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THE MINIMUM HARMONIC INDEX FOR UNICYCLIC GRAPHS WITH GIVEN DIAMETER

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Abstract

The harmonic index 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 a vertex u in G. In this paper, we present the minimum harmonic index for unicyclic graphs with given diameter and characterize the corresponding extremal graphs. This answers an unsolved problem of Zhu and Chang [26].

Keywords: harmonic index, unicyclic graphs, diameter.

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1. Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The Randić index $R(G)$, proposed by Randić [16] in 1975, is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}},$$

where $d(u)$ denotes the degree of a vertex u of G. The Randić index is one of the most successful molecular descriptors in structure-property and structure-activity relationship studies. Mathematical properties of this descriptor have been studied extensively (see [8, 12, 13] and the references cited therein).

In this paper, we consider a closely related variant of the Randić index, named the harmonic index. For a graph G, the harmonic index $H(G)$ is defined as

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

This index first appeared in [4], and it can also be viewed as a particular case of the general sum-connectivity index proposed by Zhou and Trinajstić [25].

Favaron, Mahéo and Saclé [6] considered the relation between the harmonic index and the eigenvalues of graphs. Zhong [21, 22], Zhong and Xu [24] determined the minimum and maximum harmonic indices for simple connected graphs, trees, unicyclic graphs and bicyclic graphs, and characterized the corresponding extremal graphs. Wu, Tang and Deng [19] found the minimum harmonic index for graphs (triangle-free graphs, respectively) with minimum degree at least 2, and characterized the corresponding extremal graphs. Iranmanesh and Saheli [14] computed the minimum and maximum harmonic indices for caterpillars with diameter four. Deng, Balachandran, Ayyaswamy and Venkatakrishnan [3] considered the relation between the harmonic index and the chromatic number of a graph by using the effect of removal of a minimum degree vertex on the harmonic index. Deng, Balachandran and Ayyaswamy [2] obtained several results relating the harmonic index and the largest eigenvalue of a graph. Shetty, Lokesha and Ranjini [17] considered the harmonic index of graph operations such as join, corona product, Cartesian product, composition and symmetric difference of graphs. The chemical applicability of the harmonic index was also recently investigated by Furtula, Gutman and Dehmer [7], Gutman and Tošović [9]. See [1, 5, 11, 15, 23, 26] for more information of this index.

Recently, Zhu and Chang [26] presented lower bounds of harmonic index for trees and unicyclic graphs with given diameter; however, the lower bound for unicyclic graphs in [26] is not sharp. In this paper, we determine the minimum harmonic index for unicyclic graphs with $n \geq 3$ vertices and diameter d ($1 \leq d \leq n-2$), and characterize the corresponding extremal graphs. The related problems have been well-studied for several other topological indices, such as the Randić index [18], the signless Laplacian index [10] and the Hosoya index [20].

2. Preliminaries

Let G be a graph. For any vertex $v \in V(G)$, we use $N_G(v)$ (or $N(v)$ if there is no ambiguity) to denote the set of neighbors of v in G. A pendent vertex is a vertex of degree 1. An edge incident with a pendent vertex is called a pendent edge. For two distinct vertices u and v of G, the distance $d(u, v)$ between u and v is the number of edges in a shortest path joining u and v in G. The diameter of G is the maximum distance between any two vertices of G. A unicyclic graph is a connected graph with n vertices and n edges. We use C_n to denote the cycle on n vertices. We write $A := B$ to rename B as A.

For any vertex $v \in V(G)$, we use $G - v$ to denote the graph resulting from G by deleting the vertex v and its incident edges. We define $G - uv$ to be the graph obtained from G by deleting the edge $uv \in E(G)$, and $G + uv$ to be the graph obtained from G by adding an edge uv between two non-adjacent vertices u and v of G.

We now list some lemmas which will be used in later proofs. The first lemma was proved in [23].

Lemma 1. *Let G be a nontrivial connected graph, and let $uv \in E(G)$ be such that $d_G(u), d_G(v) \geq 2$ and $N_G(u) \cap N_G(v) = \emptyset$. Let G' be the graph obtained from G by contracting the edge uv into a new vertex w and adding a new pendent edge ww' to w. Then $H(G) > H(G')$.*

Lemma 2. (i) *For $k \geq 1$, the function $f(x) = \frac{2}{x(x+1)} - \frac{2}{(x+k)(x+k+1)}$ is decreasing for $x \geq 3$.*

(ii) *The function $g(x) = \frac{x+5}{2} - \frac{4}{x+3} - \frac{2(x-1)}{x+2}$ is increasing for $x \geq 2$.*

(iii) *The function $h(x) = \frac{4}{x+2} + \frac{2(x-4)}{x+1} - \frac{2(x-3)}{x}$ is decreasing for $x \geq 3$.*

(iv) *The function $l(x) = \frac{2}{x+2} + \frac{2(x-1)}{x+1} - \frac{x}{2}$ is decreasing for $x \geq 3$.*

Proof. (i) Let $f_1(x) = \frac{2}{x(x+1)} = \frac{2}{x} - \frac{2}{x+1}$. Then $f(x) = f_1(x) - f_1(x+k)$. For $x \geq 3$, we have

$$f_1''(x) = \frac{4}{x^3} - \frac{4}{(x+1)^3} > 0,$$

and $f'(x) = f_1'(x) - f_1'(x+k) < 0$. So (i) holds.

(ii) For $x \geq 2$, we have

$$g'(x) = \frac{1}{2} + \frac{4}{(x+3)^2} - \frac{6}{(x+2)^2} > \frac{1}{2} - \frac{6}{(2+2)^2} = \frac{1}{8} > 0.$$

This proves (ii).

(iii) Let $h_1(x) = \frac{4}{x+1} + \frac{2(x-3)}{x}$. Then $h(x) = h_1(x+1) - h_1(x)$. For $x \geq 3$, we have

$$h_1''(x) = \frac{8}{(x+1)^3} - \frac{12}{x^3} = \frac{-4(x^3 + 9x^2 + 9x + 3)}{x^3(x+1)^3} < 0,$$

and $h'(x) = h_1'(x+1) - h_1'(x) < 0$. So the assertion of (iii) holds.

(iv) For $x \geq 3$, we have

$$l'(x) = -\frac{2}{(x+2)^2} + \frac{4}{(x+1)^2} - \frac{1}{2} < \frac{4}{(3+1)^2} - \frac{1}{2} = -\frac{1}{4} < 0,$$

and hence (iv) holds. This proves the lemma. ∎

Lemma 3. *Let H be a nontrivial connected graph with $u, u', v, v' \in V(H)$ such that $2 \le d_H(u) = s \le 4$, $d_H(v) = t \ge 2$, $d_H(u') = d_H(v') = 1$ and $uu', vv' \in E(H)$. Let G be the graph obtained from H by attaching $p-1$ and $q-1$ pendent edges ($p \ge q \ge 3$) to u' and v', respectively, and let G' be the graph obtained from H by attaching p and $q-2$ pendent edges to u' and v', respectively. If either $p = q$ and $s \le t$ or $p > q$, then $H(G) > H(G')$.*

Proof. Let $f(x) = \frac{2}{x(x+1)} - \frac{2}{(x+k)(x+k+1)}$ with $k \ge 1$. Then by Lemma 2(i), $f(x)$ is decreasing for $x \ge 3$. It is easy to see that

$$\begin{aligned}
H(G) - H(G') &= \left(\frac{2}{p+s} + \frac{2(p-1)}{p+1} + \frac{2(q-1)}{q+1} + \frac{2}{q+t}\right) \\
&- \left(\frac{2}{(p+1)+s} + \frac{2p}{(p+1)+1} + \frac{2(q-2)}{(q-1)+1} + \frac{2}{(q-1)+t}\right) \\
&= \left(\frac{2}{p+s} - \frac{2}{p+s+1}\right) + \left(\frac{2(p-1)}{p+1} - \frac{2p}{p+2}\right) \\
&+ \left(\frac{2(q-1)}{q+1} - \frac{2(q-2)}{q}\right) + \left(\frac{2}{q+t} - \frac{2}{q+t-1}\right) \\
&= \frac{2}{(p+s)(p+s+1)} - \frac{4}{(p+1)(p+2)} + \frac{4}{q(q+1)} \\
&- \frac{2}{(q+t-1)(q+t)}.
\end{aligned}$$

If $p = q$ and $s \le t$, then

$$\begin{aligned}
&H(G) - H(G') \\
&= 2\left(\frac{2}{p(p+1)} - \frac{2}{(p+1)(p+2)}\right) - \left(\frac{2}{(p+t-1)(p+t)} - \frac{2}{(p+s)(p+s+1)}\right) \\
&> \left(\frac{2}{p(p+1)} - \frac{2}{(p+1)(p+2)}\right) - \left(\frac{2}{(p+t-1)(p+t)} - \frac{2}{(p+t)(p+t+1)}\right) \\
&= f(p) - f(p+t-1) \ > 0 \quad (\text{with } k = 1).
\end{aligned}$$

So we may assume $p > q$. Since $2 \le s \le 4$ and $t \ge 2$, we conclude that

$$\begin{aligned}
&H(G) - H(G') \\
&\ge \frac{2}{(p+4)(p+5)} - \frac{4}{(p+1)(p+2)} + \frac{4}{q(q+1)} - \frac{2}{(q+1)(q+2)}
\end{aligned}$$

$$= \left(\frac{2}{q(q+1)} - \frac{2}{(q+1)(q+2)}\right) + \frac{2}{(p+4)(p+5)} - \frac{2}{(p+1)(p+2)}$$
$$+ \left(\frac{2}{q(q+1)} - \frac{2}{[q+(p-q+1)][q+(p-q+2)]}\right)$$
$$= \left(\frac{2}{q(q+1)} - \frac{2}{(q+1)(q+2)}\right) + \frac{2}{(p+4)(p+5)} - \frac{2}{(p+1)(p+2)} + f(q)$$
$$\text{(with } k = p-q+1 \geq 2)$$
$$> \left(\frac{2}{q(q+1)} - \frac{2}{(q+1)(q+2)}\right) + \frac{2}{(p+4)(p+5)} - \frac{2}{[(q+1)+1][(q+1)+2]}$$
$$+ \ f(q+3)$$
$$= \left(\frac{2}{q(q+1)} - \frac{2}{(q+1)(q+2)}\right) + \frac{2}{(p+4)(p+5)} - \frac{2}{(q+2)(q+3)}$$
$$+ \left(\frac{2}{(q+3)(q+4)} - \frac{2}{[(q+3)+(p-q+1)][(q+3)+(p-q+2)]}\right)$$
$$= \left(\frac{2}{q(q+1)} - \frac{2}{(q+1)(q+2)}\right) - \left(\frac{2}{(q+2)(q+3)} - \frac{2}{(q+3)(q+4)}\right)$$
$$= \frac{4}{q(q+1)(q+2)} - \frac{4}{(q+2)(q+3)(q+4)} > 0.$$

So the assertion of the lemma holds. ∎

3. THE MINIMUM HARMONIC INDEX FOR UNICYCLIC GRAPHS WITH GIVEN DIAMETER

Let $\mathscr{U}_n$ be the set of unicyclic graphs with $n \geq 3$ vertices, and let $\mathscr{U}_{n,d}$ be the set of unicyclic graphs with n vertices and diameter d, where $1 \leq d \leq n-2$. In this section, we determine the minimum harmonic index for graphs in $\mathscr{U}_{n,d}$, and characterize the corresponding extremal graphs.

Let $U_{n,2}$ be the unicyclic graph with n vertices obtained by attaching $n-3$ pendent edges to one vertex of a triangle, and let $U_{n,3}$ be the unicyclic graph with n vertices obtained by attaching $n-4$ and one pendent edges to two vertices of a triangle, respectively. For $4 \leq d \leq n-2$, let $U_{n,d}$ be the unicyclic graph with n vertices obtained by attaching $n-d-1$ pendent edges and a path of length $d-3$ to two non-adjacent vertices of C_4, respectively (see Figure 1).

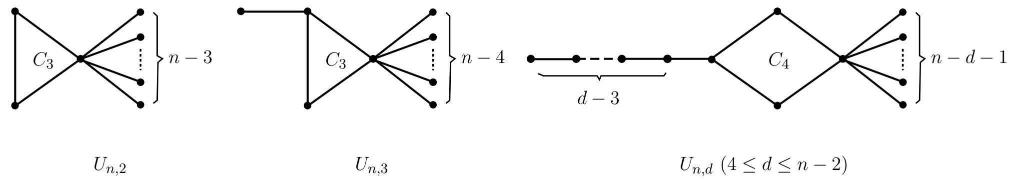

Figure 1. The graphs $U_{n,d}$ $(2 \le d \le n-2)$.

It was proved in [22, 23] that $U_{n,2}$ and $U_{n,3}$ are the extremal graphs with the minimum harmonic index $\frac{4}{n+1} + \frac{2(n-3)}{n} + \frac{1}{2}$ and the second-minimum harmonic index $\frac{2}{n+1} + \frac{2}{n} + \frac{2(n-4)}{n-1} + \frac{9}{10}$ for graphs in $\mathscr{U}_n$, respectively. Since $\mathscr{U}_{n,1} = \{C_3\}$, $U_{n,2} \in \mathscr{U}_{n,2}$ and $U_{n,3} \in \mathscr{U}_{n,3}$, we see that C_3, $U_{n,2}$ and $U_{n,3}$ are the extremal graphs with the minimum harmonic index for graphs in $\mathscr{U}_{n,1}$, $\mathscr{U}_{n,2}$ and $\mathscr{U}_{n,3}$, respectively. In the following arguments, we will show that $U_{n,d}$ is the extremal graph with the minimum harmonic index for graphs in $\mathscr{U}_{n,d}$ for $4 \le d \le n-2$. For convenience, we define the following function

$$\varphi(n,d) = H(U_{n,d}) = \frac{4}{n-d+3} + \frac{2(n-d-1)}{n-d+2} + \frac{d-5}{2} + A$$

with $A := \frac{9}{5}$ (if $d = 4$) or $A := \frac{28}{15}$ (if $5 \le d \le n-2$).

For $4 \le d \le n-2$, let $U^1_{n,d}$ be the set of unicyclic graphs in $\mathscr{U}_{n,d}$ obtained by attaching a path of length l $(l \ge 1)$ to one vertex of C_{n-l}, and let $U^2_{n,d}$ be the set of unicyclic graphs in $\mathscr{U}_{n,d}$ obtained by attaching two paths $v_1v_2\cdots v_{s+1}$ and $v_{d+1-t}\cdots v_dv_{d+1}$ of length s and t $(s,t \ge 1)$ to two vertices v_{s+1} and v_{d+1-t} of C_{n-s-t}, respectively. Note that it is possible $v_{s+1} = v_{d+1-t}$ (i.e., $s+t = d$). For $4 \le d \le n-4$, let $U^3_{n,d}$ be the set of unicyclic graphs in $\mathscr{U}_{n,d}$ obtained by connecting a path of length l between a vertex of C_{n-d-l} and a non-pendent vertex v_{s+1} of a path $v_1v_2\cdots v_sv_{s+1}v_{s+2}\cdots v_dv_{d+1}$ of length d $(l \ge 1,\ 1 \le s \le d-1)$. See Figure 2 for an illustration.

Lemma 4. *Let $G \in \mathscr{U}_{n,d}$ $(4 \le d \le n-2)$ and such that G contains at least one pendent vertex. If $G - v \in \mathscr{U}_{n-1,d-1}$ for any pendent vertex $v \in V(G)$, then $H(G) \ge \varphi(n,d)$ with equality if and only if $d = n-2$ and $G \cong U_{n,n-2}$.*

Proof. If G contains at least three pendent vertices, then there must exist some pendent vertex $v \in V(G)$ such that $G - v \in \mathscr{U}_{n-1,d}$, a contradiction. So we conclude that G contains one or two pendent vertices. This implies that $G \in U^1_{n,d} \cup U^2_{n,d} \cup U^3_{n,d}$. We consider three cases according to the structure of G.

Case 1. $G \in U^1_{n,d}$. In this case, we have

$$H(G) = \begin{cases} \frac{n}{2} - \frac{1}{5}, & \text{if } l = 1, \\ \frac{n}{2} - \frac{2}{15}, & \text{if } l \ge 2. \end{cases}$$

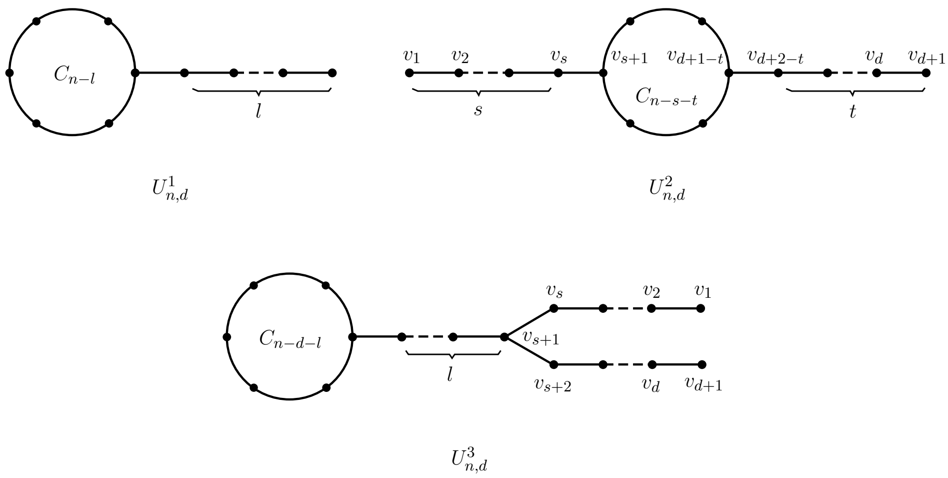

Figure 2. The graph sets $U^1_{n,d}$, $U^2_{n,d}$ $(4 \le d \le n-2)$ and $U^3_{n,d}$ $(4 \le d \le n-4)$.

Case 2. $G \in U^2_{n,d}$. By symmetry between s and t, we may assume that $s \ge t \ge 1$. If $s+t = d$, then we have $s \ge t \ge 2$; for otherwise, it is easy to see that $G - v_{d+1} \in \mathscr{U}_{n-1,d}$, which contradicts the assumption of the lemma. Hence $H(G) = \frac{n}{2} - \frac{1}{3}$. (Note that $n - d \ge 3$ in this subcase.) If $s + t = d - 1$, then we see that

$$H(G) = \begin{cases} \frac{n}{2} - \frac{3}{10}, & \text{if } s > t = 1, \\ \frac{n}{2} - \frac{7}{30}, & \text{if } s \ge t \ge 2 \text{ (and hence } d \ge 5). \end{cases}$$

If $2 \le s + t \le d - 2$, then

$$H(G) = \begin{cases} \frac{n}{2} - \frac{2}{5}, & \text{if } s = t = 1, \\ \frac{n}{2} - \frac{1}{3}, & \text{if } s > t = 1 \text{ (and hence } d \ge 5), \\ \frac{n}{2} - \frac{4}{15}, & \text{if } s \ge t \ge 2 \text{ (and hence } d \ge 6). \end{cases}$$

(Note that $n - d \ge 3$ if $s = t = 1$ and $d \ge 5$.)

Case 3. $G \in U^3_{n,d}$. In this case, we have $s, d - s \ge 3$ (and hence $d \ge 6$); otherwise, there exists some pendent vertex $v \in \{v_1, v_{d+1}\}$ such that $G - v \in \mathscr{U}_{n-1,d}$, a contradiction. Then

$$H(G) = \begin{cases} \frac{n}{2} - \frac{7}{30}, & \text{if } l = 1, \\ \frac{n}{2} - \frac{4}{15}, & \text{if } l \ge 2. \end{cases}$$

(Note that $n - d \ge 4$ in this case.)

It is easy to check that for all possible cases, we always have

$$H(G) \geq \begin{cases} \frac{n}{2} - \frac{2}{5}, & \text{if } d = 4, \\ \frac{n}{2} - \frac{1}{3}, & \text{if } d \geq 5 \text{ and } n - d = 2, \\ \frac{n}{2} - \frac{2}{5}, & \text{if } d \geq 5 \text{ and } n - d \geq 3. \end{cases}$$

If $d = 4$, then

$$\begin{aligned} H(G) - \varphi(n,4) &\geq \left(\frac{n}{2} - \frac{2}{5}\right) - \left(\frac{4}{n-4+3} + \frac{2(n-4-1)}{n-4+2} + \frac{4-5}{2} + \frac{9}{5}\right) \\ &= \left(\frac{(n-4)+5}{2} - \frac{4}{(n-4)+3} - \frac{2[(n-4)-1]}{(n-4)+2}\right) - \frac{11}{5} \\ &\geq \left(\frac{2+5}{2} - \frac{4}{2+3} - \frac{2\cdot(2-1)}{2+2}\right) - \frac{11}{5} \\ &= 0 \quad \text{(by Lemma 2(ii) with } x = n-4 \geq 2) \end{aligned}$$

with equalities if and only if $G \in U_{n,4}^2$, $s = t = 1$ and $n - 4 = 2$, i.e., $G \cong U_{6,4}$. So the assertion of the lemma holds. If $d \geq 5$ and $n - d = 2$, then

$$\begin{aligned} H(G) - \varphi(n,d) &\geq \left(\frac{n}{2} - \frac{1}{3}\right) - \left(\frac{4}{n-d+3} + \frac{2(n-d-1)}{n-d+2} + \frac{d-5}{2} + \frac{28}{15}\right) \\ &= \left(\frac{n-d+5}{2} - \frac{4}{n-d+3} - \frac{2(n-d-1)}{n-d+2}\right) - \frac{11}{5} \\ &= \left(\frac{2+5}{2} - \frac{4}{2+3} - \frac{2\cdot(2-1)}{2+2}\right) - \frac{11}{5} = 0 \end{aligned}$$

with equality if and only if $G \in U_{n,n-2}^2$, $s + t \leq n - 4$ and $s > t = 1$, i.e., $G \cong U_{n,n-2}$. Hence the lemma holds. If $d \geq 5$ and $n - d \geq 3$, then

$$\begin{aligned} H(G) - \varphi(n,d) &\geq \left(\frac{n}{2} - \frac{2}{5}\right) - \left(\frac{4}{n-d+3} + \frac{2(n-d-1)}{n-d+2} + \frac{d-5}{2} + \frac{28}{15}\right) \\ &= \left(\frac{(n-d)+5}{2} - \frac{4}{(n-d)+3} - \frac{2[(n-d)-1]}{(n-d)+2}\right) - \frac{34}{15} \\ &\geq \left(\frac{3+5}{2} - \frac{4}{3+3} - \frac{2\cdot(3-1)}{3+2}\right) - \frac{34}{15} \\ &= \frac{4}{15} > 0 \quad \text{(by Lemma 2(ii) with } x = n-d \geq 3). \end{aligned}$$

This completes the proof of the lemma. ∎

We now prove the main result of this paper.

Theorem 5. *Let* $G \in \mathscr{U}_{n,d}$ $(4 \le d \le n-2)$. *Then* $H(G) \ge \varphi(n,d)$ *with equality if and only if* $G \cong U_{n,d}$.

Proof. We prove the theorem by induction on n. If $n = d+2$, then G contains one or two pendent vertices and $G \in U^1_{n,n-2} \cup U^2_{n,n-2}$. Hence the assertion follows from the proof of Lemma 4. So we may assume $n \ge d+3$ and the result holds for smaller values of n. For convenience, we may also assume that G is the extremal graph with the minimum harmonic index for graphs in$\mathscr{U}_{n,d}$. Let C be the unique cycle in G and let $P := v_1v_2\cdots v_dv_{d+1}$ be a path of length d in G such that the distance $d(v_1, v_{d+1})$ between v_1 and v_{d+1} is d.

It was proved in [22] that C_n is the extremal graph with the maximum harmonic index for graphs in $\mathscr{U}_n$. So we deduce that G contains at least one pendent vertex. Then by Lemma 4, we may further assume that there exists at least one pendent vertex $v \in V(G)$ such that $G - v \in \mathscr{U}_{n-1,d}$. Let V^* be the set of all such pendent vertices in G (and hence $V^* \ne \emptyset$).

Let $v \in V^*$ be a pendent vertex and let $uv \in E(G)$. Then $d(u) = p \ge 2$. Since $G \in \mathscr{U}_{n,d}$, we have $p \le n-d+1$. Let $N(u) = \{v, u_1, \ldots, u_{p-1}\}$ with $d(u_i) = p_i$ for each $1 \le i \le p-1$. We choose v and u such that there are as many as possible vertices in $N(u)$ with degree at least 2. (Note that $N(u)$ contains at least one such vertex.)

Suppose there are at least two vertices in $N(u)$ with degree at least 2 (and hence $p \ge 3$). Let $G' := G - v$. Then $G' \in \mathscr{U}_{n-1,d}$. Since the function $\frac{2}{p+x} - \frac{2}{p+x-1}$ is increasing for $x \ge 1$ and by the induction hypothesis, we have

$$\begin{aligned}
H(G) &= H(G') + \frac{2}{p+1} + \sum_{i=1}^{p-1}\left(\frac{2}{p+p_i} - \frac{2}{(p-1)+p_i}\right)\\
&\ge \varphi(n-1,d) + \frac{2}{p+1} + 2\left(\frac{2}{p+2} - \frac{2}{p+1}\right) + (p-3)\left(\frac{2}{p+1} - \frac{2}{p}\right)\\
&= \left(\frac{4}{(n-1)-d+3} + \frac{2[(n-1)-d-1]}{(n-1)-d+2} + \frac{d-5}{2} + A\right)\\
&+ \left(\frac{4}{p+2} + \frac{2(p-4)}{p+1} - \frac{2(p-3)}{p}\right)\\
&\ge \left(\frac{4}{n-d+2} + \frac{2(n-d-2)}{n-d+1} + \frac{d-5}{2} + A\right)\\
&+ \left(\frac{4}{(n-d+1)+2} + \frac{2[(n-d+1)-4]}{(n-d+1)+1} - \frac{2[(n-d+1)-3]}{n-d+1}\right)\\
&\qquad \text{(by Lemma 2(iii) with } x = p \le n-d+1\text{)}
\end{aligned}$$

$$= \frac{4}{n-d+3} + \frac{2(n-d-1)}{n-d+2} + \frac{d-5}{2} + A = \varphi(n,d)$$

with equalities if and only if $G' \cong U_{n-1,d}$, $p = n-d+1$, exactly two vertices in $N(u)$ have degree 2 and the other $p-3$ vertices in $N(u)$ have degree 1, i.e., $G \cong U_{n,d}$. Hence the assertion of the theorem holds. By the choice of v and u, we may assume that

(1) for any vertex $u \in \bigcup_{v\in V^*} N(v)$, there is exactly one vertex in $N(u)$ with degree at least 2.

We claim that

(2) $u \in \{v_2, v_d\}$ for any vertex $u \in \bigcup_{v\in V^*} N(v)$.

For otherwise, suppose there exists some vertex $u \in \bigcup_{v\in V^*} N(v)$ such that $u \notin \{v_2, v_d\}$. If $u \in \{v_1, v_{d+1}\}$, say $u = v_1$, then $P' := P + uv$ (with $v \in V^*$) would be a shortest path of length $d+1$ between v and v_{d+1}, which implies that $G \notin \mathscr{U}_{n,d}$, a contradiction. Then by (1), we have $u \notin V(P) \cup V(C)$. Let G'' be the graph obtained from G by contracting the unique non-pendent edge incident with u into a new vertex w and adding a new pendent edge ww' to w. Then $G'' \in \mathscr{U}_{n,d}$. Now by Lemma 1, we see that $H(G) > H(G'')$, contradicting the assumption that G has the minimum harmonic index for graphs in $\mathscr{U}_{n,d}$. This proves (2).

By (2), we conclude that every pendent vertex in G is adjacent to either v_2 or v_d. We also claim that

(3) either $\bigcup_{v\in V^*} N(v) = \{v_2\}$ or $\bigcup_{v\in V^*} N(v) = \{v_d\}$.

Suppose to the contrary that $\bigcup_{v\in V^*} N(v) = \{v_2, v_d\}$ (by (2)). Then by (1) and (2), we know that $d(v_2), d(v_d) \geq 3$, $2 \leq d(v_3), d(v_{d-1}) \leq 4$ and all pendent vertices in G (including v_1 and v_{d+1}) are contained in V^*. Without loss of generality, we may assume by symmetry that $d(v_2) = d(v_d)$ and $d(v_3) \leq d(v_{d-1})$ or $d(v_2) > d(v_d)$. Let $G'' := G - v_dv_{d+1} + v_2v_{d+1}$. Then $G'' \in \mathscr{U}_{n,d}$. But now, it follows from Lemma 3 that $H(G) > H(G'')$, which contradicts the assumption that G has the minimum harmonic index for graphs in $\mathscr{U}_{n,d}$. So the assertion of (3) holds.

By (3) and by symmetry between v_2 and v_d, we may assume that $\bigcup_{v\in V^*} N(v) = \{v_2\}$. Let $u = v_2$ be defined as above with $v = v_1 \in V^*$ and $u_{p-1} = v_3$. Since G is a unicyclic graph and by (1) and (2), we have $3 \leq p \leq n-d$ and all vertices in $\{u_1, \ldots, u_{p-2}\}$ are pendent vertices in V^*. Let $G^* := G - \{u_1, \ldots, u_{p-2}\}$. Then $G^* \in \mathscr{U}_{n-p+2,d}$ and G^* contains at most two pendent vertices. (One pendent vertex is v_1 and the other possible pendent vertex is v_{d+1}.) This implies that $G^* \in U^1_{n-p+2,d} \cup U^2_{n-p+2,d} \cup U^3_{n-p+2,d}$. We consider three cases according to the structure of G^*.

Case 1. $G^* \in U^1_{n-p+2,d}$. In this case, we have $l \geq 2$. Then

$$H(G) = \begin{cases} \frac{2}{p+3} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{1}{5}, & \text{if } l = 2, \\ \frac{2}{p+2} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{3}{10}, & \text{if } l > 2. \end{cases}$$

Case 2. $G^* \in U^2_{n-p+2,d}$. In this case, we have $s \geq 2$ and $t \geq 1$. If $s + t = d$, then $t \geq 2$; for otherwise, it is easy to check that $G'' := G - v_{d+1} \in \mathscr{U}_{n-1,d}$, which implies that $v_{d+1} \in V^*$ and $v_d \in \bigcup_{v \in V^*} N(v)$, contradicting (3). Hence

$$H(G) = \begin{cases} \frac{2}{p+4} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{1}{3}, & \text{if } s = 2, \\ \frac{2}{p+2} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{1}{2}, & \text{if } s \geq 3. \end{cases}$$

If $s + t = d - 1$, then

$$H(G) = \begin{cases} \frac{2}{p+3} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{11}{30}, & \text{if } s = 2 \text{ and } t = 1, \\ \frac{2}{p+3} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{3}{10}, & \text{if } s = 2 \text{ and } t \geq 2, \\ \frac{2}{p+2} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{7}{15}, & \text{if } s \geq 3 \text{ and } t = 1, \\ \frac{2}{p+2} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{2}{5}, & \text{if } s \geq 3 \text{ and } t \geq 2. \end{cases}$$

If $3 \leq s + t \leq d - 2$, then

$$H(G) = \begin{cases} \frac{2}{p+3} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{2}{5}, & \text{if } s = 2 \text{ and } t = 1, \\ \frac{2}{p+3} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{1}{3}, & \text{if } s = 2 \text{ and } t \geq 2, \\ \frac{2}{p+2} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{1}{2}, & \text{if } s \geq 3 \text{ and } t = 1, \\ \frac{2}{p+2} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{13}{30}, & \text{if } s \geq 3 \text{ and } t \geq 2. \end{cases}$$

Case 3. $G^* \in U^3_{n-p+2,d}$. In this case, we have $s, d - s \geq 2$. Then

$$H(G) = \begin{cases} \frac{2}{p+3} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{3}{10}, & \text{if } s = 2 \text{ and } l = 1, \\ \frac{2}{p+3} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{1}{3}, & \text{if } s = 2 \text{ and } l \geq 2, \\ \frac{2}{p+2} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{2}{5}, & \text{if } s \geq 3 \text{ and } l = 1, \\ \frac{2}{p+2} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{13}{30}, & \text{if } s \geq 3 \text{ and } l \geq 2. \end{cases}$$

Let $B := \frac{2}{p+2} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{1}{2}$, $C := \frac{2}{p+3} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{2}{5}$ and $D := \frac{2}{p+4} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{1}{3}$. Since

$$B - C = \left(\frac{2}{p+2} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{1}{2}\right) - \left(\frac{2}{p+3} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{2}{5}\right)$$
$$= \frac{2}{(p+2)(p+3)} - \frac{1}{10} \le \frac{2}{(3+2)\cdot(3+3)} - \frac{1}{10} = -\frac{1}{30} < 0$$

and

$$B - D = \left(\frac{2}{p+2} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{1}{2}\right) - \left(\frac{2}{p+4} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{1}{3}\right)$$
$$= \frac{4}{(p+2)(p+4)} - \frac{1}{6} \le \frac{4}{(3+2)\cdot(3+4)} - \frac{1}{6} = -\frac{11}{210} < 0,$$

we deduce that $B < C$ and $B < D$. Then it is easy to calculate that for all possible cases, we always have $H(G) \ge B$. Therefore

$$H(G) - \varphi(n,d) \ge B - \varphi(n,d)$$
$$= \left(\frac{2}{p+2} + \frac{2(p-1)}{p+1} + \frac{n-p}{2} - \frac{1}{2}\right) - \left(\frac{4}{n-d+3} + \frac{2(n-d-1)}{n-d+2} + \frac{d-5}{2} + A\right)$$
$$\ge \left(\frac{2}{(n-d)+2} + \frac{2[(n-d)-1]}{(n-d)+1} + \frac{n-(n-d)}{2} - \frac{1}{2}\right)$$
$$- \left(\frac{4}{n-d+3} + \frac{2(n-d-1)}{n-d+2} + \frac{d-5}{2} + A\right)$$

(by Lemma 2(iv) with $x = p \le n-d$)

$$= \left(-\frac{4}{n-d+3} - \frac{2(n-d-2)}{n-d+2} + \frac{2(n-d-1)}{n-d+1}\right) + 2 - A$$
$$= -\frac{8}{(n-d+1)(n-d+2)(n-d+3)} + 2 - A$$
$$\ge -\frac{8}{(3+1)\cdot(3+2)\cdot(3+3)} + 2 - A = \frac{29}{15} - A > 0.$$

But this implies that $H(G) > H(U_{n,d})$, contradicting the assumption that G has the minimum harmonic index for graphs in $\mathscr{U}_{n,d}$. This finishes the proof of the theorem. ∎

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