**Subcase 2.4:** Let x = 1 and  $y \ge 2$ . 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

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

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

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

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

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

Subcase 2.5: Let  $x \ge 2$  and  $y \ge 2$ . 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

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

If u and v are non adjacent, then  $H(G')=H(U^{x,y}_{n-k,l})=\frac{n-k}{2}-\frac{4}{15}$  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

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

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

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

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.

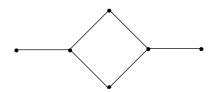


Figure 2. G

**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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