A lower bound for the harmonic index of a graph with minimum degree at least two

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Abstract. The harmonic index H(G) 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. We give a best possible lower bound for the harmonic index of a graph (a triangle-free graph, respectively) with minimum degree at least two and characterize the extremal graphs.

1. Introduction

In this work, we consider the harmonic index. For a simple graph (or a molecular graph) G = (V, E), the harmonic index H(G) is defined in [1] as $H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}$, where d(u) denotes the degree of a vertex u in G. Favaron et al. [2] considered the relation between harmonic index and the eigenvalues of graphs. Zhong [3] found the minimum and maximum values of the harmonic index for simple connected graphs and trees, and characterized the corresponding extremal graphs. Deng, Balachandran, Ayyaswamy, Venkatakrishnan [4] considered the relation relating the harmonic index H(G) and the chromatic number $\chi(G)$ and proved that $\chi(G) \leq 2H(G)$ by using the effect of removal of a minimum degree vertex on the harmonic index. It strengthens a result relating the Randić index and the chromatic number conjectured by the system AutoGraphiX and proved by Hansen et al. in [5], since we always have $H(G) \leq R(G)$ for any graph G. Deng, Tang, Zhang [6] considered the harmonic index H(G) and the radius r(G) and strengthened some results relating the Randić index and the radius in [7] [8] [9]. Deng, Balachandran, Ayyaswamy, Venkatakrishnan [10] determined the trees with the second-the sixth maximum harmonic indices, and unicyclic graphs with the second-the fifth maximum harmonic indices, and bicyclic graphs with the first-the fourth maximum harmonic indices. For other related results see [11] [12] [13] [14]. Here we will establish a best possible lower bound for the harmonic index of a graph, a triangle-free graph, respectively, with *n* vertices and minimum degree at least two and characterize the extremal graphs.

2. A lower bound for the harmonic index of a graph with minimum degree at least two

In the section, we will establish a best possible lower bound for the harmonic index of a graph with minimum degree at least two and characterize the extremal graphs.

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For an edge e = uv of a graph G, its weight is defined to be $\frac{2}{d(u)+d(v)}$. The harmonic index of G is the sum of weights over all its edges.

Lemma 2.1. *If* e *is an edge with maximal weight in* G*, then* H(G - e) < H(G)*.*

Proof. Let e = uv. Since uv is an edge with maximal weight in G, we have $d(w) \ge d(v)$ for $w \in N(u)$ and $d(w) \ge d(u)$ for $w \in N(v)$. Note that $\frac{1}{x} - \frac{1}{x-1}$ is increasing for x > 1.

$$\begin{split} H(G)-H(G-e) &= & \frac{2}{d(u)+d(v)} + \sum_{w \in N(u) \setminus \{v\}} (\frac{2}{d(u)+d(w)} - \frac{2}{d(u)+d(w)-1}) \\ &+ \sum_{w \in N(v) \setminus \{u\}} (\frac{2}{d(v)+d(w)} - \frac{2}{d(v)+d(w)-1}) \\ &\geq & \frac{2}{d(u)+d(v)} + (d(u)-1)(\frac{2}{d(u)+d(v)} - \frac{2}{d(u)+d(v)-1}) \\ &+ (d(v)-1)(\frac{2}{d(v)+d(u)} - \frac{2}{d(v)+d(u)-1}) \\ &= & \frac{2}{d(u)+d(v)-1} - \frac{2}{d(u)+d(v)} > 0 \end{split}$$

which proves the result.

Let $K_{a,b}$ be the complete bipartite graph with a and b vertices in its two partite sets, respectively. For $n \ge 4$, let $K_{2,n-2}^*$ be the graph obtained from $K_{2,n-2}$ by joining an edge between the two non-adjacent vertices of degree n-2. Obviously, $H(K_{2,n-2}^*) = h_1(n) = 4 + \frac{1}{n-1} - \frac{12}{n+1}$. Let $\delta(G)$ be the minimum degree of the graph G.

Theorem 2.2. Let G be a graph with $n \ge 3$ vertices and $\delta(G) \ge 2$. Then $H(G) \ge h_1(n)$ with equality if and only if $G = K_{2,n-2}^*$.

Proof. It is easy to check that the assertion is true for n = 4. Suppose it holds for $4 \le k < n$; we next show that it also holds for n.

Let G be a graph with n > 4 vertices. If $\delta(G) \ge 3$, then by Lemma 1, the deletion of an edge with maximal weight yields a graph G' of minimal degree at least two such that H(G') < H(G). So, we only need to prove the result is true for G with $\delta(G) = 2$.

Case 1. Every pair of adjacent vertices of degree two has a common neighbor.

Let u_1 and u_2 be a pair of adjacent vertices with degree two in G which has a common neighbor u_3 . Obviously, $2 \le d(u_3) \le n - 1$.

Subcase 1.1. If $d(u_3) = 2$, let $G_1 = G - \{u_1, u_2, u_3\}$, then $H(G_1) \ge h_1(n-3)$ by the induction hypothesis, and $H(G) = H(G_1) + \frac{3}{2} \ge h_1(n-3) + \frac{3}{2} > h_1(n)$.

Subcase 1.2. If $d(u_3) \ge 4$, let $G_2 = G - \{u_1, u_2\}$, then $H(G_2) \ge h_1(n-2)$ by the induction hypothesis. Note that $\frac{1}{x} - \frac{1}{x-2}$ is increasing for x > 2.

$$\begin{split} H(G) &= H(G_2) + \frac{1}{2} + \frac{4}{d(u_3) + 2} + \sum_{v \in N(u_3) \setminus \{u_1, u_2\}} (\frac{2}{d(u_3) + d(v)} - \frac{2}{d(u_3) + d(v) - 2}) \\ & \geq H(G_2) + \frac{1}{2} + \frac{4}{d(u_3) + 2} + (d(u_3) - 2)(\frac{2}{d(u_3) + 2} - \frac{2}{d(u_3)}) \\ &= H(G_2) + \frac{1}{2} + \frac{4}{d(u_3)} - \frac{4}{d(u_3) + 2} \\ & \geq h_1(n-2) + \frac{1}{2} + \frac{4}{d(u_3)} - \frac{4}{d(u_3) + 2} \\ & \geq h_1(n-2) + \frac{1}{2} + \frac{4}{n-1} - \frac{4}{n+1} > h_1(n). \end{split}$$

Subcase 1.3. If $d(u_3) = 3$, let u_4 be the neighbor of u_3 in G different from u_1 and u_2 , where $0 \le d(u_4) \le n-3$. (i) Suppose that $d(u_4) = 2$. Denote by u_5 the neighbor of u_4 in G different from u_3 , where $0 \le d(u_5) \le n-4$. Let $0 \le G \le d(u_4) \le d(u_5) \le n-4$. Let $0 \le G \le d(u_4) \le d(u_5) \le d($

$$H(G) = H(G_3) + \frac{2}{5} + \frac{2}{d(u_5)+2} - \frac{2}{d(u_5)+3}$$

$$\geq H(G_3) + \frac{2}{5} + \frac{2}{n-2} - \frac{2}{n-1}$$

$$\geq h_1(n-1) + \frac{2}{5} + \frac{2}{n-2} + \frac{2}{n-1} > h_1(n).$$

(ii) Suppose that $3 \le d(u_4) \le n-3$. Let $G_4 = G - u_1 - u_2 - u_3$, then $H(G_4) \ge h_1(n-3)$ by the induction hypothesis. Note that $\frac{2}{x+2} - \frac{6}{x+1} + \frac{4}{x}$ is decreasing for x > 0.

$$\begin{split} H(G) &= H(G_4) + \frac{1}{2} + \frac{4}{5} + \frac{2}{d(u_4) + 3} + \sum_{v \in N(u_4) \setminus \{u_3\}} (\frac{2}{d(u_4) + d(v)} - \frac{2}{d(u_4) + d(v) - 1}) \\ &\geq H(G_4) + \frac{13}{10} + \frac{2}{d(u_4) + 3} + (d(u_4) - 1)(\frac{2}{d(u_3) + 2} - \frac{2}{d(u_4) + 1}) \\ &= H(G_4) + \frac{13}{10} + \frac{2}{d(u_4) + 3} - \frac{6}{d(u_4) + 2} + \frac{4}{d(u_4) + 1} \\ &\geq H(G_4) + \frac{13}{10} + \frac{2}{n} - \frac{6}{n - 1} + \frac{4}{n - 2} \\ &\geq h_1(n - 3) + \frac{13}{10} + \frac{2}{n} - \frac{6}{n - 1} + \frac{4}{n - 2} > h_1(n). \end{split}$$

Case 2. There is a pair of adjacent vertices of degree two without common neighbor.

Let u_1 and u_2 be a pair of adjacent vertices with degree two in G which has no common neighbor. Denote by u_3 the neighbor of u_1 in G different from u_2 . Let $G_5 = G - u_1 + u_2 u_3$, then $H(G_5) \ge h_1(n-1)$ by the induction hypothesis, and $H(G) = H(G_5) + \frac{1}{2} \ge h_1(n-1) + \frac{1}{2} > h_1(n)$. **Case 3**. There is no pair of adjacent vertices of degree two.

Let *u* be a vertex of degree two with neighbors *v* and *w* in *G*.

Subcase 3.1. $vw \notin E$, where $3 \le d(v) \le n-2$ and $3 \le d(w) \le n-2$. Let $G_6 = G - u + vw$, then $H(G_6) \ge h_1(n-1)$ by the induction hypothesis. Note that $f(x,y) = \frac{2}{x+2} + \frac{2}{y+2} - \frac{2}{x+y} \ge f(n-2,n-2)$ for $3 \le x \le n-2$ and $3 \le y \le n-2$, since $\frac{\partial f}{\partial x} < 0$ and $\frac{\partial f}{\partial y} < 0$.

$$H(G) = H(G_6) + \frac{2}{d(v)+2} + \frac{2}{d(w)+2} - \frac{2}{d(v)+d(w)}$$

$$\geq H(G_6) + f(n-2, n-2)$$

$$\geq h_1(n-1) + \frac{4}{n} - \frac{1}{n-2} > h_1(n).$$

Subcase 3.2. $vw \in E$, where $3 \le d(v) \le n-1$ and $3 \le d(w) \le n-1$. Let $G_7 = G - u$, then $H(G_7) \ge h_1(n-1)$ by the induction hypothesis. Note that $g(x,y) = \frac{2}{x+y} + \frac{6}{x+1} + \frac{6}{y+1} - \frac{2}{x+y-2} - \frac{6}{x+2} - \frac{6}{y+2} \ge g(n-1,n-1)$ for $3 \le x \le n-1$ and $3 \le y \le n-1$, since $\frac{\partial g}{\partial y}(\frac{\partial g}{\partial x}) < 0$ and $\frac{\partial g}{\partial x} \le \frac{\partial g(x,3)}{\partial x} < 0$, and $\frac{\partial g}{\partial x}(\frac{\partial g}{\partial y}) < 0$ and $\frac{\partial g}{\partial y} \le \frac{\partial g(3,y)}{\partial y} < 0$.

$$H(G) = H(G_7) + \frac{2}{d(v) + 2} + \frac{2}{d(w) + 2} - \frac{2}{d(v) + d(w) - 2} \\ + \sum_{z \in N(w) \setminus \{u, w\}} \left(\frac{2}{d(v) + d(z)} - \frac{2}{d(v) + d(z) - 1} \right) + \sum_{z \in N(w) \setminus \{u, v\}} \left(\frac{2}{d(w) + d(z)} - \frac{2}{d(w) + d(z) - 1} \right) \\ \ge H(G_7) + \frac{2}{d(v) + 2} + \frac{2}{d(w) + 2} - \frac{2}{d(v) + d(w) - 2} \\ + (d(v) - 2) \left(\frac{2}{d(v) + 2} - \frac{2}{d(v) + 1} \right) + (d(w) - 2) \left(\frac{2}{d(w) + 2} - \frac{2}{d(w) + 1} \right) \\ \text{(with equality if and only if } d(z) = 2 \text{ for all } z \in N(v) \cup N(w) \setminus \{u, v, w\}) \\ = H(G_7) + \frac{2}{d(v) + d(w)} + \frac{6}{d(v) + 1} + \frac{6}{d(w) + 1} - \frac{2}{d(v) + d(w) - 2} - \frac{6}{d(v) + 2} \right) - \frac{6}{d(v) + 2} - \frac{6}{d(w) + 2}) \\ \ge H(G_7) + g(n - 1, n - 1) \\ \text{(with equality if and only if } d(v) = d(w) = n - 1) \\ \ge h_1(n - 1) + \frac{1}{n - 1} + \frac{12}{n} - \frac{1}{n - 2} - \frac{12}{n + 1} \\ \text{(with equality if and only if } G_7 = K_{2, n - 3}^*) \\ = h_1(n)$$

with equality if and only if $G = K_{2,n-2}^*$. Hence, the assertion is true for all $n \ge 4$.

3. A lower bound for the harmonic index of a triangle-free graph with minimum degree at least two

In the section, we will give a best possible lower bound for the harmonic index of a triangle-free graph with minimum degree at least two and characterize the extremal graphs.

Theorem 3.1. Let G be a triangle-free graph of order $n \ge 4$ with $\delta(G) \ge 2$. Then $H(G) \ge h_2(n) = 4 - \frac{8}{n}$ with equality if and only if $G = K_{2,n-2}$.

Proof. It is easy to check that the assertion is true for n = 4. Suppose it holds for $4 \le k < n$; we next show that it also holds for n.

Let G be a graph with n > 4 vertices. If $\delta(G) \ge 3$, then by Lemma 1, the deletion of an edge with maximal weight yields a graph G' of minimal degree at least two such that H(G') < H(G). So, we only need to prove the result is true for G with $\delta(G) = 2$.

Case 1. There exists a vertex *u* of degree two such that the neighbors of *u* have degree at least three.

Let $N(u) = \{u_1, u_2\}$ and $3 \le d(u_i) \le n - 2$ for i = 1, 2, then $\delta(G - u) \ge 2$ and G - u is triangle-free. $H(G - u) \ge h_2(n - 1)$ by the induction hypothesis.

$$H(G) = H(G - u) + \frac{2}{d(u_1) + 2} + \frac{2}{d(u_2) + 2} + \sum_{v \in N(u_1) \setminus \{u\}} \left(\frac{2}{d(u_1) + d(v)} - \frac{2}{d(u_1) + d(v) - 1} \right)$$

$$+ \sum_{v \in N(u_2) \setminus \{u\}} \left(\frac{2}{d(u_2) + d(v)} - \frac{2}{d(u_2) + d(v) - 1} \right)$$

$$\geq H(G - u) + \frac{2}{d(u_1) + 2} + \frac{2}{d(u_2) + 2} + (d(u_1) - 1) \left(\frac{2}{d(u_1) + 2} - \frac{2}{d(u_1) + 1} \right)$$

$$+ (d(u_2) - 1) \left(\frac{2}{d(u_2) + 2} - \frac{2}{d(u_2) + 1} \right)$$
(with equality if and only if $d(v) = 2$ for all $v \in N(u_1) \cup N(u_2) \setminus \{u\}$)
$$= H(G - u) + \frac{4}{d(u_1) + 1} - \frac{4}{d(u_1) + 2} + \frac{4}{d(u_2) + 1} - \frac{4}{d(u_2) + 2}$$

$$\geq H(G - u) + \frac{4}{n - 1} - \frac{4}{n} + \frac{4}{n - 1} - \frac{4}{n}$$
(with equality if and only if $d(u_1) = d(u_2) = n - 2$)
$$\geq h_2(n - 1) + \frac{8}{n - 1} - \frac{8}{n}$$
 (with equality if and only if $G - u = K_{2,n-3}$)
$$= h_2(n)$$

with equality if and only if $G = K_{2,n-2}$.

Case 2. Every vertex *u* of degree two has a neighbor of degree two in *G*.

Let $N(u) = \{u_1, u_2\}$ and $d(u_1) = 2$, $d(u_2) \ge 2$; $N(u_1) = \{u, v\}$.

Subcase 2.1. v is not a neighbor of u_2 .

Let $G_1 = G - u + u_1u_2$, then $\delta(G_1) \ge 2$ and G_1 is triangle-free. $H(G_1) \ge h_2(n-1)$ by the induction hypothesis.

$$H(G) = H(G_1) + \frac{1}{2} \ge h_2(n-1) + \frac{1}{2} > h_2(n).$$

Subcase 2.2. v is also a neighbor of u_2 .

(I) If $d(v) = d(u_2) = 2$, let $G_2 = G - u - v - u_1 - u_2$, then $\delta(G_2) \ge 2$ and G_2 is triangle-free, implying $n \ge 8$. $H(G_2) \ge h_2(n-4)$ by the induction hypothesis.

$$H(G) = H(G_2) + 2 \ge h_2(n-4) + 2 > h_2(n)$$
.

(II) If none of v, u_2 has degree two, then $3 \le d(v) \le n-3$ and $3 \le d(u_2) \le n-3$ since G is triangle-free. Let $G_3 = G - u - u_1$, then $\delta(G_3) \ge 2$ and G_3 is triangle-free, implying $n \ge 6$. $H(G_3) \ge h_2(n-2)$ by the induction hypothesis.

Note that $t(x, y) = \frac{2}{x+y} - \frac{2}{x+y-2} + \frac{6}{x+1} + \frac{6}{y+1} - \frac{6}{x+2} - \frac{6}{y+2} \ge t(n-3, n-3)$ for $3 \le x \le n-3$ and $3 \le y \le n-3$, since $\frac{\partial}{\partial y}(\frac{\partial t}{\partial x}) = \frac{4}{(x+y)^3} - \frac{4}{(x+y-2)^3} < 0$ and $\frac{\partial t}{\partial x} \le \frac{\partial t(x,3)}{\partial x} = -\frac{2(2x^3+21x^2+60x+49)}{(x+1)^2(x+2)^2(x+3)^2} < 0$, and $\frac{\partial t}{\partial y} < 0$, similarly.

$$H(G) = H(G_3) + \frac{1}{2} + \frac{2}{d(v)+2} + \frac{2}{d(u_2)+2} + \frac{2}{d(v)+d(u_2)} - \frac{2}{d(v)+d(u_2)-2} + \sum_{w \in N(v) \setminus \{u_1, u_2\}} \left(\frac{2}{d(w)+d(v)} - \frac{2}{d(w)+d(v)-1} \right) + \sum_{w \in N(u_2) \setminus \{u, v\}} \left(\frac{2}{d(u_2)+d(w)} - \frac{2}{d(u_2)+d(w)-1} \right)$$

$$\geq H(G_3) + \frac{1}{2} + \frac{2}{d(v)+2} + \frac{2}{d(v)+2} + \frac{2}{d(v)+d(u_2)} - \frac{2}{d(v)+d(u_2)-2} + (d(v)-2)(\frac{2}{d(v)+2} - \frac{2}{d(v)+1}) + (d(u_2)-2)(\frac{2}{d(u_2)+2} - \frac{2}{d(u_2)+1})$$

$$= H(G_3) + \frac{1}{2} + t(d(v), d(u_2))$$

$$\geq H(G_3) + \frac{1}{2} + t(n-3, n-3)$$

$$\geq h_2(n-2) + \frac{1}{2} + t(n-3, n-3)$$

$$> h_2(n).$$

- (III) If exactly one of v, u_2 has degree two, without loss of generality, assume $d(u_2) = 2$, then $3 \le d(v) \le n-3$ since *G* is triangle-free.
- (i) If $d(v) \ge 4$, let $G_4 = G u u_1 u_2$, then $\delta(G_4) \ge 2$ and G_4 is triangle-free, implying $n \ge 7$. $H(G_4) \ge h_2(n-3)$ by the induction hypothesis.

$$H(G) = H(G_4) + 1 + \frac{4}{d(v)+2} + \sum_{w \in N(v) \setminus \{u_1, u_2\}} \left(\frac{2}{d(w)+d(v)} - \frac{2}{d(w)+d(v)-2} \right)$$

$$\geq H(G_4) + 1 + \frac{4}{d(v)+2} + (d(v)-2)\left(\frac{2}{d(v)+2} - \frac{2}{d(v)}\right)$$

$$= H(G_4) + 1 + \frac{4}{d(v)} - \frac{4}{d(v)+2}$$

$$\geq H(G_4) + 1 + \frac{4}{n-3} - \frac{4}{n-1}$$

$$\geq h_2(n-3) + 1 + \frac{4}{n-3} - \frac{4}{n-1}$$

$$> h_2(n)$$

- (ii) If d(v) = 3, denote by u_3 the neighbor of v in G different from u_1 and u_2 .
- (a) If $d(u_3) = 2$, let u_4 be the neighbor of u_3 in G different from v and $G_5 = G u_3 + vu_4$, then $\delta(G_5) \ge 2$ and G_5 is triangle-free. $H(G_5) \ge h_2(n-1)$ by the induction hypothesis. And

$$H(G) = H(G_5) + \frac{2}{5} + \frac{2}{d(u_4)+2} - \frac{2}{d(u_4)+3}$$

$$\geq H(G_5) + \frac{2}{5} + \frac{2}{2+3} - \frac{2}{2+2}$$

$$= H(G_5) + \frac{1}{2} \geq h_2(n-1) + \frac{1}{2} > h_2(n).$$

(b) If $d(u_3) \ge 3$, then $d(u_3) \le n - 5$ as G is triangle-free. Let $G_6 = G - u - v - u_1 - u_2$, we have $\delta(G_6) \ge 2$ and G_6 is triangle-free, implying $n \ge 8$. $H(G_6) \ge h_2(n-4)$ by the induction hypothesis. Note that $\frac{2}{x+3} - \frac{6}{x+2} + \frac{4}{x+1}$ is decreasing for $x \ge 0$.

$$H(G) = H(G_6) + 1 + \frac{4}{5} + \frac{2}{d(u_3)+3} + \sum_{w \in N(u_3) \setminus \{v\}} \left(\frac{2}{d(u_3)+d(w)} - \frac{2}{d(u_3)+d(w)-1} \right)$$

$$\geq H(G_6) + \frac{9}{5} + \frac{2}{d(u_3)+3} + (d(u_3) - 1) \left(\frac{2}{d(u_3)+2} - \frac{2}{d(u_3)+1} \right)$$

$$= H(G_6) + \frac{9}{5} + \frac{2}{d(u_3)+3} - \frac{6}{d(u_3)+2} + \frac{4}{d(u_3)+1}$$

$$\geq H(G_6) + \frac{9}{5} + \frac{2}{n-2} - \frac{6}{n-3} + \frac{4}{n-4}$$

$$\geq h_2(n-4) + \frac{9}{5} + \frac{2}{n-2} - \frac{6}{n-3} + \frac{4}{n-4}$$

$$\geq h_2(n)$$

The proof of our theorem is completed.

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