

## On The Harmonic Index and The Minimum Degree of A Graph

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**Abstract.** The harmonic index  $H(G)$  of a graph  $G$  is the sum of  $\frac{2}{d(u) + d(v)}$  over all edges  $uv$  of  $G$ , where  $d(u)$  denotes the degree of a vertex  $u$  in  $G$ . In this paper, we give the minimum value of  $H(G)$  for graphs  $G$  with given minimum degree  $\delta(G) \geq 2$  and characterize the corresponding extremal graph. Furthermore, we prove a best-possible lower bound on the harmonic index of a triangle-free graph  $G$  with arbitrary minimum degree  $\delta(G)$ .

**Key words:** Harmonic index; triangle-free graph; minimum degree.

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### 1. Introduction

All graphs  $G = (V, E)$  will be finite, undirected and simple. The degree and the neighborhood of a vertex  $u \in V$  will be denoted by  $d(u)$  and  $N(u)$ , respectively. The minimum degree of a graph  $G$  is denoted by  $\delta(G)$ . The graph that arises from  $G$  by deleting the vertex  $u \in V$  or the edge  $uv \in E$  will be denoted by  $G - u$  or  $G - uv$ , respectively. Finally, the graph  $G + uv$  arises from  $G$  by adding an edge  $uv \notin E$  between the endpoints  $u, v \in V$ .

The Randić index of an organic molecule whose molecular graph is  $G$  was introduced by the chemist Milan Randić in 1975 [5] as

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

where 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 books [3],[5], [6]).

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

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

The term  $\frac{2}{d(u) + d(v)}$  will be called the weight of the edge  $uv \in E$ .

There are many different kinds of chemical indices. Different indices have different use in chemistry. And there are good correlations between indices and several physicochemical properties of alkanes: boiling points, surface areas, energy levels, etc. Recently, finding bounds for indices of a given class of graphs, as well as related problem of finding the graphs with extremal indices, attracted the attention of many researchers, and many results have been obtained.

The relation between the harmonic index and the eigenvalues of graphs was considered in [2]. In [8], [9], [10] and [11], the authors presented the minimum and maximum values of harmonic index on simple connected graphs, trees, unicyclic graphs and graphs with given number of pendant vertices and diameter respectively. In [4] and [7], the authors established some relationships between harmonic index and several other topological indices.

In this paper, we give the minimum value of  $H(G)$  for graphs  $G$  with given minimum degree  $\delta(G) \geq 2$  and characterize the corresponding extremal graph. Furthermore, we prove a best-possible lower bound on the harmonic index of a triangle-free graph  $G$  with arbitrary minimum degree  $\delta(G)$ .

## 2. The minimum value of $H(G)$ for graphs $G$ with $\delta(G) \geq 2$

**Lemma 2.1.** *Let  $uv$  be an edge of maximal weight in a graph  $G$ . Then*

$$H(G - uv) < H(G).$$

*Proof.* Consider the edge  $e = uv$  with maximal weight among all edges of  $G$ . Let  $d(u) = p$  and  $d(v) = q$ . Denote  $N(u) = \{v, x_1, \dots, x_{p-1}\}$  and  $N(v) = \{u, y_1, \dots, y_{q-1}\}$ . Note that we

allow  $x_i = y_j$  for some vertices  $x_i$  and  $y_j$ . Then by using  $p+q \leq p+d(x_i)$  and  $p+q \leq q+d(y_j)$ , we have

$$\begin{aligned} H(G) - H(G - uv) &= \left( \frac{2}{p+q} + \sum_{i=1}^{p-1} \frac{2}{p+d(x_i)} + \sum_{j=1}^{q-1} \frac{2}{q+d(y_j)} \right) \\ &\quad - \left( \sum_{i=1}^{p-1} \frac{2}{p-1+d(x_i)} + \sum_{j=1}^{q-1} \frac{2}{q-1+d(y_j)} \right) \\ &= \frac{2}{p+q} - \sum_{i=1}^{p-1} \frac{2}{(p+d(x_i))(p-1+d(x_i))} \\ &\quad - \sum_{j=1}^{q-1} \frac{2}{(q+d(y_j))(q-1+d(y_j))} \\ &\geq \frac{2}{p+q} - \frac{2(p+q-2)}{(p+q)(p+q-1)} > 0. \quad \square \end{aligned}$$

The unique graph which arises from a complete bipartite graph  $K_{\delta,n-\delta}$  by joining each pair of vertices in the part with  $\delta$  vertices by a new edge will be denoted by  $K_{\delta,n-\delta}^*$ . And for  $x \geq 3$ , let  $h(x) = 4 \left( 1 - \frac{3}{x+1} \right) + \frac{1}{x-1}$ .

**Theorem 2.2.** *Let  $G = (V, E)$  be a graph of order  $n \geq 4$  with  $\delta(G) \geq 2$ . Then*

$$H(G) \geq h(n)$$

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

*Proof.* We use mathematical induction on the order of graphs to prove the theorem.

When  $n = 4$ , there are only three graphs with  $\delta(G) \geq 2$ :  $K_{2,2}$ ,  $K_{2,2}^*$ ,  $K_4$ . And it is easy to verify that  $H(G) \geq h(4)$  and  $H(G) = h(4)$  if and only if  $G = K_{2,2}^*$ .

Let  $n \geq 5$  and suppose that the property holds for all graphs of order at most  $n - 1$ . If there exist graphs of order  $n$  with  $H(G) < h(n)$ , we choose such graph  $G$  among these graphs with minimal harmonic index.

If  $\delta(G) > 2$ , by Lemma 2.1, the deletion of an edge with maximal weight yields a graph  $G'$  of minimum degree at least 2 and with  $H(G') < H(G)$ , a contradiction. Hence  $\delta(G) = 2$ .

**Claim 1.** For any vertex  $x \in V$  of degree 2 with  $N(x) = \{y, z\}$ , we have  $yz \in E$ .

*Proof.* If  $yz \notin E$ , by the induction hypothesis we have  $H(G') \geq h(n - 1)$ ,  $G' = G - x + yz$ . For

$2 \leq d_1 = d(y) \leq n - 2$ ,  $2 \leq d_2 = d(z) \leq n - 2$  we have

$$\begin{aligned}
 H(G) &= H(G') - \frac{2}{d_1 + d_2} + \frac{2}{d_1 + 2} + \frac{2}{d_2 + 2} \\
 &\geq h(n-1) - \frac{2}{d_1 + d_2} + \frac{2}{d_1 + 2} + \frac{2}{d_2 + 2} \\
 &\geq \frac{4(n-3)}{n} + \frac{1}{n-2} + \frac{2}{n} \\
 &= 4\left(1 - \frac{3}{n+1}\right) + \frac{1}{n-1} + \frac{1}{n-2} + \frac{12}{n+1} - \frac{1}{n-1} - \frac{10}{n} \\
 &= h(n) + \frac{2n\left(n - \frac{15}{4}\right)^2 + \frac{55}{8}n - 20}{(n+1)n(n-1)(n-2)} > h(n),
 \end{aligned}$$

which is a contradiction.  $\square$

**Claim 2.** For any vertex  $u \in V$  of degree 2 with  $N(u) = \{x, y\}$ , we have  $d(x) \geq 3$ ,  $d(y) \geq 3$ .

*Proof.* Let  $d(x) = 2$ . We have  $2 \leq d = d(y) \leq n - 1$ . Now we consider the following cases.

**Case 1.**  $d = 2$ .

In this case,  $n \geq 6$ . By the induction hypothesis, the graph  $G' = G - u - x - y$  satisfies  $H(G') \geq h(n-1)$  and

$$\begin{aligned}
 H(G) &= H(G') + \frac{3}{2} \geq h(n-3) + \frac{3}{2} \\
 &\geq 4\left(1 - \frac{3}{n-2}\right) + \frac{1}{n-4} + \frac{3}{2} > 4\left(1 - \frac{3}{n-2}\right) + \frac{1}{n-1} + \frac{3}{2} \\
 &= 4\left(1 - \frac{3}{n+1}\right) + \frac{1}{n-1} + \frac{3}{2} - \frac{12}{n-2} + \frac{12}{n+1} \\
 &= h(n) + \frac{3}{2} - \frac{36}{(n+1)(n-2)} > h(n),
 \end{aligned}$$

a contradiction.

**Case 2.**  $d = 3$ .

In this case, we assume that  $N(y) = \{u, x, z\}$ . By Claim 1, we have  $d' = d(z) \geq 3$ . It follows that  $n \geq 6$ . Denote  $N(z) = \{y, \omega_1, \dots, \omega_{d'-1}\}$ . By the induction hypothesis we have

$H(G') \geq h(n-3)$ ,  $G' = G - u - x - y$ . And for  $d' \leq n-2$ ,  $d_{\omega_i} \geq 2$ , we have

$$\begin{aligned} H(G) &= H(G') + \sum_{i=1}^{d'-1} \frac{2}{d' + d(\omega_i)} - \sum_{i=1}^{d'-1} \frac{2}{d' - 1 + d(\omega_i)} + \frac{1}{2} + \frac{4}{5} + \frac{2}{3 + d'} \\ &\geq h(n-3) + \frac{1}{2} + \frac{4}{5} + \frac{2}{3 + d'} - \sum_{i=1}^{d'-1} \frac{2}{(d' + d(\omega_i))(d' - 1 + d(\omega_i))} \\ &\geq 4\left(1 - \frac{3}{n-2}\right) + \frac{1}{n-4} + \frac{1}{2} + \frac{4}{5} + \frac{2(d'+5)}{(d'+1)(d'+2)(3+d')} \\ &> 4\left(1 - \frac{3}{n-2}\right) + \frac{1}{n-1} + \frac{1}{2} + \frac{4}{5} + \frac{2(n+3)}{(n-1)n(n+1)} \\ &= 4\left(1 - \frac{3}{n+1}\right) + \frac{1}{n-1} + \frac{13}{10} + \frac{12}{n+1} - \frac{12}{n-2} + \frac{2(n+3)}{(n-1)n(n+1)} \\ &= h(n) + \frac{13}{10} - \frac{34n^2 - 38n + 12}{(n-2)(n-1)n(n+1)} \geq h(n) + \frac{13}{10} - \frac{12}{10} > h(n). \end{aligned}$$

The inequality  $\frac{2(d'+5)}{(d'+1)(d'+2)(3+d')} \geq \frac{2(n+3)}{(n-1)n(n+1)}$  holds since the function  $f(x) = \frac{2(x+5)}{(x+1)(x+2)(x+3)}$  is monotonously decreasing in  $x$  and  $3 \leq d' \leq n-2$ . The inequality  $-\frac{34n^2 - 38n + 12}{(n-2)(n-1)n(n+1)} \geq -\frac{12}{10}$  holds since the function  $g(x) = -\frac{34x^2 - 38x + 12}{(x-2)(x-1)x(x+1)}$  is monotonously increasing in  $x$  and  $n \geq 6$ .

**Case 3.**  $d \geq 4$ .

In this case, we have  $n \geq 5$ . Let  $N(y) = \{u, x, u_1, \dots, u_{d-2}\}$ . The graph  $G' = G - u - x$  satisfies  $H(G') \geq h(n-2)$  by the induction hypothesis and for  $d \leq n-1$ ,  $d_{u_i} \geq 2$ , we have

$$\begin{aligned} H(G) &= H(G') + \sum_{i=1}^{d-2} \frac{2}{d + d(u_i)} - \sum_{i=1}^{d-2} \frac{2}{d - 2 + d(u_i)} + \frac{1}{2} + \frac{4}{2 + d} \\ &\geq h(n-2) + \frac{1}{2} + \frac{4}{2 + d} - \sum_{i=1}^{d-2} \frac{4}{(d + d(u_i))(d - 2 + d(u_i))} \\ &\geq 4\left(1 - \frac{3}{n-1}\right) + \frac{1}{n-3} + \frac{1}{2} + \frac{8}{d(d+2)} \\ &= h(n) + \frac{1}{2} + \left(\frac{12}{n+1} - \frac{12}{n-1}\right) + \left(\frac{1}{n-3} - \frac{1}{n-1}\right) + \frac{8}{d(d+2)} \\ &\geq h(n) + \frac{1}{2} - \frac{16}{n^2 - 1} + \frac{2}{(n-3)(n-1)} = h(n) + \frac{1}{2} - \frac{14n - 50}{(n^2 - 1)(n-3)} > h(n). \end{aligned}$$

The inequality  $\frac{14n - 50}{(n^2 - 1)(n-3)} < \frac{1}{2}$  holds since the function  $\frac{14x - 50}{(x^2 - 1)(x-3)}$  is monotonously decreasing in  $x$  and  $n \geq 5$ . Then  $H(G) > h(n)$  for  $n \geq 5$ , a contradiction.

Therefore, all cases lead to a contradiction. Then  $d(x) \geq 3$ . By symmetry,  $d(y) \geq 3$ . The proof of Claim 2 is completed.  $\square$

Now let  $u \in V$  with  $d(u) = 2$  and  $N(u) = \{u_1, u_2\}$ . By Claim 2, we have  $d_1 = d(u_1) \geq 3$ ,  $d_2 = d(u_2) \geq 3$ . Let  $N(u_1) = \{u, u_2, v_1, \dots, v_{d_1-2}\}$  and  $N(u_2) = \{u, u_1, v'_1, \dots, v'_{d_2-2}\}$ . Then

$$\begin{aligned} H(G) - H(G - u) &= \frac{2}{d_1 + 2} + \frac{2}{d_2 + 2} + \frac{2}{d_1 + d_2} + \sum_{i=1}^{d_1-2} \frac{2}{d_1 + d(v_i)} + \sum_{i=1}^{d_2-2} \frac{2}{d_2 + d(v'_i)} \\ &\quad - \frac{2}{d_1 - 1 + d_2 - 1} - \sum_{i=1}^{d_1-2} \frac{2}{d_1 - 1 + d(v_i)} - \sum_{i=1}^{d_2-2} \frac{2}{d_2 - 1 + d(v'_i)} \\ &\geq \frac{2}{d_1 + 2} + \frac{2}{d_2 + 2} - \frac{4}{(d_1 + d_2)(d_1 + d_2 - 2)} - \frac{2(d_1 - 2)}{(d_1 + 1)(d_1 + 2)} \\ &\quad - \frac{2(d_2 - 2)}{(d_2 + 1)(d_2 + 2)} \\ &= \frac{6}{(d_1 + 1)(d_1 + 2)} + \frac{6}{(d_2 + 1)(d_2 + 2)} - \frac{4}{(d_1 + d_2)(d_1 + d_2 - 2)}. \end{aligned}$$

$$\text{Let } f(d_1, d_2) = \frac{6}{(d_1 + 1)(d_1 + 2)} + \frac{6}{(d_2 + 1)(d_2 + 2)} - \frac{4}{(d_1 + d_2)(d_1 + d_2 - 2)}.$$

Then

$$\begin{aligned} \frac{\partial}{\partial d_1} f(d_1, d_2) &= \frac{6}{(d_1 + 2)^2} - \frac{6}{(d_1 + 1)^2} + \frac{2}{(d_1 + d_2 - 2)^2} - \frac{2}{(d_1 + d_2)^2}, \\ \frac{\partial}{\partial d_2} \frac{\partial}{\partial d_1} f(d_1, d_2) &= \frac{4}{(d_1 + d_2)^3} - \frac{4}{(d_1 + d_2 - 2)^3} < 0. \end{aligned}$$

So

$$\begin{aligned} \frac{\partial}{\partial d_1} f(d_1, d_2) &\leq \frac{\partial}{\partial d_1} f(d_1, 3) = \frac{6}{(d_1 + 2)^2} - \frac{4}{(d_1 + 1)^2} - \frac{2}{(d_1 + 3)^2} \\ &= \frac{-4d_1^3 - 42d_1^2 - 120d_1 - 98}{(d_1 + 1)^2(d_1 + 2)^2(d_1 + 3)^2} < 0. \end{aligned}$$

By symmetry,  $\frac{\partial}{\partial d_2} f(d_1, d_2) < 0$ .

Hence  $f(d_1, d_2) \geq f(n-1, n-1) = \frac{12}{n(n+1)} + \frac{1}{n-1} - \frac{1}{n-2}$

and

$$H(G) \geq H(G - u) + f(d_1, d_2) \geq h(n-1) + \frac{12}{n(n+1)} + \frac{1}{n-1} - \frac{1}{n-2} = h(n).$$

$H(G) = h(n)$  implies that equality holds in the above inequality, that is  $G = K_{2,n-2}^*$ . Conversely, it is obvious that  $H(K_{2,n-2}^*) = h(n)$ .  $\square$

### 3. The minimum value of $H(G)$ for triangle-free graphs $G$

In this part, we consider triangle-free graphs. and we get a lower bound on  $H(G)$  in terms of  $\delta$  by a new method.

An edge of  $G$ , connecting a vertex of degree  $i$  with a vertex of degree  $j$  will be called an  $(i, j)$ -edge. The number of  $(i, j)$ -edges will be denoted by  $x_{i,j}$ .

**Lemma 3.1.** *The harmonic index of a graph  $G$  without isolated vertices can be rewritten as*

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)} = \frac{n}{2} - \frac{1}{2} \sum_{1 \leq i < j \leq n-1} \left( \frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) x_{i,j}.$$

*Proof.*  $H(G)$  can be rewritten as

$$H(G) = \sum_{1 \leq i < j \leq n-1} \frac{2x_{i,j}}{i+j} = \sum_{1 \leq i < j \leq n-1} \frac{2x_{i,j}}{i+j} + \sum_{i=1}^{n-1} \frac{x_{i,i}}{i}.$$

Denote by  $n_i$  the number of vertices of  $G$  having degree  $i$ . Then  $\sum_{j=1, j \neq i}^n x_{i,j} + 2x_{i,i} = in_i$ , that is,

$$n_i = \frac{1}{i} \left( \sum_{j=1, j \neq i}^n x_{i,j} + 2x_{i,i} \right).$$

We have  $n_1 + n_2 + \dots + n_{n-1} = n$  and  $x_{i,j} = x_{j,i}$ , so

$$\sum_{1 \leq i < j \leq n-1} \left( \frac{1}{i} + \frac{1}{j} \right) x_{i,j} + 2 \sum_{i=1}^{n-1} \frac{x_{i,i}}{i} = n.$$

It follows that  $n - 2H(G) = \sum_{1 \leq i < j \leq n-1} \left( \frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) x_{i,j}$ , that is,

$$H(G) = \frac{n}{2} - \frac{1}{2} \sum_{1 \leq i < j \leq n-1} \left( \frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) x_{i,j}. \quad \square$$

**Theorem 3.2.** *Let  $G = (V, E)$  be a triangle-free graph of order  $n$  with  $\delta(G) \geq k \geq 1$ . Then*

$$H(G) \geq \frac{2k(n-k)}{n}$$

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

*Proof.* Let  $m$  be the number of edges of  $G$ . If  $m > k(n-k)$ , since  $G$  is triangle-free, we have  $d(u) + d(v) \leq n$  for any edge  $uv \in E$  and  $H(G) > \frac{2k(n-k)}{n}$  and equality is not possible.

Hence we may assume that  $m \leq k(n-k)$ . For  $G$  is triangle-free, the maximum degree of  $G$  is at most  $n - \delta$ . By Lemma 3.1,  $H(G)$  can be rewritten as

$$\begin{aligned} H(G) &= \frac{n}{2} - \frac{1}{2} \sum_{\delta \leq i < j \leq n-\delta} \left( \frac{1}{i} + \frac{1}{j} - \frac{4}{i+j} \right) x_{i,j} \\ &\geq \frac{n}{2} - \frac{1}{2} \sum_{\delta \leq i < j \leq n-\delta} \left( \frac{1}{i} + \frac{1}{n-i} - \frac{4}{n} \right) x_{i,j} = \frac{n}{2} + \frac{1}{2} \sum_{\delta \leq i < j \leq n-\delta} \left( \frac{4}{n} - \frac{n}{i(n-i)} \right) x_{i,j} \\ &\geq \frac{n}{2} + \frac{1}{2} \sum_{\delta \leq i < j \leq n-\delta} \left( \frac{4}{n} - \frac{n}{\delta(n-\delta)} \right) x_{i,j} = \frac{n}{2} - \frac{m(n-2\delta)^2}{2n\delta(n-\delta)} \\ &\geq \frac{n}{2} - \frac{k(n-k)(n-2\delta)^2}{2n\delta(n-\delta)} \\ &\geq \frac{n}{2} - \frac{k(n-k)(n-2k)^2}{2nk(n-k)} = \frac{2k(n-k)}{n}. \end{aligned}$$

The first inequality holds since the function  $\frac{4}{i+j} - \frac{1}{j}$  is monotonously decreasing in  $j$  for  $j > i$  and  $j \leq n-i$ . The second inequality holds since the function  $-\frac{n}{i(n-i)}$  is monotonously increasing in  $i$  for  $\delta \leq i \leq \frac{n}{2}$ . The last inequality holds since the function  $-\frac{(n-2\delta)^2}{n\delta(n-\delta)}$  is monotonously increasing in  $\delta$  and  $k \leq \delta \leq \frac{n}{2}$ .

In the above inequality chain equality holds throughout if and only if  $m = k(n-k) = x_{k,n-k}$ , which implies that  $G = K_{k,n-k}$ .  $\square$

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