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The Harmonic Index for Unicyclic Graphs with Given Girth

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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 work, we present the minimum, second-minimum, maximum and second-maximum harmonic indices for unicyclic graphs with given girth, and characterize the corresponding extremal graphs.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The Randić index $R(G)$, proposed by Randić [18] in 1975, is defined as the sum of the weights $\frac{1}{\sqrt{d(u)d(v)}}$ over all edges uv of G, that is,

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

where $d(u)$ (or $d_G(u)$) 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 [11, 15, 16] and the references cited therein). Motivated by the success of the Randić index, various generalizations and modifications were introduced, such as the generalized Randić index [1], the atom-bond connectivity index [5, 6], the sum-connectivity index [19, 30] and the general sum-connectivity index [4, 31].

In this paper, we consider another 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 [7], and it can also be viewed as a particular case of the general sum-connectivity index. Favaron, Mahéo and Saclé [8] considered the relation between the harmonic index and the eigenvalues of graphs. Zhong [26, 27], Zhong and Xu [29] determined the minimum and maximum harmonic

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indices for simple connected graphs, trees, unicyclic graphs and bicyclic graphs, and characterized the corresponding extremal graphs. Wu, Tang and Deng [20] found the minimum harmonic index for graphs (triangle-free graphs, respectively) with minimum degree at least 2, and characterized the corresponding extremal graphs. The same authors [21] also considered the relation between the harmonic index and the girth of a graph. 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. Ilić [14], Xu [23], Zhong and Xu [28] established some relationships between the harmonic index and several other topological indices. The chemical applicability of the harmonic index was also recently investigated [10, 12]. See [2, 13, 24, 32] for more information of this index.

In this work, we consider the minimum, second-minimum, maximum and second-maximum harmonic indices for unicyclic graphs with $n \geq 5$ vertices and girth k ($3 \leq k \leq n$), and characterize the corresponding extremal graphs. We also present the second-minimum, second-maximum, third-maximum and fourth-maximum harmonic indices for unicyclic graphs with $n \geq 5$ vertices. The similar techniques have been used to determine the extremal graphs with respect to some other topological indices for a certain classes of graphs, which is one of the important directions in chemical graph theory. Liu, Zhu and Cai [17] found the minimum Randić index for unicyclic graphs with given girth. Yu and Feng [25], Feng, Ilić and Yu [9] determined the extremal graphs with the minimum, second-minimum, maximum and second-maximum Wiener indices for unicyclic graphs with given girth. Xu and Das [22] considered the minimum and maximum multiplicative sum Zagreb indices for trees, unicyclic graphs and bicyclic graphs, and characterized the corresponding extremal graphs.

We conclude this section with some notation and terminology. 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, and $G - v$ to denote the graph resulting from G by deleting the vertex v and its incident edges. A pendent vertex is a vertex of degree 1. An edge incident with a pendent vertex is called a pendent edge. 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 write $A := B$ to rename B as A.

Let $\mathscr{U}_n$ be the set of unicyclic graphs with $n \geq 5$ vertices, and let $\mathscr{U}_{n,k}$ be the set of unicyclic graphs with $in \geq 5$ vertices and girth k, where $3 \leq k \leq n$. Clearly, $\mathscr{U}_n = \bigcup_{k=3}^{n} \mathscr{U}_{n,k}$. We use C_n and $U_{n,n-1}$ to denote the cycle with n vertices and the unique unicyclic graph with n vertices and girth $n-1$, respectively. Since $\mathscr{U}_{n,n} = \{C_n\}$ and $\mathscr{U}_{n,n-1} = \{U_{n,n-1}\}$, we only consider $3 \leq k \leq n-2$ in the following arguments.

2. The Minimum and Second-Minimum Harmonic Indices for Graphs in $\mathscr{U}_{n,k}$

In this section, we present the minimum and second-minimum harmonic indices for graphs in $\mathscr{U}_{n,k}$, and characterize the corresponding extremal graphs. The extremal graph with the second-minimum harmonic index for graphs in $\mathscr{U}_n$ is also obtained. We first prove the following two lemmas.

Lemma 2.1. *Let G be a nontrivial connected graph, and let $uv \in E(G)$ 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 $H(G) > H(G')$.*

Proof. Let $N_G(u) = \{v, u_1, \ldots, u_{p-1}\}$ ($p \geq 2$) with $d_G(u_i) = d_{G'}(u_i) = p_i$ for each $1 \leq i \leq p-1$, and let $N_G(v) = \{u, v_1, \ldots, v_{q-1}\}$ ($q \geq 2$) with $d_G(v_j) = d_{G'}(v_j) = q_j$ for each $1 \leq j \leq q-1$. Then $N_{G'}(w) = \{u_1, \ldots, u_{p-1}, v_1, \ldots, v_{q-1}, w'\}$. Hence

$$H(G) - H(G') = \left(\sum_{i=1}^{p-1} \frac{2}{p + p_i} + \sum_{j=1}^{q-1} \frac{2}{q + q_j} \right) - \left(\sum_{i=1}^{p-1} \frac{2}{(p+q-1) + p_i} + \sum_{j=1}^{q-1} \frac{2}{(p+q-1) + q_j} \right)$$
$$= \sum_{i=1}^{p-1} \left(\frac{2}{p + p_i} - \frac{2}{(p+q-1) + p_i} \right) + \sum_{j=1}^{q-1} \left(\frac{2}{q + q_j} - \frac{2}{(p+q-1) + q_j} \right) > 0.$$

This proves the lemma. □

Lemma 2.2. *(i) For integer $q \geq 3$, the function $f(x) = \frac{2}{q+x} - \frac{2}{q+x-1}$ is increasing for $x \geq 1$.*

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

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

(iv) The function $l(x) = \frac{4}{(x+2)^2} - \frac{8}{(x+1)^2} + \frac{4}{x^2} > 0$ for $x \geq 3$.

Proof. (i) For $x \geq 1$, we have

$$f'(x) = -\frac{2}{(q+x)^2} + \frac{2}{(q+x-1)^2} > 0,$$

and hence (i) holds.

(ii) Let $g_1(x) = \frac{4}{x+1} + \frac{2(x-3)}{x}$, then $g(x) = g_1(x+1) - g_1(x)$. For $x \geq 3$, we have

$$g_1''(x) = \frac{8}{(x+1)^3} - \frac{12}{x^3} = \frac{-4(x^3 + 9x^2 + 9x + 3)}{x^3(x+1)^3} < 0,$$

and $g'(x) = g_1'(x+1) - g_1'(x) < 0$. This proves (ii).

(iii) Let $h_1(x) = \frac{2}{x+1} + \frac{2(x-3)}{x}$, then $h(x) = h_1(x+1) - h_1(x)$. For $x \geq 3$, we see that

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

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

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

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

which implies that (iv) holds. □

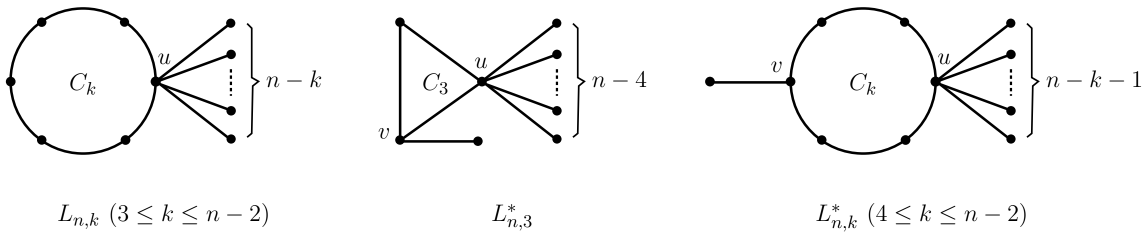

Figure 1: The graphs $L_{n,k}$ and $L^*_{n,k}$ $(3 \leq k \leq n-2)$.

For each $3 \leq k \leq n-2$, let $L_{n,k}$ be the unicyclic graph with n vertices obtained by attaching $n-k$ pendent edges to one vertex u of C_k (see Figure 1).

Theorem 2.3. *Let $G \in \mathscr{U}_{n,k}$. Then $H(G) \geq \frac{k-2}{2} + \frac{4}{n-k+4} + \frac{2(n-k)}{n-k+3}$ with equality if and only if $G \cong L_{n,k}$.*

Proof. We prove the theorem by induction on n. If $n = k+2$, then it is easy to calculate that the assertion of the theorem holds. So we may assume that $n > k+2$ 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 $\mathscr{U}_{n,k}$.

Let $w \in V(G)$ be a pendent vertex and let $vw \in E(G)$. Then $d(v) = q \geq 2$. Since $G \in \mathscr{U}_{n,k}$, we have $q \leq n-k+2$. Let $N(v) = \{w, v_1, \ldots, v_{q-1}\}$ with $d(v_i) = q_i$ for each $1 \leq i \leq q-1$. Note that there exists at least one vertex in $\{v_1, \ldots, v_{q-1}\}$ with degree at least 2.

Suppose there is exactly one vertex in $\{v_1, \ldots, v_{q-1}\}$ with degree at least 2, say u. Then by Lemma 2.1, there exists a graph $G' \in \mathscr{U}_{n,k}$ such that $H(G) > H(G')$, contradicting the assumption that G has the minimum harmonic index for graphs in $\mathscr{U}_{n,k}$.

So we may further assume that there are at least two vertices in $\{v_1, \ldots, v_{q-1}\}$ with degree at least 2 (and hence $q \geq 3$). Let $G'' := G - w$, then $G'' \in \mathscr{U}_{n-1,k}$. Now by applying Lemma 2.2(i), Lemma 2.2(ii) and the induction hypothesis, we have

$$\begin{aligned}
H(G) &= H(G'') + \frac{2}{q+1} + \sum_{i=1}^{q-1} \left(\frac{2}{q+q_i} - \frac{2}{(q-1)+q_i} \right) \\
&\geq H(G'') + \frac{2}{q+1} + 2\left(\frac{2}{q+2} - \frac{2}{q+1} \right) + (q-3)\left(\frac{2}{q+1} - \frac{2}{q} \right) \\
&= H(G'') + \left(\frac{4}{q+2} + \frac{2(q-4)}{q+1} - \frac{2(q-3)}{q} \right) \\
&\geq \left(\frac{k-2}{2} + \frac{4}{(n-1)-k+4} + \frac{2[(n-1)-k]}{(n-1)+k+3} \right) + \left(\frac{4}{q+2} + \frac{2(q-4)}{q+1} - \frac{2(q-3)}{q} \right) \\
&\geq \left(\frac{k-2}{2} + \frac{4}{n-k+3} + \frac{2(n-k-1)}{n-k+2} \right) + \left(\frac{4}{(n-k+2)+2} + \frac{2[(n-k+2)-4]}{(n-k+2)+1} - \frac{2[(n-k+2)-3]}{n-k+2} \right) \\
&= \frac{k-2}{2} + \frac{4}{n-k+4} + \frac{2(n-k)}{n-k+3}
\end{aligned}$$

with equalities if and only if $G'' \cong L_{n-1,k}$, $d(v) = q = n-k+2$, exactly two vertices in $\{v_1, \ldots, v_{q-1}\}$ have degree 2 and the other $q-3$ vertices in $\{v_1, \ldots, v_{q-1}\}$ have degree 1, i.e., $G \cong L_{n,k}$. This completes the proof of the theorem. □

In order to determine the second-minimum harmonic index for graphs in $\mathscr{U}_{n,k}$, we need the following auxiliary lemmas.

Lemma 2.4. *Let H be a nontrivial connected graph, and let $uv \in E(H)$ such that $d_H(u) = d_H(v) = 2$ and the other neighbors of u and v have degree at least 2 in H. Let G be the graph obtained from H by attaching $p-2$ and $q-2$ pendent edges ($p \geq q \geq 3$) to u and v, respectively, and let G' be the graph obtained from H by attaching $p+q-4$ pendent edges to u. Then $H(G) > H(G')$.*

Proof. Let $N_H(u) = \{v, w\}$ with $d_H(w) = s \geq 2$, and let $N_H(v) = \{u, w'\}$ with $d_H(w') = t \geq 2$. Since $p \geq q \geq 3$, we have

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

If $p = q = 3$, then

$$H(G) - H(G') > 2 \cdot (3-2) \cdot \left(\frac{3-2}{(3+1)\cdot(3+3-1)} - \frac{1}{4\cdot(3+2)} \right) = 0.$$

So we may assume that $p \geq 4$. Hence

$$\begin{aligned} H(G) - H(G') &> 2(q-2)\left(\frac{p-2}{(q+2)(p+p-1)} - \frac{1}{4(q+2)}\right) \\ &= \frac{2(q-2)}{q+2}\left(\frac{p-2}{2p-1} - \frac{1}{4}\right) \\ &= \frac{2(q-2)}{q+2} \cdot \frac{2p-7}{4(2p-1)} > 0. \end{aligned}$$

This proves Lemma 2.4. □

Lemma 2.5. *Let H be a nontrivial connected graph, and let $uv \in E(H)$ such that $d_H(u) = d_H(v) = 2$ and the other neighbors of u and v also have degree 2 in H. Let G be the graph obtained from H by attaching $p-2$ and $q-2$ pendent edges ($p \geq q \geq 3$) to u and v, respectively, and let G' be the graph obtained from H by attaching $p-1$ and $q-3$ pendent edges to u and v, respectively. Then $H(G) > H(G')$.*

Proof. Let $h(x) = \frac{2}{x+2} + \frac{2(x-3)}{x+1} - \frac{2(x-3)}{x}$. Then by Lemma 2.2(iii), $h(x)$ is decreasing for $x \geq 3$. Since $p \geq q \geq 3$, we conclude that

$$\begin{aligned} & H(G) - H(G') \\ &= \left(\frac{2}{p+2} + \frac{2(p-2)}{p+1} + \frac{2(q-2)}{q+1} + \frac{2}{q+2}\right) - \left(\frac{2}{(p+1)+2} + \frac{2(p-1)}{(p+1)+1} + \frac{2(q-3)}{(q-1)+1} + \frac{2}{(q-1)+2}\right) \\ &= \left(\frac{2}{q+2} + \frac{2(q-3)}{q+1} - \frac{2(q-3)}{q}\right) - \left(\frac{2}{p+3} + \frac{2(p-2)}{p+2} - \frac{2(p-2)}{p+1}\right) \\ &= h(q) - h(p+1) > 0. \end{aligned}$$

So the assertion of the lemma holds. □

Lemma 2.6. *Let H be a nontrivial connected graph, and let u, v be two distinct vertices in H such that $uv \notin E(H)$, $d_H(u) = d_H(v) = 2$ and all neighbors of u and v also have degree 2 in H. Let G be the graph obtained from H by attaching $p-2$ and $q-2$ pendent edges ($p \geq q \geq 3$) to u and v, respectively, and let G' be the graph obtained from H by attaching $p-1$ and $q-3$ pendent edges to u and v, respectively. Then $H(G) > H(G')$.*

Proof. Let $g(x) = \frac{4}{x+2} + \frac{2(x-4)}{x+1} - \frac{2(x-3)}{x}$. Then by Lemma 2.2(ii), $g(x)$ is decreasing for $x \geq 3$. Since $p \geq q \geq 3$, we see that

$$\begin{aligned} & H(G) - H(G') \\ &= \left(\frac{4}{p+2} + \frac{2(p-2)}{p+1} + \frac{2(q-2)}{q+1} + \frac{4}{q+2}\right) - \left(\frac{4}{(p+1)+2} + \frac{2(p-1)}{(p+1)+1} + \frac{2(q-3)}{(q-1)+1} + \frac{4}{(q-1)+2}\right) \\ &= \left(\frac{4}{q+2} + \frac{2(q-4)}{q+1} - \frac{2(q-3)}{q}\right) - \left(\frac{4}{p+3} + \frac{2(p-3)}{p+2} - \frac{2(p-2)}{p+1}\right) \\ &= g(q) - g(p+1) > 0. \end{aligned}$$

This proves the lemma. □

For each $3 \leq k \leq n-2$, let $L_{n,k}^1$ be the set of unicyclic graphs with n vertices obtained by attaching p and q pendent edges ($p \geq q \geq 1$ and $p + q = n - k$) to two distinct vertices u, v of C_k, respectively, and let $L_{n,k}^2$ be the set of unicyclic graphs with n vertices obtained by attaching q pendent edges ($1 \leq q \leq n-k-1$) to a pendent vertex v of $L_{n-q,k}$ (see Figure 2 for an illustration).

Lemma 2.7. *Let $G \in L_{n,k}^1$.*

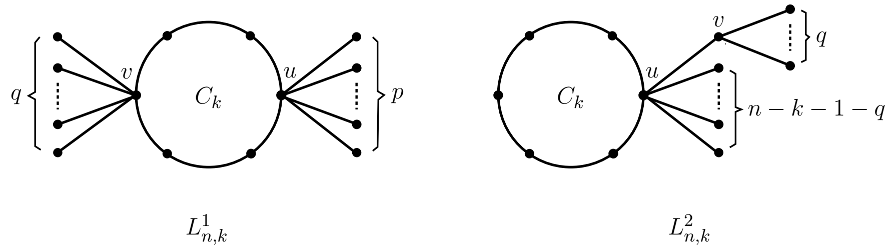

Figure 2: The graph sets $L^1_{n,k}$ and $L^2_{n,k}$ $(3 \le k \le n-2)$.

(*i*) *If* $k = 3$, *then* $H(G) \ge \frac{2}{n+1} + \frac{2}{n} + \frac{2(n-4)}{n-1} + \frac{9}{10}$ *with equality if and only if* $q = 1$.

(*ii*) *If* $4 \le k \le n-2$, *then* $H(G) \ge \frac{k-3}{2} + \frac{4}{n-k+3} + \frac{2(n-k-1)}{n-k+2} + \frac{4}{5}$ *with equality if and only if* $uv \notin E(G)$ *and* $q = 1$.

Proof. First suppose that $k = 3$. Then $uv \in E(G)$. By applying Lemma 2.5, we have $H(G) \ge \frac{2}{n+1} + \frac{2}{n} + \frac{2(n-4)}{n-1} + \frac{9}{10}$ with equality if and only if $p = n-4$ and $q = 1$. This proves (i).

Now assume that $4 \le k \le n-2$. If $uv \in E(G)$, then by Lemma 2.5, we conclude that $H(G) \ge \frac{k-2}{2} + \frac{2}{n-k+4} + \frac{2}{n-k+3} + \frac{2(n-k-1)}{n-k+2} + \frac{2}{5}$ with equality if and only if $p = n-k-1$ and $q = 1$. If $uv \notin E(G)$, then by Lemma 2.6, we have $H(G) \ge \frac{k-3}{2} + \frac{4}{n-k+3} + \frac{2(n-k-1)}{n-k+2} + \frac{4}{5}$ with equality if and only if $p = n-k-1$ and $q = 1$. Since

$$\begin{aligned}
&\left(\frac{k-2}{2} + \frac{2}{n-k+4} + \frac{2}{n-k+3} + \frac{2(n-k-1)}{n-k+2} + \frac{2}{5}\right) - \left(\frac{k-3}{2} + \frac{4}{n-k+3} + \frac{2(n-k-1)}{n-k+2} + \frac{4}{5}\right)\\
&= \left(\frac{2}{n-k+4} - \frac{2}{n-k+3}\right) + \frac{1}{10}\\
&= -\frac{2}{(n-k+3)(n-k+4)} + \frac{1}{10}\\
&\ge -\frac{2}{(2+3)\cdot(2+4)} + \frac{1}{10} > 0,
\end{aligned}$$

we see that (ii) holds. This finishes the proof of the lemma. □

Lemma 2.8. *Let* $G \in L^2_{n,k}$. *Then* $H(G) \ge \frac{k-2}{2} + \frac{6}{n-k+3} + \frac{2(n-k-2)}{n-k+2} + \frac{2}{3}$ *with equality if and only if* $q = 1$.

Proof. It is easy to see that the assertion of the lemma holds for $n-k = 2$ (since there is only one such graph in $L^2_{n,k}$). So we may assume that $n-k \ge 3$. Let

$$f(q) = H(G) = \frac{k-2}{2} + \frac{2}{n-k+3} + \frac{4}{n-k+4-q} + \frac{2(n-k-1-q)}{n-k+3-q} + \frac{2q}{q+2}$$

with $1 \le q \le n-k-1$. Hence

$$f'(q) = \frac{4}{(n-k+4-q)^2} - \frac{8}{(n-k+3-q)^2} + \frac{4}{(q+2)^2}.$$

If $1 \le q \le \lfloor\frac{n-k}{2}\rfloor$ (i.e., $q+2 \le n-k+2-q$), then by Lemma 2.2(iv) (with $x = n-k+2-q \ge 3$), we have

$$\begin{aligned}
f'(q) &= \left(\frac{4}{(n-k+4-q)^2} - \frac{8}{(n-k+3-q)^2} + \frac{4}{(n-k+2-q)^2}\right) + \left(\frac{4}{(q+2)^2} - \frac{4}{(n-k+2-q)^2}\right)\\
&\ge \frac{4}{(n-k+4-q)^2} - \frac{8}{(n-k+3-q)^2} + \frac{4}{(n-k+2-q)^2}\\
&= \frac{4}{(x+2)^2} - \frac{8}{(x+1)^2} + \frac{4}{x^2} > 0.
\end{aligned}$$

If $\lceil \frac{n-k+1}{2} \rceil \leq q \leq n-k-1$ (i.e., $q+2 \geq n-k+3-q$), we know that

$$f'(q) = \left(\frac{4}{(n-k+4-q)^2} - \frac{4}{(n-k+3-q)^2} \right) + \left(\frac{4}{(q+2)^2} - \frac{4}{(n-k+3-q)^2} \right) < 0.$$

This implies that $f(q)$ is increasing for $1 \leq q \leq \lfloor \frac{n-k}{2} \rfloor$ and decreasing for $\lceil \frac{n-k+1}{2} \rceil \leq q \leq n-k-1$. Therefore the minimum value of $f(q)$ is $\min\{f(1), f(n-k-1)\}$. Since $n-k \geq 3$, we have

$$\begin{aligned}
f(n-k-1) - f(1) &= \left(\frac{k-2}{2} + \frac{2}{n-k+3} + \frac{2(n-k-1)}{n-k+1} + \frac{4}{5} \right) - \left(\frac{k-2}{2} + \frac{6}{n-k+3} + \frac{2(n-k-2)}{n-k+2} + \frac{2}{3} \right) \\
&= \left(-\frac{4}{n-k+3} - \frac{2(n-k-2)}{n-k+2} + \frac{2(n-k-1)}{n-k+1} \right) + \frac{2}{15} \\
&= \left(-\frac{4}{n-k+3} + \frac{8}{n-k+2} - \frac{4}{n-k+1} \right) + \frac{2}{15} \\
&= -\frac{8}{(n-k+1)(n-k+2)(n-k+3)} + \frac{2}{15} \\
&\geq -\frac{8}{(3+1)\cdot(3+2)\cdot(3+3)} + \frac{2}{15} > 0.
\end{aligned}$$

So the assertion of Lemma 2.8 holds. $\square$

Let $L^*_{n,3}$ be the unicyclic graph with n vertices obtained by attaching $n-4$ and one pendent edges to two adjacent vertices u, v of a triangle, respectively. For each $4 \leq k \leq n-2$, let $L^*_{n,k}$ be the set of unicyclic graphs with n vertices obtained by attaching $n-k-1$ and one pendent edges to two non-adjacent vertices u, v of C_k, respectively (see Figure 1). Note that $L^*_{n,k} \subseteq L^1_{n,k}$ and there are $\lfloor \frac{k}{2} \rfloor - 1$ unicyclic graphs in $L^*_{n,k}$ for each $4 \leq k \leq n-2$. We can now determine the second-minimum harmonic index for graphs in $\mathscr{U}_{n,k}$.

Theorem 2.9. *Let $G \in \mathscr{U}_{n,k}$ and $G \ncong L_{n,k}$.*

(*i*) *If $k = 3$, then $H(G) \geq \frac{2}{n+1} + \frac{2}{n} + \frac{2(n-4)}{n-1} + \frac{9}{10}$ with equality if and only if $G \cong L^*_{n,3}$.*

(*ii*) *If $4 \leq k \leq n-2$, then $H(G) \geq \frac{k-3}{2} + \frac{4}{n-k+3} + \frac{2(n-k-1)}{n-k+2} + \frac{4}{5}$ with equality if and only if $G \in L^*_{n,k}$.*

Proof. Let $C := v_1 v_2 \ldots v_k v_1$ be the unique cycle in G. Then there exists at least one vertex in $\{v_1, v_2, \ldots, v_k\}$ with degree at least 3. For convenience of the proof, let $A := \frac{2}{n+1} + \frac{2}{n} + \frac{2(n-4)}{n-1} + \frac{9}{10}$ (if $k = 3$) or $A := \frac{k-3}{2} + \frac{4}{n-k+3} + \frac{2(n-k-1)}{n-k+2} + \frac{4}{5}$ (if $4 \leq k \leq n-2$), and let $B := \frac{k-2}{2} + \frac{6}{n-k+3} + \frac{2(n-k-2)}{n-k+2} + \frac{2}{3}$.

Suppose there are at least three vertices in $\{v_1, v_2, \ldots, v_k\}$ with degree at least 3. Then by applying Lemma 2.1, Lemma 2.4 (or Lemma 2.6) and Lemma 2.7, there exists a graph $G_1 \in L^1_{n,k}$ such that $H(G) > H(G_1) \geq A$.

If there are exactly two vertices in $\{v_1, v_2, \ldots, v_k\}$ with degree at least 3, then by Lemma 2.1, Lemma 2.5 (or Lemma 2.6) and Lemma 2.7, there exists a graph $G_2 \in L^1_{n,k}$ such that $H(G) \geq H(G_2) \geq A$ with equalities if and only if $G \cong L^*_{n,k}$.

So we may assume that there is exactly one vertex in $\{v_1, v_2, \ldots, v_k\}$ with degree at least 3. Since $G \ncong L_{n,k}$, we know that there exists at least one non-pendent vertex outside C. If there are at least two non-pendent vertices outside C, then by Lemma 2.1 and Lemma 2.8, there exists a graph $G_3 \in L^2_{n,k}$ such that $H(G) > H(G_3) \geq B$. Hence we may further assume that there is only one non-pendent vertex outside C, which implies that $G \in L^2_{n,k}$. Then by Lemma 2.8, we have $H(G) \geq B$ with equality if and only if $q = 1$.

To prove the theorem, it suffices to compare the two values A and B. If $k = 3$, then

$$\begin{aligned}
B - A &= \left(\frac{3-2}{2} + \frac{6}{n-3+3} + \frac{2(n-3-2)}{n-3+2} + \frac{2}{3}\right) - \left(\frac{2}{n+1} + \frac{2}{n} + \frac{2(n-4)}{n-1} + \frac{9}{10}\right) \\
&= \left(-\frac{2}{n+1} + \frac{4}{n} - \frac{2}{n-1}\right) + \frac{4}{15} \\
&= -\frac{4}{n(n-1)(n+1)} + \frac{4}{15} \\
&\geq -\frac{4}{5\cdot(5-1)\cdot(5+1)} + \frac{4}{15} > 0.
\end{aligned}$$

So (i) holds. If $4 \leq k \leq n-2$, then

$$\begin{aligned}
B - A &= \left(\frac{k-2}{2} + \frac{6}{n-k+3} + \frac{2(n-k-2)}{n-k+2} + \frac{2}{3}\right) - \left(\frac{k-3}{2} + \frac{4}{n-k+3} + \frac{2(n-k-1)}{n-k+2} + \frac{4}{5}\right) \\
&= \left(\frac{2}{n-k+3} - \frac{2}{n-k+2}\right) + \frac{11}{30} \\
&= -\frac{2}{(n-k+2)(n-k+3)} + \frac{11}{30} \\
&\geq -\frac{2}{(2+2)\cdot(2+3)} + \frac{11}{30} > 0.
\end{aligned}$$

This proves (ii), and hence completes the proof of the theorem. □

By applying Theorem 2.3 and Theorem 2.9, we have the following result.

Corollary 2.10. *Let $L_{n,k}$ and $L^*_{n,k}$ be the graphs defined as above.*

(*i*) *If $n = 5$, then*

$$H(L_{5,3}) < H(L^*_{5,3}) < H(U_{5,4}) < H(C_5).$$

(*ii*) *If $n \geq 6$, then*

$$H(L_{n,3}) < H(L^*_{n,3}) < H(L_{n,4}) < H(L^*_{n,4}) < \cdots < H(L_{n,n-2}) < H(L^*_{n,n-2}) < H(U_{n,n-1}) < H(C_n).$$

Proof. Since $H(L^*_{5,3}) = \frac{32}{15} < H(U_{5,4}) = \frac{23}{10} < H(C_5) = \frac{5}{2}$, we know that (i) holds.

We now prove (ii). By Theorem 2.3 and Theorem 2.9, we have $H(L_{n,k}) < H(L^*_{n,k})$ for each $3 \leq k \leq n-2$. Since $H(L^*_{n,n-2}) = \frac{n}{2} - \frac{2}{5} < H(U_{n,n-1}) = \frac{n}{2} - \frac{1}{5} < H(C_n) = \frac{n}{2}$, in order to prove (ii), it suffices to show that $H(L^*_{n,k}) < H(L_{n,k+1})$ for each $3 \leq k \leq n-3$. If $k = 3$, then we have

$$\begin{aligned}
H(L^*_{n,3}) - H(L_{n,4}) &= \left(\frac{2}{n+1} + \frac{2}{n} + \frac{2(n-4)}{n-1} + \frac{9}{10}\right) - \left(\frac{4-2}{2} + \frac{4}{n-4+4} + \frac{2(n-4)}{n-4+3}\right) \\
&= \left(\frac{2}{n+1} - \frac{2}{n}\right) - \frac{1}{10} < 0.
\end{aligned}$$

This implies that $H(L^*_{n,3}) < H(L_{n,4})$. For each $4 \leq k \leq n-3$ (and hence $n \geq 7$), we have

$$\begin{aligned}
&H(L^*_{n,k}) - H(L_{n,k+1}) \\
&= \left(\frac{k-3}{2} + \frac{4}{n-k+3} + \frac{2(n-k-1)}{n-k+2} + \frac{4}{5}\right) - \left(\frac{(k+1)-2}{2} + \frac{4}{n-(k+1)+4} + \frac{2[n-(k+1)]}{n-(k+1)+3}\right) \\
&= -\frac{1}{5} < 0.
\end{aligned}$$

So the assertion of the corollary holds. □

It was shown in [27] that $L_{n,3}$ is the unique graph with the minimum harmonic index for graphs in $\mathscr{U}_n$. By Theorem 2.3, Theorem 2.9 and Corollary 2.10, we conclude that $L^*_{n,3}$ is the unique graph with the second-minimum harmonic index for graphs in $\mathscr{U}_n$.

3. The Maximum and Second-Maximum Harmonic Indices for Graphs in $\mathscr{U}_{n,k}$

In this section, we consider the maximum and second-maximum harmonic indices for graphs in $\mathscr{U}_{n,k}$, and characterize the corresponding extremal graphs. The extremal graphs with the second-maximum, third-maximum and fourth-maximum harmonic indices for graphs in $\mathscr{U}_n$ are also determined. First, we prove the following two lemmas.

Lemma 3.1. *Let H be a nontrivial connected graph with $u \in V(H)$. Let G be the graph obtained from H by attaching two paths $P := uu_1 \ldots u_s$ and $Q := uv_1 \ldots v_t$ $(s \geq t \geq 1)$ at u, and let $G' := G - uv_1 + u_s v_1$. Then $H(G) < H(G')$.*

Proof. Let $d_G(u) = p \geq 3$, and let $N_H(u) = N_G(u) \setminus \{u_1, v_1\} = \{w_1, \ldots, w_{p-2}\}$ with $d_H(w_i) = d_G(w_i) = p_i$ for each $1 \leq i \leq p-2$. We consider three cases according to the values of s and t.

Case 1. $s = t = 1$.

In this case, $d_G(u_1) = d_G(v_1) = 1$. Then

$$\begin{aligned} H(G) - H(G') &= \left(\sum_{i=1}^{p-2} \frac{2}{p+p_i} + \frac{4}{p+1}\right) - \left(\sum_{i=1}^{p-2} \frac{2}{(p-1)+p_i} + \frac{2}{(p-1)+2} + \frac{2}{3}\right) \\ &= \sum_{i=1}^{p-2} \left(\frac{2}{p+p_i} - \frac{2}{(p-1)+p_i}\right) + \frac{2}{p+1} - \frac{2}{3} \\ &< \frac{2}{p+1} - \frac{2}{3} \leq \frac{2}{3+1} - \frac{2}{3} < 0. \end{aligned}$$

Case 2. $s > t = 1$.

In this case, $d_G(u_1) = 2$ and $d_G(v_1) = 1$. Hence we have

$$\begin{aligned} H(G) - H(G') &= \left(\sum_{i=1}^{p-2} \frac{2}{p+p_i} + \frac{2}{p+2} + \frac{2}{p+1} + \frac{2}{3}\right) - \left(\sum_{i=1}^{p-2} \frac{2}{(p-1)+p_i} + \frac{2}{(p-1)+2} + \frac{1}{2} + \frac{2}{3}\right) \\ &= \sum_{i=1}^{p-2} \left(\frac{2}{p+p_i} - \frac{2}{(p-1)+p_i}\right) + \frac{2}{p+2} - \frac{1}{2} \\ &< \frac{2}{p+2} - \frac{1}{2} \leq \frac{2}{3+2} - \frac{1}{2} < 0. \end{aligned}$$

Case 3. $s \geq t > 1$.

Now $d_G(u_1) = d_G(v_1) = 2$. Therefore

$$\begin{aligned} H(G) - H(G') &= \left(\sum_{i=1}^{p-2} \frac{2}{p+p_i} + \frac{4}{p+2} + \frac{2}{3}\right) - \left(\sum_{i=1}^{p-2} \frac{2}{(p-1)+p_i} + \frac{2}{(p-1)+2} + 1\right) \\ &= \sum_{i=1}^{p-2} \left(\frac{2}{p+p_i} - \frac{2}{(p-1)+p_i}\right) + \frac{4}{p+2} - \frac{2}{p+1} - \frac{1}{3} \\ &< \frac{4}{p+2} - \frac{2}{p+1} - \frac{1}{3} = -\frac{(p-1)(p-2)}{3(p+1)(p+2)} < 0. \end{aligned}$$

So the assertion of the lemma holds. □

Lemma 3.2. *Let H be a nontrivial connected graph, and let u, v be two distinct vertices in H with $d_H(u), d_H(v) \geq 2$. Moreover, suppose that the two neighbors of v have degree sum at most 9 in H if $d_H(v) = 2$. Let G be the graph obtained from H by attaching the paths $P := uu_1 \ldots u_s$ and $Q := vv_1 \ldots v_t$ ($s \geq t \geq 1$) at u and v, respectively, and let $G' := G - vv_1 + u_s v_1$. Then $H(G) < H(G')$.*

Proof. Since $N_G(u) = N_H(u) \cup \{u_1\}$, $N_G(v) = N_H(v) \cup \{v_1\}$ and $d_H(u), d_H(v) \geq 2$, we have $d_G(u) = p \geq 3$ and $d_G(v) = q \geq 3$. Let $N_H(v) = N_G(v) \setminus \{v_1\} = \{w_1, \ldots, w_{q-1}\}$ with $d_G(w_i) = q_i$ for each $1 \leq i \leq q-1$. If $uv \in E(G)$, we further assume that $w_1 = u$. Similar to Lemma 3.1, we consider three cases according to the values of s and t.

Case 1. $s = t = 1$.

Since $d_G(u_1) = d_G(v_1) = 1$, we have

$$\begin{aligned}
H(G) - H(G') &= \left(\sum_{i=1}^{q-1} \frac{2}{q+q_i} + \frac{2}{q+1} + \frac{2}{p+1}\right) - \left(\sum_{i=1}^{q-1} \frac{2}{(q-1)+q_i} + \frac{2}{p+2} + \frac{2}{3}\right) \\
&= \sum_{i=1}^{q-1}\left(\frac{2}{q+q_i} - \frac{2}{(q-1)+q_i}\right) + \frac{2}{(p+1)(p+2)} + \frac{2}{q+1} - \frac{2}{3} \\
&< \frac{2}{(p+1)(p+2)} + \frac{2}{q+1} - \frac{2}{3} \\
&\leq \frac{2}{(3+1)\cdot(3+2)} + \frac{2}{3+1} - \frac{2}{3} < 0.
\end{aligned}$$

Case 2. $s > t = 1$.

Now $d_G(u_1) = 2$ and $d_G(v_1) = 1$. Hence

$$\begin{aligned}
H(G) - H(G') &= \left(\sum_{i=1}^{q-1} \frac{2}{q+q_i} + \frac{2}{q+1} + \frac{2}{3}\right) - \left(\sum_{i=1}^{q-1} \frac{2}{(q-1)+q_i} + \frac{1}{2} + \frac{2}{3}\right) \\
&= \sum_{i=1}^{q-1}\left(\frac{2}{q+q_i} - \frac{2}{(q-1)+q_i}\right) + \frac{2}{q+1} - \frac{1}{2} \\
&< \frac{2}{q+1} - \frac{1}{2} \leq \frac{2}{3+1} - \frac{1}{2} = 0.
\end{aligned}$$

Case 3. $s \geq t > 1$.

In this case, $d_G(u_1) = d_G(v_1) = 2$. Then

$$\begin{aligned}
H(G) - H(G') &= \left(\sum_{i=1}^{q-1} \frac{2}{q+q_i} + \frac{2}{q+2} + \frac{2}{3}\right) - \left(\sum_{i=1}^{q-1} \frac{2}{(q-1)+q_i} + 1\right) \\
&= \sum_{i=1}^{q-1}\left(\frac{2}{q+q_i} - \frac{2}{(q-1)+q_i}\right) + \frac{2}{q+2} - \frac{1}{3} \\
&= -\sum_{i=1}^{q-1} \frac{2}{(q+q_i)(q-1+q_i)} + \frac{2}{q+2} - \frac{1}{3}.
\end{aligned}$$

If $q \geq 4$, then

$$H(G) - H(G') < \frac{2}{q+2} - \frac{1}{3} \leq \frac{2}{4+2} - \frac{1}{3} = 0.$$

So we may assume that $q = 3$. Then by the assumption of the lemma, we have $q_1 + q_2 \leq 10$ (since it is possible that $w_1 = u$ and hence $q_1 = d_G(u) = d_H(u) + 1$). Therefore

$$\begin{aligned} H(G) - H(G') &= -\frac{2}{(3+q_1)(2+q_1)} - \frac{2}{(3+q_2)(2+q_2)} + \frac{2}{3+2} - \frac{1}{3} \\ &\leq -\frac{2}{(3+5)\cdot(2+5)} - \frac{2}{(3+5)\cdot(2+5)} + \frac{2}{5} - \frac{1}{3} < 0. \end{aligned}$$

This proves Lemma 3.2. $\square$

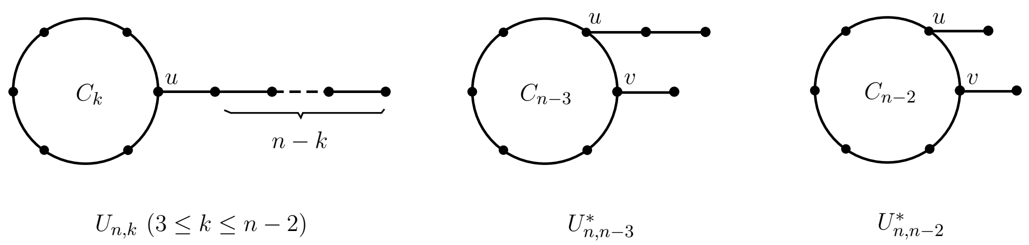

Figure 3: The graphs $U_{n,k}$ $(3 \leq k \leq n-2)$, $U^*_{n,n-3}$ and $U^*_{n,n-2}$.

For each $3 \leq k \leq n-2$, let $U_{n,k}$ be the unicyclic graph with n vertices obtained by attaching a path of length $n-k$ to one vertex u of C_k (see Figure 3).

Theorem 3.3. *Let $G \in \mathscr{U}_{n,k}$. Then $H(G) \leq \frac{n}{2} - \frac{2}{15}$ with equality if and only if $G \cong U_{n,k}$.*

Proof. Let $C := v_1v_2\ldots v_kv_1$ be the unique cycle in G. Then there exists at least one vertex in $\{v_1, v_2, \ldots, v_k\}$ with degree at least 3.

Suppose there are at least two vertices in $\{v_1, v_2, \ldots, v_k\}$ with degree at least 3. Then by Lemma 3.1 and Lemma 3.2, we have $H(G) < H(U_{n,k})$.

So we may assume that there is exactly one vertex in $\{v_1, v_2, \ldots, v_k\}$ with degree at least 3, say v_i. If $d(v_i) \geq 4$, then by Lemma 3.1, we also have $H(G) < H(U_{n,k})$. Hence we may further assume that $d(v_i) = 3$. Then by Lemma 3.1, we see that $H(G) \leq H(U_{n,k})$ with equality if and only if $G \cong U_{n,k}$. It is easy to calculate that $H(U_{n,k}) = \frac{n}{2} - \frac{2}{15}$. This finishes the proof of Theorem 3.3. $\square$

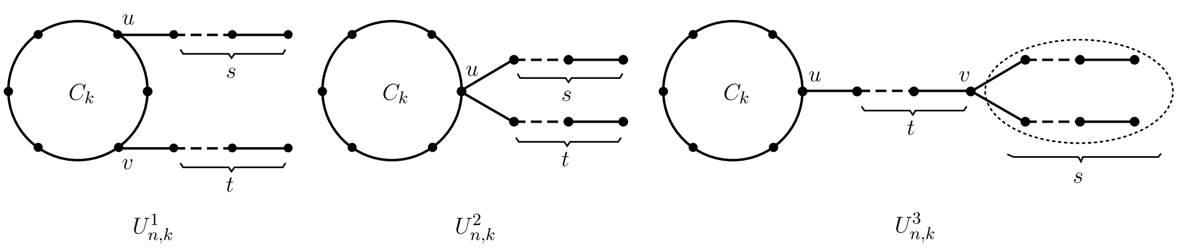

Figure 4: The graph sets $U^1_{n,k}$, $U^2_{n,k}$ $(3 \leq k \leq n-2)$ and $U^3_{n,k}$ $(3 \leq k \leq n-3)$.

For each $3 \leq k \leq n-2$, let $U^1_{n,k}$ be the set of unicyclic graphs with n vertices obtained by attaching two paths of length s and t ($s \geq t \geq 1$ and $s+t = n-k$) to two distinct vertices u, v of C_k, respectively, and let $U^2_{n,k}$ be the set of unicyclic graphs with n vertices obtained by attaching two paths of length s and t ($s \geq t \geq 1$ and $s+t = n-k$) to one vertex u of C_k. For each $3 \leq k \leq n-3$, let $U^3_{n,k}$ be the set of unicyclic graphs with n vertices obtained by connecting a path of length t between a vertex u of C_k and a non-pendent vertex v of a path of length s ($s \geq 2$, $t \geq 1$ and $s+t = n-k$). See Figure 4 for an illustration.

Lemma 3.4. *Let $G \in U^1_{n,k} \bigcup U^2_{n,k}$ with $3 \le k \le n-4$. Then $H(G) \le \frac{n}{2} - \frac{7}{30}$ with equality if and only if $G \in U^1_{n,k}$, $uv \in E(G)$ and $s \ge t > 1$.*

Proof. First suppose that $G \in U^1_{n,k}$. If $uv \in E(G)$, then

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

If $uv \notin E(G)$, then

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

Now assume that $G \in U^2_{n,k}$. Then

$$H(G) = \begin{cases} \frac{n}{2} - \frac{13}{30}, & \text{if } s > t = 1, \\ \frac{n}{2} - \frac{1}{3}, & \text{if } s \ge t > 1. \end{cases}$$

Since $\frac{n}{2} - \frac{13}{30} < \frac{n}{2} - \frac{1}{3} < \frac{n}{2} - \frac{3}{10} < \frac{n}{2} - \frac{4}{15} < \frac{n}{2} - \frac{7}{30}$, we see that the assertion of Lemma 3.4 holds. □

Lemma 3.5. *Let $G \in U^3_{n,k}$ with $3 \le k \le n-4$. Then $H(G) \le \frac{n}{2} - \frac{7}{30}$ with equality if and only if $uv \in E(G)$ (i.e., $t = 1$) and v is not adjacent to any pendent vertex.*

Proof. First assume that $t = 1$. Then $s \ge 3$ and v is adjacent to at most one pendent vertex. Hence

$$H(G) = \begin{cases} \frac{n}{2} - \frac{3}{10}, & \text{if } v \text{ is adjacent to one pendent vertex}, \\ \frac{n}{2} - \frac{7}{30}, & \text{if } v \text{ is not adjacent to any pendent vertex}. \end{cases}$$

Now suppose that $t > 1$. Then

$$H(G) = \begin{cases} \frac{n}{2} - \frac{2}{5}, & \text{if } v \text{ is adjacent to two pendent vertices}, \\ \frac{n}{2} - \frac{1}{3}, & \text{if } v \text{ is adjacent to one pendent vertex}, \\ \frac{n}{2} - \frac{4}{15}, & \text{if } v \text{ is not adjacent to any pendent vertex}. \end{cases}$$

Since $\frac{n}{2} - \frac{2}{5} < \frac{n}{2} - \frac{1}{3} < \frac{n}{2} - \frac{3}{10} < \frac{n}{2} - \frac{4}{15} < \frac{n}{2} - \frac{7}{30}$, we see that the assertion of the lemma holds. □

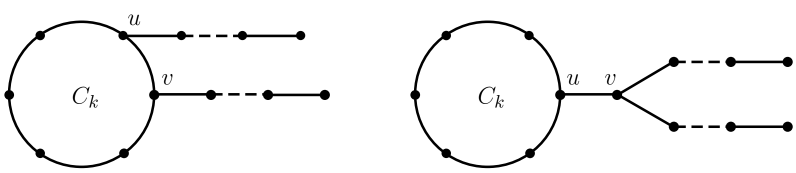

Figure 5: The two types of graphs in $U^*_{n,k}$ ($3 \le k \le n-4$).

For each $3 \le k \le n-4$, let $U^*_{n,k}$ be the set of unicyclic graphs with n vertices obtained either by attaching two paths of length at least 2 to two adjacent vertices u, v of C_k, respectively, or by connecting an edge between a vertex u of C_k and a vertex v of a path of length $n-k-1$ such that v is not adjacent to any pendent vertex (see Figure 5). Note that $U^*_{n,k} \subseteq U^1_{n,k} \bigcup U^3_{n,k}$ and $H(U^*_{n,k}) = \frac{n}{2} - \frac{7}{30}$. Let $U^*_{n,n-3}$ be the unicyclic graph with n vertices obtained by attaching a path of length 2 and a pendent edge to two adjacent vertices u, v of C_{n-3}, respectively, and let $U^*_{n,n-2}$ be the unicyclic graph with n vertices obtained by attaching two pendent edges to two adjacent vertices u, v of C_{n-2}, respectively (see Figure 3). By the similar arguments as in the proof of Thereom 3.3, we now determine the second-maximum harmonic index for graphs in $\mathscr{U}_{n,k}$.

Theorem 3.6. *Let $G \in \mathscr{U}_{n,k}$ and $G \ncong U_{n,k}$.*

(*i*) *If $3 \le k \le n-4$, then $H(G) \le \frac{n}{2} - \frac{7}{30}$ with equality if and only if $G \in U^*_{n,k}$.*

(*ii*) *If $k = n-3$, then $H(G) \le \frac{n}{2} - \frac{3}{10}$ with equality if and only if $G \cong U^*_{n,n-3}$.*

(*iii*) *If $k = n-2$, then $H(G) \le \frac{n}{2} - \frac{11}{30}$ with equality if and only if $G \cong U^*_{n,n-2}$.*

Proof. Let $C := v_1 v_2 \ldots v_k v_1$ be the unique cycle in G. Then there exists at least one vertex in $\{v_1, v_2, \ldots, v_k\}$ with degree at least 3.

We first consider the case that $3 \le k \le n-4$. Suppose there are at least three vertices in $\{v_1, v_2, \ldots, v_k\}$ with degree at least 3. Then by applying Lemma 3.1, Lemma 3.2 and Lemma 3.4, there exists a graph $G_1 \in U^1_{n,k}$ such that $H(G) < H(G_1) \le \frac{n}{2} - \frac{7}{30}$.

If there are exactly two vertices in $\{v_1, v_2, \ldots, v_k\}$ with degree at least 3, then by Lemma 3.1 and Lemma 3.4, there exists a graph $G_2 \in U^1_{n,k}$ such that $H(G) \le H(G_2) \le \frac{n}{2} - \frac{7}{30}$ with equalities if and only if $G \in U^1_{n,k} \bigcap U^*_{n,k}$.

So we may assume that there is exactly one vertex in $\{v_1, v_2, \ldots, v_k\}$ with degree at least 3, say v_i. If $d(v_i) \ge 5$, then by Lemma 3.1 and Lemma 3.4, there exists a graph $G_3 \in U^2_{n,k}$ such that $H(G) < H(G_3) < \frac{n}{2} - \frac{7}{30}$. If $d(v_i) = 4$, then by applying Lemma 3.1 and Lemma 3.4, there exists a graph $G_4 \in U^2_{n,k}$ such that $H(G) \le H(G_4) < \frac{n}{2} - \frac{7}{30}$. Hence we may also assume that $d(v_i) = 3$. Since $G \ncong U_{n,k}$, we see that there exists at least one vertex with degree at least 3 outside C. If there are at least two vertices with degree at least 3 outside C, then by Lemma 3.1 and Lemma 3.5, there must exist a graph $G_5 \in U^3_{n,k}$ such that $H(G) < H(G_5) \le \frac{n}{2} - \frac{7}{30}$. Therefore we may further assume that there is only one vertex with degree at least 3 outside C, which implies that $G \in U^3_{n,k}$. Then by Lemma 3.5, we have $H(G) \le \frac{n}{2} - \frac{7}{30}$ with equality if and only if $G \in U^*_{n,k}$. Since $U^*_{n,k} \subseteq U^1_{n,k} \bigcup U^3_{n,k}$, we know that (i) holds.

For the cases that $k = n-3$ or $k = n-2$, by the similar arguments as above, it is easy to calculate that (ii) and (iii) hold. This completes the proof of Theorem 3.6. □

Since $H(U_{n,n-1}) = \frac{n}{2} - \frac{1}{5}$ and $H(C_n) = \frac{n}{2}$, by Theorem 3.3 and Theorem 3.6, we immediately obtain the following result.

Corollary 3.7. *Let $U_{n,k}$ and $U^*_{n,k}$ be the graphs defined as above.*

(*i*) *If $n = 5$, then*

$$H(U^*_{5,3}) < H(U_{5,4}) < H(U_{5,3}) < H(C_5).$$

(*ii*) *If $n = 6$, then*

$$H(U^*_{6,4}) < H(U^*_{6,3}) < H(U_{6,5}) < H(U_{6,3}) = H(U_{6,4}) < H(C_6).$$

(*iii*) *If $n \ge 7$, then*

$$\begin{aligned} H(U^*_{n,n-2}) < H(U^*_{n,n-3}) < H(U^*_{n,n-4}) = \cdots = H(U^*_{n,3}) \\ < H(U_{n,n-1}) < H(U_{n,3}) = \cdots = H(U_{n,n-2}) < H(C_n). \end{aligned}$$

It was proved in [27] that C_n is the unique graph with the maximum harmonic index for graphs in $\mathscr{U}_n$. Now by Theorem 3.3, Theorem 3.6 and Corollary 3.7, we deduce that $U_{n,k}$ $(3 \le k \le n-2)$ are the unique graphs with the second-maximum harmonic index, and $U_{n,n-1}$ is the unique graph with the third-maximum harmonic index for graphs in $\mathscr{U}_n$. Furthermore, $U^*_{5,3}$ is the unique graph with the fourth-maximum harmonic index for graphs in $\mathscr{U}_5$, $U^*_{6,3}$ is the unique graph with the fourth-maximum harmonic index for graphs in $\mathscr{U}_6$, and the graphs in $U^*_{n,k}$ $(3 \le k \le n-4)$ are the unique graphs with the fourth-maximum harmonic index for graphs in $\mathscr{U}_n$ if $n \ge 7$.

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