ON THE HARMONIC INDEX AND DIAMETER OF UNICYCLIC GRAPHS

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Communicated by Vasile Brînzănescu

The harmonic index of a graph G is defined as $H(G) = \sum_{uv \in E(G)} \frac{2}{d(u)+d(v)}$, where $E(G)$ is the edge set of G, $d(u)$ and $d(v)$ are the degrees of vertices u and v, respectively. A. Jerline and B. Michaelraj proved that if G is a unicyclic graph of order $n \geq 7$ and diameter $D(G)$, then $H(G) - D(G) \geq \frac{5}{3} - \frac{n}{2}$ (see [1]) and $\frac{H(G)}{D(G)} \geq \frac{1}{2} + \frac{2}{3(n-2)}$ (see [2]). We prove a stronger result by presenting sharp lower bounds on the harmonic index of unicyclic graphs with respect to diameter $D(G)$ for every $D(G) \geq 2$. We show that if G is any unicyclic graph of order $n \geq 7$ and diameter $D(G) \geq 2$, then $H(G) \geq \frac{D(G)}{2} + \frac{2}{3}$ and the bound is best possible. Results obtained by A. Jerline and B. Michaelraj are corollaries of our bound.

AMS 2010 Subject Classification: 05C35, 05C07, 05C12.

Key words: harmonic index, unicyclic graph, diameter, degree.

1. INTRODUCTION

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The order n of a graph G is the number of vertices of G. The degree of a vertex $v \in V(G)$, $d(v)$, is the number of edges incident with v. A pendant vertex is a vertex of degree one. The distance between two vertices is the number of edges in a shortest path connecting them and the diameter $D(G)$ of G is the distance between any two furthest vertices in G. A diametral path is a shortest path in G connecting two vertices whose distance is $D(G)$. A unicyclic graph is a connected graph containing exactly one cycle. A subgraph G' of a graph G is a graph whose set of vertices is a subset of $V(G)$ and set of edges is a subset of $E(G)$.

Topological indices have been used and have been shown to give a high degree of predictability of pharmaceutical properties. The harmonic index of a graph G is defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u)+d(v)}.$$

This index has been extensively studied. Zhong [8, 9] gave lower and upper bounds on the harmonic indices for simple connected graphs, trees and unicyclic graphs of given order. Wu, Tang and Deng [7] presented a lower bound for the harmonic index of graphs with minimum degree at least 2. Deng *et al.* [3] considered the relation between the harmonic index and the chromatic number of a graph.

Lv, Li and Shiu [6] determined the graph with minimum harmonic index among all unicyclic graphs with a given matching number. Zhong and Cui [10] presented the minimum and maximum harmonic indices for unicyclic graphs with given girth. The harmonic index of unicyclic graphs was studied also in [4]. Liu [5] conjectured that for any connected graph G of order $n \geq 4$ and diameter $D(G)$, we have

$$H(G) - D(G) \geq \frac{5}{6} - \frac{n}{2} \quad \text{and} \quad \frac{H(G)}{D(G)} \geq \frac{1}{2} + \frac{1}{3(n-1)}.$$

Liu [5] proved that this conjecture is true for trees and A. Jerline and B. Michaelraj [1, 2] proved the conjecture for unicyclic graphs.

THEOREM 1.1 ([1]). *Let G be a unicyclic graph of order $n \geq 7$ and diameter $D(G)$. Then*

$$H(G) - D(G) \geq \frac{5}{3} - \frac{n}{2}.$$

THEOREM 1.2 ([2]). *Let G be a unicyclic graph of order $n \geq 7$ and diameter $D(G)$. Then*

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

We prove a stronger result than Theorems 1.1 and 1.2. We show that for any unicyclic graph of diameter $D(G) \geq 5$, we have $H(G) \geq \frac{D(G)}{2} + \frac{2}{3}$ and the bound is best possible. We also present sharp bounds on the harmonic index of unicyclic graphs with respect to diameter $D(G)$ for $D(G) = 2, 3$ and 4. Theorems 1.1 and 1.2 are corollaries of our results.

2. RESULTS

We use Lemma 2.1 in the proofs of Theorems 2.1 and 2.2. Let us denote by $i(G)$ the number of pendant vertices in a graph G.

LEMMA 2.1. *Let G be any unicyclic graph and let U be a diametral path of G. If G contains a pendant vertex v not in U, then there is a unicyclic graph $G' \subset G$ not containing v, such that $D(G') = D(G)$, $i(G') = i(G) - 1$ and $H(G') < H(G)$.*

Proof. Let U be a diametral path of G and let $v \in V(G)$ be a pendant vertex not in U. We denote by u the closest vertex to v which is not of degree 2. Let G' be a subgraph of G obtained by the removal of the path connecting u and v from G. Let u' be the neighbour of u on the $u-v$ path (if the path has only one edge, then $u' = v$). Clearly, G' is a unicyclic graph, $D(G') = D(G)$ and $i(G') = i(G) - 1$. Moreover,

$$H(G) - H(G') \geq \frac{2}{d(u)+1} + \sum_{w \in N(u)\setminus\{u'\}} \left(\frac{2}{d(u)+d(w)} - \frac{2}{d(u)+d(w)-1} \right),$$

since the Harmonic index of the path uv is at least $\frac{2}{d(u)+1}$. Note that $\frac{1}{d(u)+d(w)} - \frac{1}{d(u)+d(w)-1} \geq \frac{1}{d(u)+1} - \frac{1}{d(u)}$ for every $w \in N(u) \setminus \{u'\}$, thus we obtain

$$H(G) - H(G') \geq \frac{2}{d(u)+1} + (d(u)-1)\left(\frac{2}{d(u)+1} - \frac{2}{d(u)} \right),$$

which means that $H(G) > H(G')$. $\square$

From Lemma 2.1 it follows that for any unicyclic graph G, if U is a diametral path of G, then there is a unicyclic graph $G' \subset G$ containing only pendant vertices of U, where $D(G') = D(G)$ and $H(G') < H(G)$.

Let us present a bound on the harmonic index of any unicyclic graph of diameter at least 5.

THEOREM 2.1. *Let G be any unicyclic graph of diameter $D(G) \geq 5$. Then $H(G) \geq \frac{D(G)}{2} + \frac{2}{3}$ and the bound is best possible.*

Proof. We distinguish a few cases.

Case 1: G does not contain any pendant vertex.

Then G is the cycle either with $2D(G)$ or $2D(G)+1$ vertices, which implies that $H(G) \geq 2D(G)(\frac{2}{4}) = D(G) > \frac{D(G)}{2} + \frac{2}{3}$.

Case 2: G contains one pendant vertex.

Then G consists of the cycle C_k of length $k \geq 3$ and the path P having $p \geq 1$ edges, where $C_k \cap P$ consists of one vertex which has degree 3 in G. This degree will be included in the computation of $H(C_k)$ and $H(P)$. We have $H(G) = H(C_k) + H(P)$, where

$$H(C_k) = \sum_{uv \in E(C_k)} \frac{2}{d_G(u)+d_G(v)} = (k-2)\frac{2}{4} + 2\left(\frac{2}{5}\right) = \frac{k}{2} - \frac{1}{5}.$$

and

$$H(P) = \sum_{uv \in E(P)} \frac{2}{d_G(u)+d_G(v)} = (p-2)\frac{2}{4} + \frac{2}{3} + \frac{2}{5} = \frac{p}{2} + \frac{1}{15}$$

if $p \geq 2$, and $H(P) = \frac{1}{2}$ if $p = 1$. So $H(P) \geq \frac{p}{2}$ for every $p \geq 1$ and the equality holds if $p = 1$.

If $k \geq 4$, then $D(G) \leq \frac{k}{2} + p$ and

$$H(G) \geq \frac{k}{2} - \frac{1}{5} + \frac{p}{2} \geq \frac{D(G)}{2} + \frac{k}{4} - \frac{1}{5} \geq \frac{D(G)}{2} + \frac{4}{5}.$$

If $k = 3$, then $D(G) = p + 1$ and

$$H(G) \geq \frac{3}{2} - \frac{1}{5} + \frac{p}{2} = \frac{D(G)}{2} + \frac{4}{5} > \frac{D(G)}{2} + \frac{2}{3}.$$

Case 3: G contains 2 pendant vertices.

Then G consists of the cycle C_k of length $k \geq 3$ and two paths P_1 and P_2 having $p_1 \geq 1$ and $p_2 \geq 1$ edges, respectively. We can assume that $C_k \cap P_1$ consists of one vertex and P_2 is attached either to an internal vertex of P_1 or to a vertex of C_k.

Case 3a: $P_1 \cap P_2 = \emptyset$.

We have $H(G) = H(C_k) + H(P_1) + H(P_2)$. For $i = 1, 2$,

$$H(P_i) = \sum_{uv \in E(P_i)} \frac{2}{d_G(u) + d_G(v)} = (p_i - 2)\frac{2}{4} + \frac{2}{3} + \frac{2}{5} = \frac{p_i}{2} + \frac{1}{15}$$

if $p_i \geq 2$, and $H(P_i) = \frac{1}{2}$ if $p_i = 1$. If P_1 and P_2 are attached to non-adjacent vertices of C_k, then

$$H(C_k) = (k - 4)\frac{2}{4} + 4\left(\frac{2}{5}\right) = \frac{k}{2} - \frac{2}{5}.$$

If P_1 and P_2 are attached to adjacent vertices of C_k, then

$$H(C_k) = (k - 3)\frac{2}{4} + 2\left(\frac{2}{5}\right) + \frac{2}{6} = \frac{k}{2} - \frac{11}{30} > \frac{k}{2} - \frac{2}{5}.$$

If $p_1 = p_2 = 1$, then $D(G) \leq \frac{k}{2} + 2$ and

$$H(G) \geq \frac{k}{2} - \frac{2}{5} + \frac{1}{2} + \frac{1}{2} = D(G) - \frac{7}{5} > \frac{D(G)}{2} + \frac{2}{3}.$$

So we can assume that p_1 or p_2 is at least 2. We have $H(P_1) + H(P_2) \geq \frac{p_1}{2} + \frac{p_2}{2} + \frac{1}{15}$ (the equality holds if p_1 or p_2 is 1). If $k \geq 4$, then $D(G) \leq \frac{k}{2} + p_1 + p_2$ and

$$H(G) \geq \frac{k}{2} - \frac{2}{5} + \frac{p_1}{2} + \frac{p_2}{2} + \frac{1}{15} \geq \frac{D(G)}{2} + \frac{k}{4} - \frac{1}{3} \geq \frac{D(G)}{2} + \frac{2}{3}.$$

If $k = 3$, then $D(G) \leq p_1 + p_2 + 1$ and

$$H(G) \geq \frac{3}{2} - \frac{2}{5} + \frac{p_1}{2} + \frac{p_2}{2} + \frac{1}{15} \geq \frac{D(G)}{2} + \frac{2}{3}.$$

Case 3b: $P_1 \cap P_2$ is nonempty and there is a diametral path containing both pendant vertices of G.

Let U be the diametral path containing both pendant vertices of G. Then $U \subseteq P_1 \cup P_2$. One of the internal vertices, say x, of U is of degree 3 or 4 in G. If x is adjacent to a pendant vertex of U, then

$$H(U) = \sum_{uv \in E(U)} \frac{2}{d_G(u) + d_G(v)} \geq (D(G) - 3)\frac{2}{4} + \frac{2}{3} + \frac{2}{5} + \frac{2}{6} = \frac{D(G)}{2} - \frac{1}{10}.$$

If x is not adjacent to a pendant vertex of U, then

$$H(U) \geq (D(G) - 4)\frac{2}{4} + 2\left(\frac{2}{3}\right) + 2\left(\frac{2}{6}\right) = \frac{D(G)}{2}.$$

Note that G contains also the cycle C_k, where one of the vertices is of degree 3 or 4 in G. We have

$$H(C_k) \geq (k - 2)\frac{2}{4} + 2\left(\frac{2}{6}\right) = \frac{k}{2} - \frac{1}{3} \geq \frac{7}{6},$$

which implies that $H(G) \geq H(U) + H(C_k) \geq \frac{D(G)}{2} - \frac{1}{10} + \frac{7}{6} > \frac{D(G)}{2} + \frac{2}{3}$.

Case 3c: $P_1 \cap P_2$ is nonempty and there is a diametral path containing only one pendant vertex of G.

There is a diametral path U containing only one pendant vertex of G. Since the other pendant vertex is not in U, by Lemma 2.1, there is a unicyclic graph G' having one pendant vertex, such that $D(G') = D(G)$ and $H(G) > H(G')$ and we know that $H(G') > \frac{D(G)}{2} + \frac{2}{3}$.

Case 4: G contains at least 3 pendant vertices.

Let U be a diametral path of G. Clearly, this path contains at most 2 pendant vertices of G. Since G contains $m \geq 3$ pendant vertices, we have at least $m - 2$ pendant vertices not in U. By Lemma 2.1, there is a unicyclic graph $G' \subset G$ having only the pendant vertices of U (at most 2 vertices), such that $D(G') = D(G)$, $i(G') = i(G) - 1$ and $H(G) > H(G')$. From the previous cases it follows that $H(G') \geq \frac{D(G)}{2} + \frac{2}{3}$.

It is easy to show that the bound $H(G) \geq \frac{D(G)}{2} + \frac{2}{3}$ is best possible, since the graph F, where $V(F) = \{u, v_0, v_1, v_2, \ldots, v_{D(F)}\}$ and $E(F) = \{v_0v_1, v_1v_2, \ldots, v_{D(F)-1}v_{D(F)}, uv_1, uv_3\}$ has harmonic index $H(F) = (D(F) - 4)\frac{2}{4} + 5(\frac{2}{5}) + \frac{2}{3} = \frac{D(F)}{2} + \frac{2}{3}$. The proof is complete. $\square$

We give a lower bound on the harmonic index for unicyclic graphs of small diameter.

Theorem 2.2. *Let G be any unicyclic graph of diameter $D(G)$.*
(i) *If $D(G) = 2$, then $H(G) \geq \frac{9}{5}$.*
(ii) *If $D(G) = 3$, then $H(G) \geq \frac{32}{15}$.*
(iii) *If $D(G) = 4$, then $H(G) \geq \frac{13}{5}$.*
The bounds are best possible.

Proof. The proof of Theorem 2.1 holds also for $D(G) = 3$ and $D(G) = 4$ except for Case 3a, where $p_1 = p_2 = 1$.

Let $D(G) = 4$. We have $H(G) \geq D(G) - \frac{7}{5}$ (as presented in the proof of Theorem 2.1, which is $\frac{13}{5}$. From the other cases we obtain $H(G) \geq \frac{D(G)}{2} + \frac{2}{3} = \frac{8}{3} > \frac{13}{5}$, which implies that $H(G) \geq \frac{13}{5}$.

Let $D(G) = 3$. The bound $H(G) \geq D(G) - \frac{7}{5}$ (obtained in the proof of Theorem 2.1, Case 3a if $p_1 = p_2 = 1$) is not sufficient now, so we give a better bound in this case. Since $p_1 = p_2 = 1$ and $D(G) = 3$, then P_1 and P_2 must be attached to adjacent vertices of C_k, which means that $H(C_k) = \frac{k}{2} - \frac{11}{30}$ (given in the proof of Theorem 2.1). Since $k \geq 3$, we obtain

$$H(G) = H(C_k) + H(P_1) + H(P_2) = \frac{k}{2} - \frac{11}{30} + \frac{1}{2} + \frac{1}{2} \geq \frac{32}{15}.$$

Let $D(G) = 2$. Except for C_5 and C_4, the only unicyclic graphs F of diameter 2 are formed by the cycle C_3, where $p \geq 1$ pendant vertices are adjacent to one of the vertices of C_3. Let $V(C_3) = \{v_1, v_2, v_3\}$. We can assume that the pendant vertices $u_1, u_2, \ldots, u_p$ are adjacent to v_1. Then $U = v_2 v_1 u_1$ is a diametral path of F and from Lemma 2.1 it follows that there is a unicyclic graph $F' \subseteq F$, which contains only one pendant vertex u_1 (the pendant vertex in U), where $H(F) \geq H(F')$. Since $H(F') = 2(\frac{2}{5}) + 2(\frac{2}{4}) = \frac{9}{5}$, $H(C_4) = 2$ and $H(C_5) = \frac{5}{2}$, we obtain the bound $H(G) \geq \frac{9}{5}$.

It remains to show that the bounds are best possible. The graph G', where $V(G') = \{v_0, v_1, v_2, v_3, v_4, u\}$ and $E(G') = \{v_0v_1, v_1v_2, v_2v_3, v_3v_4, uv_1, uv_3\}$ has diameter 4 and $H(G') = \frac{13}{5}$. The graph G', where $V(G') = \{v_0, v_1, v_2, v_3, u\}$ and $E(G') = \{v_0v_1, v_1v_2, v_2v_3, uv_1, uv_2\}$ has diameter 3 and $H(G') = \frac{32}{15}$. The graph F' presented in the previous paragraph has diameter 2 and $H(F') = \frac{9}{5}$. $\square$

Corollary 2.1. *Let G be any unicyclic graph of order $n \geq 7$ and diameter $D(G) \geq 2$. Then $H(G) \geq \frac{D(G)}{2} + \frac{2}{3}$.*

Proof. By Theorem 2.1, for $D(G) \geq 5$ and any n, we have $H(G) \geq \frac{D(G)}{2} + \frac{2}{3}$. By Theorem 2.2, for $D(G) = 2$ and any n, we have $H(G) \geq \frac{9}{5}$, which is greater than $\frac{D(G)}{2} + \frac{2}{3}$.

It remains to prove Corollary 2.1 for $n \geq 7$ and $3 \leq D(G) \leq 4$. The proof of Theorem 2.1 holds also for $D(G) = 3$ and $D(G) = 4$ except for Case

3a, where $p_1 = p_2 = 1$. We show that if $n \geq 7$, then $H(G) \geq \frac{D(G)}{2} + \frac{2}{3}$ also in that case. If $n \geq 7$ and $p_1 = p_2 = 1$, then G contains the cycle C_k for $k \geq 5$ and $H(C_k) \geq \frac{k}{2} - \frac{2}{5}$ (given in the proof of Theorem 2.1, Case 3a). Since $H(P_1) = H(P_2) = \frac{1}{2}$, we obtain $H(G) = H(C_k) + H(P_1) + H(P_2) \geq \frac{31}{10}$, which is greater than $\frac{D(G)}{2} + \frac{2}{3}$ for $D(G) = 3$ and $D(G) = 4$. □

COROLLARY 2.2. *Let G be any unicyclic graph of order $n \geq 7$ and diameter $D(G) \geq 2$. Then*

$$\frac{H(G)}{D(G)} \geq \frac{1}{2} + \frac{2}{3(n-2)} \quad \text{and} \quad H(G) - D(G) \geq \frac{5}{3} - \frac{n}{2}.$$

Proof. By Corollary 2.1, we have $H(G) \geq \frac{D(G)}{2} + \frac{2}{3}$, which implies that

$$\frac{H(G)}{D(G)} \geq \frac{1}{2} + \frac{2}{3D(G)} \geq \frac{1}{2} + \frac{2}{3(n-2)}$$

since $D(G) \leq n - 2$ for any graph G except for the path.

Similarly, we obtain

$$H(G) - D(G) \geq \frac{2}{3} - \frac{D(G)}{2} \geq \frac{2}{3} - \frac{n-2}{2} = \frac{5}{3} - \frac{n}{2}.$$

The proof is complete. □

Acknowledgements. The work of the second author has been supported by the National Research Foundation of South Africa; grant numbers: 91499, 90793.

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Received 3 March 2017

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