The harmonic index on bicyclic graphs*

Yan Zhu[1†], Renying Chang[2] and Xiang Wei[3]

[1] Department of Mathematics, East China University of Science and Technology, Shanghai, 200237, China

[2] Department of Mathematics, Linyi University, Linyi, Shandong, 276005, China

[3] Department of Enginerring, University of Honghe, Honghe, Yunnan, 661100, China

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 give sharp lower and upper bounds for harmonic index of bicyclic graphs and characterize the corresponding extremal graphs.

Keywords: Harmonic index; bicyclic graph; degree.

AMS subject classification: 05C35

1 Introduction

The Randić index of an organic molecule whose molecular graph is G was introduced by the chemist Milan Randić in 1975 [4] as $R(G) = \sum_{uv} \frac{1}{\sqrt{d(u)d(v)}}$, where

*This work is supported by the Fundamental Research Funds for the Central Universities and the National Natural Science Foundation of China (61070230).

†Corresponding author: operationzy@163.com

$d(u)$ and $d(v)$ stand for the degrees of the vertices u and v, respectively, and the summation goes over all edges uv of G. This topological index is one of the most popular molecular descriptors, the mathematical properties of this descriptor have also been studied extensively (see recent book [4]).

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 [1]) as

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

In [2], the authors considered the relation between the harmonic index and the eigenvalues of graphs. In [6] and [7], Zhong presented the minimum and maximum values of harmonic index on simple connected graphs, trees and unicyclic graphs respectively. In [3] and [5], the authors established some relationships between harmonic index and several other topological indices.

Bicyclic graphs are connected graphs in which the number of edges equals the number of vertices plus one. A pendant vertex is a vertex of degree 1. The bicyclic graphs of order n without pendant vertex are characterized in Figure 1:

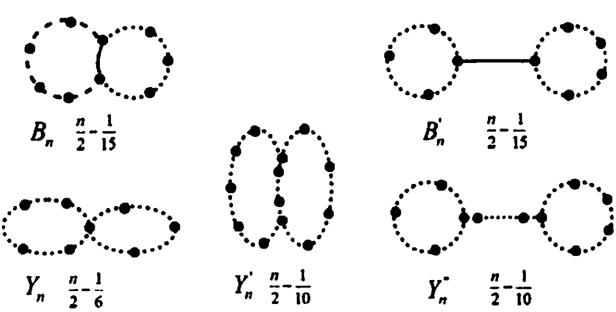

Figure 1: Bicyclic graphs without pendant vertex with their harmonic indices.

In this paper, we will give sharp lower and upper bounds on the harmonic index of bicyclic graphs and characterize the corresponding extremal graphs.

2 Upper bound

Let n be a positive integer with $n \geq 4$. We denote by $\mathscr{B}(n)$ the set of all bicyclic graphs on n vertices. In this section, we consider the maximum value of the harmonic index for bicyclic graphs with n vertices, and we show that the extremal graph is one of the type of $\{B_n, B'_n\}$. In the proof of this result, we use the following theorem.

Theorem 2.1. *([3]) Let w be a vertex of a nontrival connected graph G. For nonnegative integers p and q, let $G(p,q)$ denote the graph obtained from G by attaching to the vertex w pendant paths $P = wv_1v_2\dots v_p$ and $Q = wu_1u_2\dots u_q$ of length p and q, respectively. Then $H(G(p,q)) < H(G(p+q,0))$.*

Theorem 2.2. *Among connected bicyclic graphs on n vertices, $n \geq 4$, the graph of the type B_n and B'_n have maximum harmonic index, and $H(B_n) = H(B'_n) = \frac{n}{2} - \frac{1}{15}$.*

Proof. Assume that $G \in \mathscr{B}(n)$ with $n \geq 4$. If G has no pendant vertex, then G is one of the type of $\{B_n, B'_n, Y_n, Y'_n, Y''_n\}$. For convenient, we denote by $\mathscr{B}^*(n)$ the set of all bicyclic graphs on n vertices without pendant vertices. It is easy to prove that $\max\{H(B_n), H(B'_n), H(Y_n), H(Y'_n), H(Y''_n)\} = H(B_n, B'_n) = \frac{n}{2} - \frac{1}{15}$. Hence, in the next proof, we assume that G has at least one pendant vertex. By repetitive application of Theorem 2.1, we can conclude that the bicyclic graph with the maximum value of harmonic index has the form as follow: there is at most one pendant path attached to each vertex of $\mathscr{B}^*(n)$. Assume that $v \in \mathscr{B}^*(n)$ and there is a pendant path $P = vu_1u_2\dots u_p$ attaching to v in the graph G. Denote $d_G(v) = d$ and $N(v) = \{w, u_1, x_1, \dots, x_{d-2}\}$, where $w \in \mathscr{B}^*(n)$. Then $3 \leq d \leq 5$, $2 \leq d_G(w) \leq 5$, $2 \leq d_G(x_i) \leq 5$, $i \in \{1, 2, \dots, d-2\}$. If $p = 1$, that is, $P = vu_1$. Define $G_1 = G - \{wv\} + \{wu_1\}$, clearly, G_1 is also a bicyclic graph with order n, then $H(G_1) = H(G) + \frac{2}{d_G(w)+2} - \frac{2}{d_G(w)+d} + \frac{2}{d-1+2} - \frac{2}{d+1} + \sum_{i=1}^{d-2} \frac{2}{d_G(x_i)+d-1} - \sum_{i=1}^{d-2} \frac{2}{d_G(x_i)+d} > H(G)$. Now we consider the length of pendant path is at least 2, let $P = vu_1u_2\dots u_{p-1}u_p$.

Then $d_G(u_{p-1}) = 2$, $d_G(u_p) = 1$. Define $G_2 = G - \{wv\} + \{wu_p\}$, clearly, G_2 is also a bicyclic graph with order n, and we have

$$\begin{aligned} H(G_2) &= H(G) + \frac{2}{d_G(w)+2} - \frac{2}{d_G(w)+d} + \frac{2}{d+1} - \frac{2}{d+2} \\ &\quad + \sum_{i=1}^{d-2} \frac{2}{d_G(x_i)+d-1} - \sum_{i=1}^{d-2} \frac{2}{d_G(x_i)+d} - \frac{1}{6} \\ &\geq H(G) + \frac{2(d-2)}{(5+2)(5+d)} + \frac{2}{(d+1)(d+2)} + \frac{2(d-2)}{(5+d-1)(5+d)} - \frac{1}{6} \\ &= H(G) + \frac{5}{42} + \frac{-10(d+\frac{9}{10})^2 + \frac{241}{10}}{(d+1)(d+2)(d+4)(d+5)} > H(G). \end{aligned}$$

Repeating this process on G_1 and G_2, we can obtain that bicyclic graphs with maximum harmonic index cannot possess acyclic branches. ∎

3 Lower bound

In this section, we consider the minimum value of the harmonic index for bicyclic graphs of order n and characterize the extremal graph. Graph B_4 is the unique bicyclic graph with 4 vertices. We define a bicyclic graph $B^*(n)$ with n vertices as follow: $B^*(n)$ is obtained from B_4 by attaching $n-4$ pendant vertices on the 3-vertex of graph B_4. Similarly, we can define $B^*_+(n)$ and $B^*_-(n)$ (see Figure 2). Denote $\varphi(n) = \frac{14}{5} - \frac{8}{n} + \frac{4}{n+1} + \frac{2}{n+2}$. We have the following results.

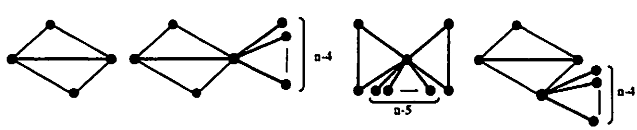

Figure 2: The four graphs from left to right are: B_4, $B^*(n)$, $B^*_+(n)$, $B^*_-(n)$

Theorem 3.1. *Let G be a bicyclic graph of order $n \geq 4$. Then $H(G) \geq \varphi(n)$ with equality if and only if $G \cong B^*(n)$.*

Proof. We apply induction on n. For $n = 4$, $G \cong B_4$, then $H(G) = \varphi(4)$. If $n = 5$, then the theorem holds clearly by the facts that there are only five graphs in $\mathscr{B}(5)$ (see Figure 3) and $\varphi(5) = \frac{226}{105}$.

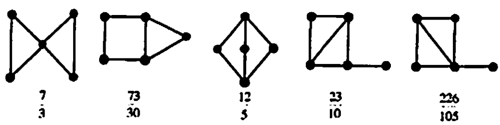

Figure 3: The only five graphs in $\mathscr{B}(5)$ with their harmonic indices.

For $n \geq 6$, assume that $G \in \mathscr{B}(n)$ with $n \geq 6$. If G has no pendant vertex, then G is one of the type of $\{B_n, B'_n, Y_n, Y'_n, Y''_n\}$. It is easy to prove that

$$\min\{H(B_n), H(B'_n), H(Y_n), H(Y'_n), H(Y''_n)\} = H(Y_n) = \frac{n}{2} - \frac{1}{6} > \varphi(n).$$

Hence, in the next proof, we assume that G has at least one pendant vertex. Denote $V_1 = \{u \in V(G) | d(u) = 1\}$, then $V_1 \neq \emptyset$. Let $u \in V_1$ and v is the neighbor of u. Then $d(v) \geq 2$. Set $W(u) = \{y | y \in N(v) \setminus \{u\}, d(y) = 1\}$. Choose $u_0 \in V_1$ such that

(i) the number of the set $W(u_0)$ is as large as possible;

(ii) subject to (i), d(v) is as small as possible.

Denote $d(v) = d$ and $N(v) = \{y_1, y_2, \ldots, y_{d-1}, u_0\}$. Let $G' = G - u_0$. Then $G' \in \mathscr{B}(n-1)$. By induction assumption, we have

$$\begin{aligned} H(G) &= H(G') + \frac{2}{1+d} + \sum_{i=1}^{d-1} \frac{2}{d+d(y_i)} - \sum_{i=1}^{d-1} \frac{2}{d+d(y_i)-1} \\ &\geq \varphi(n) - \frac{8}{n-1} + \frac{12}{n} - \frac{2}{n+1} - \frac{2}{n+2} + \frac{2}{1+d} \\ &\quad -2\sum_{i=1}^{d-1} \frac{1}{(d+d(y_i))(d+d(y_i)-1)}. \quad (*) \end{aligned}$$

Now we consider the following two cases.

Case 1. $d(y_i) \geq 2$ for $i = 1, 2, \cdots, d-1$.

By the choice of u_0 and $G \in \mathscr{B}(n)$ (it has at least one pendant vertex), we have $W(u) = \emptyset$ for all $u \in V_1$. By the structure of bicyclic graphs, we know that $d(v) \leq 5$. Since, if $d(v) \geq 6$, then there is at least one vertex in $\{y_1, y_2, \ldots, y_{d-1}\}$, say y_1, such that the component H of $G - v$ which containing y_1 is a tree and $|V(H)| \geq 2$. Since $W(u) = \emptyset$ for all $u \in V_1$, there exists $u' \in V(H) \cap V_1$ and $u'v' \in E(G)$ such that $d(v') = 2$, a contradiction with the choice of u_0. Thus $d(v) = d \leq 5$. By (*), we have

$$\begin{aligned} H(G) &\geq \varphi(n) - \frac{8}{n-1} + \frac{12}{n} - \frac{2}{n+1} - \frac{2}{n+2} + \frac{2}{1+d} - \frac{2(d-1)}{(d+2)(d+1)} \\ &\geq \varphi(n) - \frac{8}{n-1} + \frac{12}{n} - \frac{2}{n+1} - \frac{2}{n+2} + \frac{6}{(5+2)(5+1)}. \end{aligned}$$

Denote $f(n) = -\frac{8}{n-1} + \frac{12}{n} - \frac{2}{n+1} - \frac{2}{n+2} + \frac{1}{7}$, then $f(n) > -\frac{8}{n-1} + \frac{8}{n} + \frac{1}{7}$, it is easy to show that $f(n) > 0$ when $n \geq 8$, for $n = 6$ and $n = 7$, clearly $f(n) > 0$. So, in this case, $H(G) > \varphi(n)$.

Case 2. There exists some i $(1 \leq i \leq d-1)$ such that $d(y_i) = 1$.

Without loss of generality, assume that $d(y_1) = d(y_2) = \cdots = d(y_k) = 1$ and $d(y_i) \geq 2$ for $k+1 \leq i \leq d-1$, where $k \geq 1$. By (*), we have

$$\begin{aligned} H(G) &\geq \varphi(n) - \frac{8}{n-1} + \frac{12}{n} - \frac{2}{n+1} - \frac{2}{n+2} + \frac{2}{1+d} - \frac{2k}{(1+d)d} - \frac{2(d-1-k)}{(d+2)(d+1)} \\ &= \varphi(n) - \frac{8}{n-1} + \frac{12}{n} - \frac{2}{n+1} - \frac{2}{n+2} + \frac{6d-4k}{d(d+1)(d+2)}. \qquad (**) \end{aligned}$$

Now we consider the following three subcases.

Subcase 2.1. $d(v) = d = n-1$, then $G \cong B^*(n)$ or $G \cong B^*_+(n)$. Clearly, $H(B^*(n)) = \varphi(n)$, and $H(B^*_+(n)) = 3 - \frac{10}{n} + \frac{8}{n+1} > \varphi(n)$. This implies that $H(G) = \varphi(n)$ holds if and only if $G \cong B^*(n)$.

Subcase 2.2. $d(v) = d \leq n-2$ and v is a vertex of a cycle in bicyclic graph G.

Then $k \le d-3$ and $d \le n-2$. By the structure of bicyclic graphs, since v is a vertex of a cycle in bicyclic graph G, when $k = d-3$ and $d = n-2$ hold simultaneously, $G \cong B^*_-(n)$. Clearly, $H(B^*_-(n)) - \varphi(n) = \frac{47}{15} - \frac{6}{n-1} + \frac{4}{n+1} - \varphi(n) > 0$. In the following proof of this subcase, by (**), we divide into two parts:

(i) $d = n-2$ and $k \le d-4$;

$$\begin{aligned} H(G) &\ge \varphi(n) - \frac{2n^2+22n+24}{(n-1)n(n+1)(n+2)} + \frac{6d-4(d-4)}{d(d+1)(d+2)} \\ &= \varphi(n) + \frac{60n+72}{(n-2)(n-1)n(n+1)(n+2)} > \varphi(n). \end{aligned}$$

(ii) $d \le n-3$ and $k \le d-3$.

$$\begin{aligned} H(G) &\ge \varphi(n) - \frac{2n^2+22n+24}{(n-1)n(n+1)(n+2)} + \frac{2d+12}{d(d+1)(d+2)} \\ &\ge \varphi(n) - \frac{2n^2+22n+24}{(n-1)n(n+1)(n+2)} + \frac{2n+6}{(n-3)(n-2)(n-1)} \\ &= \varphi(n) + \frac{96n^2-144}{(n-3)(n-2)(n-1)n(n+1)(n+2)} > \varphi(n), \end{aligned}$$

where the second inequality holds since $\frac{2d+12}{d(d+1)(d+2)}$ is monotonously decreasing in d.

Subcase 2.3. v is not a vertex of two cycles in bicyclic graph G.

Then $d \le n-4$. If $k \le d-3$, by the subcase 2.2, we have $H(G) > \varphi(n)$. If $k = d-2$, there is only one vertex in $N(v)$ we say y_{d-1} such that $d(y_{d-1}) \ge 2$. The vertices in $\{y_1, y_2, \cdots, y_{d-2}, u_0\}$ are all pendant vertices. Denote $d(y_{d-1}) = d'$, $N(y_{d-1}) = \{v, x_1, x_2, \cdots, x_{d'-1}\}$ and $d(x_i) = d_i$ for all $i = 1, 2, \cdots, d'-1$. Let $G_1 = G - \{vu_0, vy_1, \cdots, vy_{d-2}\} + \{y_{d-1}u_0, y_{d-1}y_1, \cdots, y_{d-1}y_{d-2}\}$. Clearly, G_1 is also a bicyclic graph with order n, and we have

$H(G) = H(G_1) + \sum_{i=1}^{d'-1} \frac{2}{d_i+d'} - \sum_{i=1}^{d'-1} \frac{2}{d_i+d'+d-1} + \frac{2}{d'+d} + \frac{2(d-1)}{d+1} - \frac{2d}{d'+d} > H(G_1)$,

where the last inequality holds since $d' > 1$ and $d > 1$.

We consider the vertex y_{d-1} in graph G_1. Then one of the above three subcases must be happened on y_{d-1} in graph G_1.

If subcase 2.1 and 2.2 happened, we have $H(G) > H(G_1) \geq \varphi(n)$.

If subcase 2.3 happened, similarly, we can obtain another graph G_2 and a vertex w_2 of G_2 satisfying one of the above three subcases. Repeating this process on G_2, and we can obtain a graph G_p and a vertex w_p of G_p satisfying subcase 2.1 or 2.2. So we have $H(G) > H(G_1) > \cdots > H(G_p) \geq \varphi(n)$. ∎

References

[1] S. Fajtlowicz, On conjectures of Graffti-II, Congr. Numer., **60** (1987), 187–197.

[2] O. Favaron, M. Mahó and J.F. Saclé, Some eigenvalue properties in graphs (conjectures of Graffi-II), Discrete Math., **111** (1993), 197–220.

[3] A. Ilić, Note on the harmonic index of a graph, arXiv:1204.3313v1 [math.CO], (2012).

[4] X. Li and I. Gutman, Mathematical Aspects of Randić-Type Molecular Structure Descriptors, Mathematical Chemistry Monographs, No. 1, University of Kragujevac and Faculty of Science Kragujevac, pp.VI+330, (2006).

[5] X. Xu, Relationships between harmonic index and other topological indices, Applied Mathematical Sciences, **41** (2012), 2013–2018.

[6] L. Zhong, The harmonic index for graphs, Appl. Math. Lett., **25** (2012), 561–566.

[7] L. Zhong, The harmonic index on unicyclic graphs, Ars Combin., **104** (2012), 261–269.