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On the Harmonic Index of Unicyclic Conjugated Molecules

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Abstract. The harmonic index $H(G)$ of a graph G is defined as the sum of weights $\dfrac{2}{d(u)+d(v)}$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G. In this paper, we first present a sharp lower bound on the harmonic index of unicyclic conjugated graphs (unicyclic graphs with a perfect matching). Also a sharp lower bound on the harmonic index of unicyclic graphs is given in terms of the order and given size of matching.

Keywords: Harmonic index; unicyclic graph; given size of matching.

AMS subject classification: 05C35

1. Introduction

We first introduce some terminologies and notations of graphs. Undefined terminologies and notations may refer to [1]. We only consider finite, undirected and simple graphs. Denote by C_n the cycle of n vertices. Unicyclic graphs are connected graphs with n vertices and n edges. For a vertex x of a graph G, we denote the neighborhood and the degree of x by $N(x)$ and $d(x)$, respectively. A pendant vertex is a vertex of degree 1. Denote by PV the set of pendant vertices of G. Let $d_G(x, y)$ denote the length of a shortest (x, y)-path in G. We will use $G - x$ to denote the graph that arises from G by deleting the vertex $x \in V(G)$ together with its incident edges. An edge e of G is said to be *contracted* if it is deleted and its ends are identified, the resulting graph is denoted by $G \cdot e$. A subset $M \subseteq E(G)$ is called a *matching* in G if its elements are edges and no two are adjacent in G. A matching M saturates a vertex v, and v is said to be M-saturated, if an edge of M is incident with v. If every vertex of G is M-saturated, the matching M is *perfect*. A matching M is said to be an *m-matching* (or a *maximum matching*), if $|M| = m$ and for every matching $M^{'}$ in G, $|M^{'}| \leq m$. Denote $\mathscr{U}_{n,m}$=$\{G$: G is a unicyclic graph with n vertices and an m-matching$\}$.

The Randić index of an organic molecule whose molecular graph is G was introduced by the chemist Milan Randić in 1975 [11] as

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

where $d(u)$ and $d(v)$ stand for the degrees of the vertices u and v, respectively, and the summation goes over all edges uv of G. Recently, finding bounds for the Randić index of a given class of graphs, as well as related problem of finding the graphs with extremal Randić index, attracted the attention of many researchers, and many results have been obtained (see recent books [6] and [8]).

In this paper, we consider another variant of the Randić index, named the harmonic index. For a graph G, the harmonic index $H(G)$ is defined (see [4]) as

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

In [5], the authors considered the relation between the harmonic index and the eigenvalues of graphs. In [15], [16] and [17], the authors presented the minimum and maximum values of harmonic index on simple connected graphs, trees, unicyclic graphs and bicyclic graphs respectively. In [3], the authors gave the minimum value of harmonic index for graphs with given minimum degree and characterize the corresponding extremal graph. In [7] and [12], the authors established some relationships between harmonic index and several other topological indices, such as the Zagreb index and the atom-bond connectivity index. In [13], the authors gave explicit computing formulae for harmonic index of nanocones and triangular benzenoid graphs, respectively.

In this paper, we first present a sharp lower bound on the harmonic index of unicyclic conjugated graphs (unicyclic graphs with a perfect matching). Also a sharp lower bound on the harmonic index of unicyclic graphs is given in terms of the order and given size of matching.

2. Some lemmas

Lemma 2.1. *[2] Let $G \in \mathscr{U}_{2m,m}$, $m \geq 3$, and let T be a tree in G attached to a root r. If $v \in V(T)$ is a vertex furthest from the root r with $d_G(v,r) \geq 2$, then v is a pendant vertex and adjacent to a vertex u of degree 2.*

Lemma 2.2. *[10] Let $G \in \mathscr{U}_{2m,m}$. If $PV \neq \emptyset$, then for any vertex $u \in V(G)$, $|N(u) \cap PV| \leq 1$.*

Lemma 2.3. *[14] Let $G \in \mathscr{U}_{n,m}$ $(n > 2m)$ and $G \ncong C_n$. Then there is an m-matching M and a pendant vertex v such that M does not saturate v.*

Lemma 2.4. *Let x, y be positive integers with $1 \leq x \leq y - 1$. Denote $\kappa(x, y) = \frac{2x+2}{y+1} + \frac{2(y-x-1)}{y+2}$. Then the function $\kappa(x-1, y) - \kappa(x, y+1)$ is monotonously increasing in $x \geq 1$ and $y \geq 0$, respectively.*

Proof. $\kappa(x-1, y) - \kappa(x, y+1) = \frac{2x}{y+1} + \frac{2y-4x-2}{y+2} - \frac{2y-2x}{y+3}$. We consider some partial derivatives. Since

$$\begin{aligned}
\frac{\partial[\kappa(x-1,y) - \kappa(x,y+1)]}{\partial y} &= \frac{-2x}{(y+1)^2} + \frac{4x+6}{(y+2)^2} - \frac{2x+6}{(y+3)^2} \\
&= \frac{-12xy^2 - 48xy - 44x + 12y^3 + 54y^2 + 72y + 30}{(y+1)^2(y+2)^2(y+3)^2} \\
&\geq \frac{-12(y-1)y^2 - 48(y-1)y - 44(y-1) + 12y^3 + 54y^2 + 72y + 30}{(y+1)^2(y+2)^2(y+3)^2} \\
&= \frac{18y^2 + 76y + 74}{(y+1)^2(y+2)^2(y+3)^2} > 0,
\end{aligned}$$

$\kappa(x-1, y) - \kappa(x, y+1)$ is monotonously increasing in y. On the other hand,

$$\frac{\partial[\kappa(x-1,y) - \kappa(x,y+1)]}{\partial x} = \frac{2}{y+1} - \frac{4}{y+2} + \frac{2}{y+3} = \frac{4}{(y+1)(y+2)(y+3)} > 0.$$

Thus $\kappa(x-1, y) - \kappa(x, y+1)$ is monotonously increasing in x. ∎

3. On the harmonic index of unicyclic conjugated molecules

Let n and m be positive integers with $n \geq 2m$. Let $U_{n,m}$ be a graph with n vertices obtained from C_3 by attaching $n - 2m + 1$ pendant edges and $m - 2$ paths of length 2 to one vertex of C_3 (see Figure 3.1). Denote $\varphi(n, m) = \frac{2(m-2)}{3} + \frac{2m}{n-m+3} + \frac{2(n-2m+1)}{n-m+2} + \frac{1}{2}$.

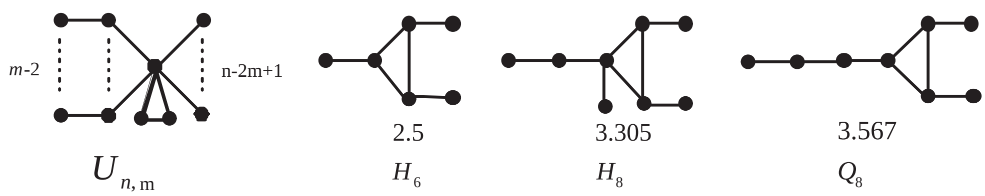

Fig. 3.1.

Theorem 3.1. *Let $G \in \mathscr{U}_{2m,m} \backslash \{H_6, H_8\}$ $(m \geq 2)$. Then*

$$H(G) \geq \varphi(2m, m),$$

with equality holds if and only if $G \cong U_{2m,m}$.

Proof. First we note that if $G \cong U_{2m,m}$, then $H(G) = \varphi(2m, m)$. We apply induction on m. For $m = 2$, $G \cong C_4$ or $U_{4,2}$, it is easy to check that $H(G) \geq \varphi(4, 2)$. In the following proof, we assume that $m \geq 3$ and that the result holds for all smaller values of m.

If $G \cong C_{2m}$, then:

$$H(C_{2m}) - \varphi(2m, m) = \frac{m}{3} - \frac{2m}{m+3} - \frac{2}{m+2} + \frac{5}{6} = \frac{2m^2(m+1) + (m-2)(m+3)}{6(m+2)(m+3)} > 0.$$

So in the following proof, we assume that $G \ncong C_{2m}$. By Lemmas 2.1 and 2.2, we only consider the following two cases.

Case 1. G has a pendant vertex v which is adjacent to a vertex w of degree 2.

In this case, there is a unique vertex $u \neq v$ such that $uw \in E(G)$. Denote $d(u) = t$ and $N(u) = \{w, y_1, \ldots, y_{t-1}\}$, then $t \geq 2$. Since G is a unicyclic graph with a perfect matching, then $t \leq m + 1$. By Lemma 2.2, there exists at most one vertex in $\{y_i\}$ $(i = 1, 2, \ldots, t-1)$ having degree one, say $i = 1$, such that $d(y_1) \geq 1$, the degree of other vertices are at least two. Let $G' = G - v - w$. Then $G \in \mathscr{U}_{2m-2,m-1}$.

If $G' \cong H_6$, then $G \cong Q_8$ and $H(Q_8) = 3.567 > \varphi(8, 4) = 3.310$.

If $G' \cong H_8$, then $G \in \{G_i | 1 \leq i \leq 6\}$, where G_i $(1 \leq i \leq 6)$ are illustrated in Figure 3.2. By $\varphi(10, 5) = 4.036$, it is easy to check that $H(G_i) > \varphi(10, 5)$ $(1 \leq i \leq 6)$.

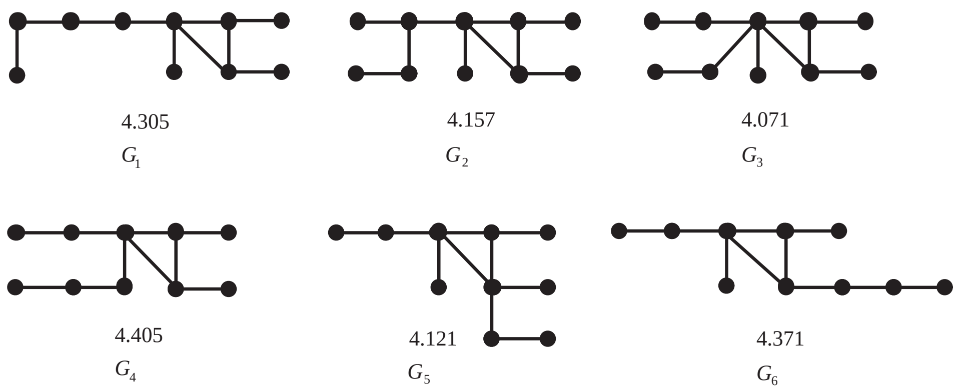

Fig. 3.2. G_i with their harmonic indices.

Otherwise, if $G^{'} \ncong \{H_6, H_8\}$, then

$$\begin{aligned} H(G) &= H(G^{'}) + \frac{2}{3} + \frac{2}{t+2} + \sum_{i=1}^{t-1} \frac{2}{t+d(y_i)} - \sum_{i=1}^{t-1} \frac{2}{t+d(y_i)-1} \\ &\geq \varphi(2m-2, m-1) + \frac{2}{3} + \frac{2}{t+2} - \frac{2}{t(t+1)} - \frac{2(t-2)}{(t+1)(t+2)} \\ &= \varphi(2m-2, m-1) + \frac{2}{3} + \frac{4t-4}{t(t+1)(t+2)}. \end{aligned}$$

Since $\frac{4t-4}{t(t+1)(t+2)}$ is strictly monotonously decreasing in t and $t \leq m+1$, we have

$$H(G) \geq \varphi(2m, m) - \frac{2m}{m+3} + \frac{2m-4}{m+2} + \frac{2}{m+1} + \frac{4m}{(m+1)(m+2)(m+3)} = \varphi(2m, m).$$

The equality $H(G) = \varphi(2m, m)$ holds if and only if equality holds throughout the above inequalities, that is if and only if $G^{'} \cong U_{2m-2,m-1}$, $d(y_1) = 1$, $d(y_i) = 2$ for $i = 2, 3, \ldots, t-1$ and $t = m+1$. Thus $G \cong U_{2m,m}$.

Case 2. G is a cycle C together with some pendant edges attached to some vertices on C. For convenience, we label the vertices of C with $u_1, u_2, \ldots, u_p$ one by one clockwise.

If each vertex of C is attached by a pendant edge, then $m \geq 4$ as $G \ncong H_6$. If $m = 4$, then $H(G) = 3.333 > \varphi(8, 4) = 3.310$. If $m \geq 5$, then $H(G) - \varphi(2m, m) = \frac{5m}{6} - \varphi(2m, m) = \frac{m}{6} - \frac{2m}{m+3} - \frac{2}{m+2} + \frac{5}{6} = \frac{m(m+2)(m-4) + 3(m-2)}{6(m+2)(m+3)} > 0$.

Otherwise, there is at least a vertex of degree two on C. Since $G \ncong C_n$, there exists some $i \in \{1, 2, \ldots, p\}$ such that $d_G(u_i) = 3$ and $d_G(u_{i+1}) = 2$, where $u_{p+1} = u_1$. Without loss of generality, assume $d_G(u_2) = 3$ and $d_G(u_3) = 2$. Denote by v_2 the pendant vertex adjacent to u_2. Obviously, every pair of vertices of degree three cannot be adjacent to a common vertex of degree two (since G has a perfect matching). Then each vertex of degree two on C must be adjacent to another vertex of degree two. Thus $d_G(u_4) = 2$.

Let $G^{'} = (G \cdot u_2v_2) \cdot u_2u_3$ be a graph obtained from G by contracting u_2v_2 and u_2u_3 consecutively. Then $G^{'} \in \mathscr{U}_{2m-2,m-1} \backslash \{H_6, H_8\}$. We have

$$\begin{aligned} H(G) &= H(G^{'}) + \frac{9}{10} + \frac{2}{d_G(u_1)+3} - \frac{2}{d_G(u_1)+2} \\ &\geq \varphi(2m-2, m-1) + \frac{9}{10} - \frac{2}{(d_G(u_1)+2)(d_G(u_1)+3)} \\ &\geq \varphi(2m, m) + \frac{2}{15} + \frac{2}{m+1} + \frac{2m-4}{m+2} - \frac{2m}{m+3} \\ &= \varphi(2m, m) + \frac{2m(m-3)(m+9) + 16m + 12}{15(m+1)(m+2)(m+3)} > \varphi(2m, m), \end{aligned}$$

where the second inequality holds since $d_G(u_1) \geq 2$. ∎

Note 1. It is easy to calculate that $H(H_6) = 2.5 < \varphi(6,3) = 2.567$ and $H(H_8) = 3.305 < \varphi(8,4) = 3.310$, where H_6 and H_8 are shown in Figure 3.1. Thus, by Theorem 3.1, H_6 has the minimum harmonic index in $\mathscr{U}_{6,3}$ and H_8 has the minimum harmonic index in $\mathscr{U}_{8,4}$.

Theorem 3.2. *Let $G \in \mathscr{U}_{n,m}$ $(n \geq 2m, m \geq 5)$. Then*

$$H(G) \geq \varphi(n,m),$$

with equality holds if and only if $G \cong U_{n,m}$.

Proof. We apply induction on n. Suppose $n = 2m$. Then the theorem holds by Theorem 3.1. Now we suppose that $n > 2m$ and the result holds for smaller values of n.

If $G \cong C_n$, then $n = 2m+1$ since G has an m-matching. Thus $H(G) - \varphi(2m+1,m) = \frac{2m+1}{2} - \varphi(2m+1,m) = \frac{m-2}{3} + \frac{8}{m+4} - \frac{4}{m+3} = \frac{m^3+5m^2+10m}{3(m+3)(m+4)} > 0$. So in the following proof, we assume that $G \ncong C_n$.

By Lemma 2.3, G has an m-matching M and a pendant vertex v such that M does not saturate v. Let $uv \in E(G)$ with $d(u) = t$. Denote $N(u) \cap PV = \{v, x_1, \ldots, x_r\}$ and $N(u) \backslash PV = \{y_1, \ldots, y_{t-r-1}\}$. Then all $d(y_i) \geq 2$ $(1 \leq i \leq t-r-1)$. Let $G' = G - v$. Then $G' \in \mathscr{U}_{n-1,m}$. We have

$$\begin{aligned}
H(G) &= H(G') + \frac{2r+2}{t+1} - \frac{2r}{t} + \sum_{i=1}^{t-r-1} \frac{2}{t+d(y_i)} - \sum_{i=1}^{t-r-1} \frac{2}{t+d(y_i)-1} \\
&\geq \varphi(n-1,m) + \frac{2r+2}{t+1} + \frac{2(t-r-1)}{t+2} - \frac{2r}{t} - \frac{2(t-r-1)}{t+1} \\
&= \varphi(n,m) + \frac{2(n-2m)}{n-m+1} + \frac{2m}{n-m+2} - \frac{2(n-2m+1)}{n-m+2} - \frac{2m}{n-m+3} \\
&\quad + \frac{2r+2}{t+1} + \frac{2(t-r-1)}{t+2} - \frac{2r}{t} - \frac{2(t-r-1)}{t+1} \\
&= \varphi(n,m) + [\kappa(n-2m-1, n-m) - \kappa(n-2m, n-m+1)] - \\
&\quad -[\kappa(r-1,t-1) - \kappa(r,t)],
\end{aligned}$$

where $\kappa(x,y)$ is defined in Lemma 2.4. Since the unicyclic graph G has an m-matching, $n-m+1 \geq t$ and $n-2m \geq r$. By Lemma 2.4 and $t \geq r+1$, we have

$$H(G) \geq \varphi(n,m) + [\kappa(r-1,n-m) - \kappa(r,n-m+1)] - [\kappa(r-1,t-1) - \kappa(r,t)] \geq \varphi(n,m).$$

The equality $H(G) = \varphi(n,m)$ holds if and only if equality holds throughout the above inequalities, that is if and only if $G' \cong U_{n-1,m}$, $d(y_1) = \ldots = d(y_{t-r-1}) = 2$, $n-m+1 = t$ and $n-2m = r$. Thus $G \cong U_{n,m}$. ∎

Note 2. In [16], Zhong gave the maximum value of harmonic index for unicyclic graphs with n vertices and proved that the extremal graph is the cycle C_n. Then if $G \in \mathscr{U}_{2m,m}$, then $H(G) \leq m$ with equality if and only if $G \cong C_{2m}$. Similarly, if $G \in \mathscr{U}_{2m+1,m}$, then $H(G) \leq m + \frac{1}{2}$ with equality if and only if $G \cong C_{2m+1}$. As to $G \in \mathscr{U}_{n,m}$, for $n \geq 2m+2$, we do not know the sharp upper bounds on $H(G)$. This case maybe much more complicated.

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