The Harmonic Index on Unicyclic Graphs *

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Abstract

The Harmonic index $H(G)$ of a graph G is defined as the sum of 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 consider the Harmonic index of unicyclic graphs with a given order. We give the lower and upper bounds for Harmonic index of unicyclic graphs and characterize the corresponding extremal graphs.

Keywords: Harmonic index; unicyclic graph; degree

1 Introduction

For a graph $G = (V, E)$, the Harmonic index $H(G)$ of a graph G is defined as the sum of 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, i.e.,

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

In recent years, many researchers focus on topological indices of graphs, such as Randić index, Wiener index, Hosoya index. For a comprehensive survey of mathematical properties of the topological indices, see the book of Li and Gutman [4]. Favaron, Mahéo and Saclé [3] disproved some conjectures in [2] about the eigenvalues and Harmonic index. In [5], the lower and

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upper bounds for Harmonic index on trees and general graphs are obtained. In this paper, we consider the lower and upper bounds for Harmonic index on unicyclic graphs.

For a vertex u of a graph G, we use $N_G(u)$ (or $N(u)$) and $d_G(u)$ (or $d(u)$) to denote the neighborhood and the degree of u, respectively. If $d(u) = 1$, then we call u a pendent vertex. For two vertices v_i and v_j $(i \neq j)$, the distance between v_i and v_j in G is the number of edges in a shortest path joining v_i and v_j. We use $G - uv$ to denote the graph obtained from G by deleting the edge $uv \in E(G)$. Similarly, $G + uv$ is the graph that arises from G by adding an edge $uv \notin E(G)$, where $u, v \in V(G)$. We denote by S_n^+ the unicyclic graph obtained from the star S_n on n vertices by joining its two pendent vertices, and denote by C_n the cycle on n vertices. A path $P = u_0u_1 \dots u_k$ $(k \geq 2)$ in G is called a pendent path if $d(u_0) \geq 3$, $d(u_1) = d(u_2) = \dots = d(u_{k-1}) = 2$ and $d(u_k) = 1$. For $n = 3$, C_n is the unique unicyclic graph, so we only consider $n \geq 4$ in the following. For convenience, let $\mathcal{G}(n)$ be the set of unicyclic graphs with $n \geq 4$ vertices.

For terminology and notations not defined here, we refer the readers to [1].

2 The lower bound for Harmonic index on unicyclic graphs

Denote by G^* the graph in $\mathcal{G}(n)$ such that $H(G^*) \leq H(G)$ for any graph $G \in \mathcal{G}(n)$.

Lemma 1 *Let $C = v_1v_2 \dots v_kv_1$ $(k \geq 3)$ be the unique cycle in G^*, then $k = 3$.*

Proof. Suppose to the contrary that $k \geq 4$. Since G^* is a unicyclic graph, we have $N(v_1) \cap N(v_2) = \emptyset$. Let $N(v_1) = \{u_1, u_2, \dots, u_x\}$ and $N(v_2) = \{w_1, w_2, \dots, w_y\}$, where $u_1 = v_2$, $u_2 = v_k$, $w_1 = v_1$ and $w_2 = v_3$.

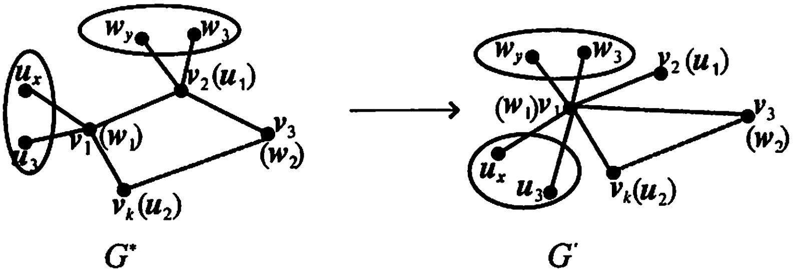

Figure 2.1 G^* and G'.

Let $G' = G^* - \{v_2w_2, \ldots, v_2w_y\} + \{v_1w_2, \ldots, v_1w_y\}$, see Figure 2.1. Then $G' \in \mathcal{G}(n)$ and we have

$$\begin{aligned}
&H(G^*) - H(G') \\
=&\sum_{i=2}^{x} \frac{2(y-1)}{(d(u_i)+x)(d(u_i)+x+y-1)} + \sum_{j=2}^{y} \frac{2(x-1)}{(d(w_i)+y)(d(w_i)+x+y-1)} \\
>&0,
\end{aligned}$$

a contradiction. Hence $k = 3$ and the assertion of the lemma holds. ∎

Lemma 2 *Let $C = uvwu$ be the unique cycle in G^*. If $d(u) \geq 3$, then every vertex in $N(u) \setminus \{v, w\}$ has degree exactly one.*

Proof. Suppose for a contradiction that some vertex in $N(u) \setminus \{v, w\}$, say u_1, has degree at least 2. Without loss of generality, suppose $d(u_1) = k \geq 2$ and $N(u_1) \setminus \{u\} = \{u_2, \ldots, u_k\}$. Since G^* is a unicyclic graph, we have $\{v, w\} \cap \{u_2, \ldots, u_k\} = \emptyset$.

Let $G' = G^* - \{u_1u_2, u_1u_3, \ldots, u_1u_k\} + \{uu_2, uu_3, \ldots, uu_k\}$, see Figure 2.2 for an illustration. Then $G' \in \mathcal{G}(n)$ and it is easy to calculate that $H(G^*) > H(G')$, which contradicts the assumption that $H(G^*) \leq H(G')$. This proves Lemma 2. ∎

By the same arguments as in the proof of Lemma 2, we can obtain the same conclusion for the vertices v and w.

Lemma 3 *Let $x \geq 1$ be an integer, then $f(x) = 46x^2 - 6x - 16 > 0$, and both $g(x) = \frac{11x-7}{x(x+1)(2x+1)}$ and $h(x) = \frac{x+3}{x(x+1)(x+2)}$ are monotone decreasing functions.*

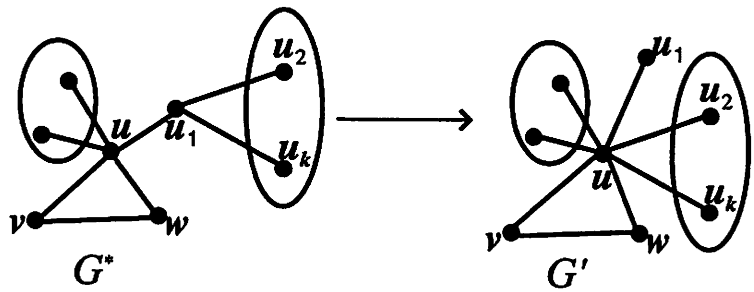

Figure 2.2 G^* and G'.

Proof. For $x \geq 1$, $f(x) \geq 46x^2 - 6x^2 - 16x^2 = 24x^2 > 0$,

$$g(x+1) - g(x) = \frac{-42x^2 - 13x - 42}{x(x+1)(x+2)(2x+1)(2x+3)} < 0,$$

$$h(x+1) - h(x) = \frac{-2x - 9}{x(x+1)(x+2)(x+3)} < 0.$$

This finishes the proof of Lemma 3. ∎

Lemma 4 *Let $C = uvwu$ be the unique cycle in G^* with $d(u) \geq d(v) \geq d(w) \geq 2$, then $d(v) = d(w) = 2$.*

Proof. Without loss of generality, suppose that $d(u) = x$, $d(v) = y$ and $d(w) = z$.

If $d(w) = z \geq 3$, then $x \geq y \geq z \geq 3$. Let $N(u)\backslash\{w, v\} = \{u_1, \ldots, u_{x-2}\}$ and $N(w)\backslash\{u, v\} = \{w_1, \ldots, w_{z-2}\}$. Then by Lemma 2, we have $d(u_i) = 1$ for $1 \leq i \leq x-2$, and $d(w_i) = 1$ for $1 \leq i \leq z-2$.

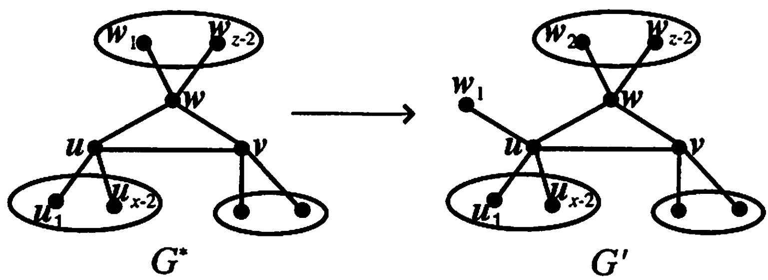

Figure 2.3 G^* and G'.

Let $G' = G^* - ww_1 + uw_1$, see Figure 2.3. Then $G' \in \mathcal{G}(n)$ and we get

$$
\begin{aligned}
& H(G^*) - H(G') \\
=& \frac{2(x-2)}{x+1} + \frac{2(z-2)}{z+1} + \frac{2}{x+y} + \frac{2}{y+z} - \frac{2(x-1)}{x+2} - \frac{2(z-3)}{z} - \frac{2}{x+y+1} \\
& - \frac{2}{y+z-1} \\
=& - \frac{6}{(x+1)(x+2)} + \frac{6}{z(z+1)} + \frac{2}{(x+y)(x+y+1)} - \frac{2}{(y+z)(y+z-1)} \\
\geq& - \frac{6}{(x+1)(x+2)} + \frac{6}{z(z+1)} + \frac{2}{2x(2x+1)} - \frac{2}{2z(2z-1)} \\
=& \frac{-11x^2 - 3x + 2}{x(x+1)(x+2)(2x+1)} + \frac{11z-7}{z(z+1)(2z-1)} \\
\geq& \frac{-11x^2 - 3x + 2}{x(x+1)(x+2)(2x+1)} + \frac{11x-7}{x(x+1)(2x-1)} \\
=& \frac{46x^2 - 6x - 16}{x(x+1)(x+2)(2x-1)(2x+1)} > 0,
\end{aligned}
$$

a contradiction. Therefore $d(w) = 2$.

In the following argument, we will further show that $d(v) = 2$.

Suppose to the contrary that $d(v) = y \geq 3$. Let $N(u) \setminus \{w, v\} = \{u_1, \ldots, u_{x-2}\}$ and $N(v) \setminus \{w, u\} = \{v_1, \ldots, v_{y-2}\}$. Then by Lemma 2, we have $d(u_i) = 1$ for $1 \leq i \leq x-2$, and $d(v_i) = 1$ for $1 \leq i \leq y-2$.

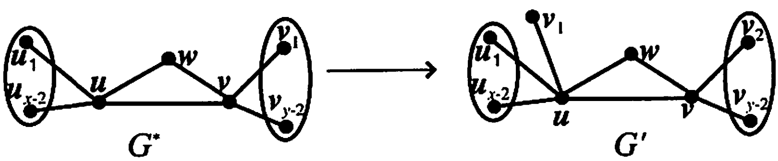

Figure 2.4 G^* and G'.

Let $G' = G^* - vv_1 + uv_1$, see Figure 2.4 for an illustration. Then $G' \in \mathcal{G}(n)$ and we have

$$\begin{aligned}
&H(G^*) - H(G')\\
=&\frac{2(x-2)}{x+1} + \frac{2(y-3)}{y+1} + \frac{4-2x}{x+2} + \frac{2}{y+2} - \frac{2(y-3)}{y} - \frac{2}{x+3}\\
=&\frac{-4(x+4)}{(x+1)(x+2)(x+3)} + \frac{4(y+3)}{y(y+1)(y+2)}\\
\geq&\frac{-4(x+4)}{(x+1)(x+2)(x+3)} + \frac{4(x+3)}{x(x+1)(x+2)}\\
=&\frac{4(2x+9)}{x(x+1)(x+2)(x+3)} > 0,
\end{aligned}$$

again a contradiction. Hence $d(w) = 2$. This completes the proof of Lemma 4. ∎

It follows immediately from Lemma 2 and Lemma 4 that the following theorem holds.

Theorem 1 *Let $G \in \mathcal{G}(n)$, then $H(G) \geq \frac{5}{2} - \frac{2(n+3)}{n(n+1)}$ with equality if and only if $G \cong S_n^+$.*

3 The upper bound for Harmonic index on unicyclic graphs

Theorem 2 *Let $G \in \mathcal{G}(n)$, then $H(G) \leq \frac{n}{2}$ and the equality holds if and only if $G \cong C_n$.*

Proof. We denote by $\tilde{G}$ the graph in $\mathcal{G}(n)$ such that $H(\tilde{G}) \geq H(G)$ for any graph $G \in \mathcal{G}(n)$. Let $C = v_1v_2\dots v_kv_1$ $(k \geq 3)$ be the unique cycle in $\tilde{G}$. To prove Theorem 2, it suffices to show that $k = n$.

Suppose for a contradiction that $k < n$. Then there exists some vertex in $\{v_1, v_2, \dots, v_k\}$ with degree at least 3. Without loss of generality, we may assume that $d_{\tilde{G}}(v_1) \geq 3$ and $N_{\tilde{G}}(v_1) \setminus \{v_2, v_k\} = \{u_1, u_2, \dots, u_s\}$ $(s \geq 1)$.

Case 1. For some vertex u_i $(1 \leq i \leq s)$, we have $d_{\tilde{G}}(u_i) = 1$.

Let $d_{\tilde{G}}(v_1) = x \geq 3$, $d_{\tilde{G}}(v_2) = y \geq 2$, and assume the degrees of $N(v_1) \setminus \{v_2, u_i\}$ are $\{p_1, p_2, \dots, p_{x-2}\}$. Construct $G' = \tilde{G} - v_1v_2 + u_iv_2$, then $G' \in \mathcal{G}(n)$ and $C = v_1u_iv_2v_3\dots v_kv_1$ is the unique cycle in G'. But now, we have

$$\begin{aligned}&H(\tilde{G}) - H(G')\\ =&\sum_{i=1}^{x-2}\frac{2}{p_i+x}+\frac{2}{x+y}-\sum_{i=1}^{x-2}\frac{2}{p_i+x-1}-\frac{2}{y+2}\\ =&-\sum_{i=1}^{x-2}\frac{2}{(p_i+x)(p_i+x-1)}-\frac{2(x-2)}{(x+y)(y+2)}<-\frac{2(x-2)}{(x+y)(y+2)}<0,\end{aligned}$$

a contradiction.

Case 2. For every vertex u_i $(1 \le i \le s)$, we have $d_{\tilde{G}}(u_i) \ge 2$.

In this case, the graph $\tilde{G} - v_1v_2 - v_1v_k$ has two components, say G_1 and G_1'. Let G_1 be the component containing v_1. Then $d_{G_1}(v_1) = x - 2$ and $d_{G_1}(v) = d_{\tilde{G}}(v)$ for every vertex $v \in V(G_1) \setminus \{v_1\}$.

We claim that $d_{\tilde{G}}(v_1) = 3$ (i.e., $d_{G_1}(v_1) = 1$) and G_1 is a path of length at least 2. Suppose this is not true. Since $d_{\tilde{G}}(u_1) = d_{G_1}(u_1) \ge 2$, we have $d_{G_1}(v_1) \ge 2$ or there exists some vertex in $V(G_1) \setminus \{v_1\}$ with degree at least 3. It is easy to see that in both cases, there exist at least two pendent vertices in $G_1 \setminus \{v_1\}$.

Without loss of generality, we may assume that $d_{G_1}(w_1) = d_{G_1}(w_2) = 1$. Suppose w_1 and w_2 have the common neighbor, say w. Since G_1 is a tree and $d_{\tilde{G}}(u_i) = d_{G_1}(u_i) \ge 2$ $(1 \le i \le s)$, we have $w \ne v_1$ and $d(w) = t \ge 3$. Let $G' = \tilde{G} - ww_1 + w_1w_2$ and assume the degrees of $N_{\tilde{G}}(w) \setminus \{w_1, w_2\}$ are $\{p_1, p_2, \dots, p_{t-2}\}$, then

$$\begin{aligned}&H(G') - H(\tilde{G})\\ =&\sum_{i=1}^{t-2}\frac{2}{p_i+t-1}+\frac{2}{t+1}+\frac{2}{3}-\sum_{i=1}^{t-2}\frac{2}{p_i+t}-\frac{4}{t+1}\\ =&\sum_{i=1}^{t-2}\frac{2}{(p_i+t)(p_i+t-1)}+\frac{2}{3}-\frac{2}{t+1}>\frac{2}{3}-\frac{2}{t+1}\ge 0,\end{aligned}$$

contradicting the assumption that $H(\tilde{G}) \ge H(G)$. So we deduce that w_1 and w_2 have distinct neighbors. Let $N_{G_1}(w_1) = \{w\}$ and $N_{G_1}(w_2) = \{w'\}$ such that $w \ne w'$. Then $d(w) = r \ge 2$ and $d(w') = t \ge 2$. By symmetry, we may assume that $r \ge t \ge 2$, and the degrees of $N_{\tilde{G}}(w) \setminus \{w_1\}$ are

$\{q_1, q_2, \ldots, q_{r-1}\}$. Let $G' = \tilde{G} - ww_1 + w_1w_2$, then $G' \in \mathcal{G}(n)$ and we have

$$\begin{aligned} & H(G') - H(\tilde{G}) \\ =& \sum_{i=1}^{r-1} \frac{2}{q_i + r - 1} + \frac{2}{t+2} + \frac{2}{3} - \sum_{i=1}^{r-1} \frac{2}{q_i + r} - \frac{2}{r+1} - \frac{2}{t+1} \\ =& \sum_{i=1}^{r-1} \frac{2}{(q_i + r)(q_i + r - 1)} + \frac{2}{3} - \frac{2}{r+1} - \frac{2}{(t+1)(t+2)}. \end{aligned}$$

If $r \geq 3$, then it is easy to calculate that the above equation is greater than 0, a contradiction. Therefore $r = t = 2$. By the choice of w_1 and w_2, we know that every pendent vertex is adjacent to a vertex of degree 2 in G_1.

We now consider two subcases to finish the proof of the above claim.

Subcase 2.1. $d_{G_1}(v_1) = x - 2 \geq 2$ and $d_{G_1}(v) \leq 2$ for every vertex $v \in V(G_1) \setminus \{v_1\}$.

For $i = 1, 2$, let P_i be the pendent path linking v_1 and w_i in $\tilde{G}$ (also in G_1), then $v_1u_i \in E(P_i)$. Construct $G' = \tilde{G} - v_1u_2 + w_1u_2$, see Figure 3.1 for an illustration. Then $G' \in \mathcal{G}(n)$ and $H(G') - H(\tilde{G}) = \frac{1}{6} - \frac{x}{(x+1)(x+2)} > 0$ for $x \geq 3$, a contradiction.

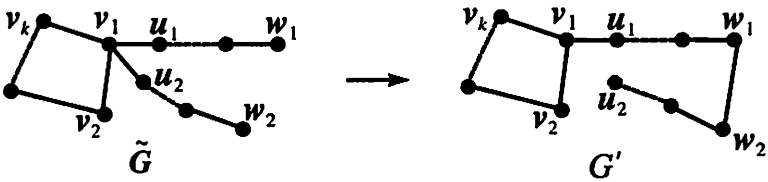

Figure 3.1 $\tilde{G}$ and G'.

Subcase 2.2. There exists some vertex in $V(G_1) \setminus \{v_1\}$ with degree at least 3.

In this case, it is easy to see that there always exist two pendent paths which are attached to a same vertex of degree at least 3 (since every pendent vertex is adjacent to a vertex of degree 2 in G_1). Hence by a similar argument as in the proof of Subcase 2.1, we can obtain the same contradiction.

Hence the claim holds. If $d_{\tilde{G}}(v_2) \geq 3$, then by the same argument as above, we can show that v_2 has the same property as that for v_1: $d_{\tilde{G}}(v_2) = 3$ and the component of $\tilde{G} - v_1v_2 - v_2v_3$ containing v_2, say G_2, is a path of length at least 2.

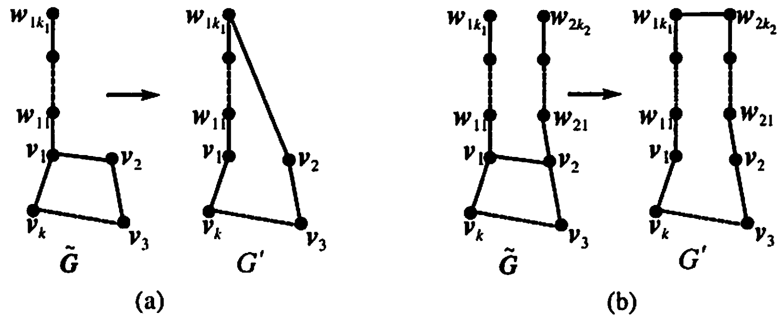

Figure 3.2 $\tilde{G}$ and G'.

By the claim, let $G_1 = v_1 w_{11} w_{12} \ldots w_{1k_1}$ $(k_1 \geq 2)$ and let $G_2 = v_2 w_{21} w_{22} \ldots w_{2k_2}$ with $k_2 \geq 2$ if $d_{\tilde{G}}(v_2) = 3$. We can now prove Theorem 2.

Suppose $d_{\tilde{G}}(v_2) = 2$. Let $G' = \tilde{G} - v_1v_2 + w_{1k_1}v_2$, see Figure 3.2(a). Then $G' \in \mathcal{G}(n)$ and we have $H(G') - H(\tilde{G}) = \frac{2}{(2+d(v_k))(3+d(v_k))} + \frac{1}{30} > 0$, a contradiction. So we conclude that $d_{\tilde{G}}(v_2) = 3$. Let $G' = \tilde{G} - v_1v_2 + w_{1k_1}w_{2k_2}$, see Figure 3.2(b). But now, $H(G') - H(\tilde{G}) = \frac{2}{(2+d(v_k))(3+d(v_k))} > 0$, again a contradiction. ∎

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