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A Lower Bound for the Harmonic Index of a Graph with Minimum Degree at Least Three

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Abstract. The harmonic index $H(G)$ of a graph G is 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. In this work, a lower bound for the harmonic index of a graph with minimum degree at least three is obtained and the corresponding extremal graph is characterized.

1. Introduction

In this article, we study the harmonic index of a graph. Let G be a simple, undirected and connected graph with vertex set $V(G)$ and edge set $E(G)$. We denote the number of vertices of G by $n(G)$, for simplicity, we denote n. For a vertex u of G, the degree of u is written by $d_G(u)$, or just for short $d(u)$. We use $N_G(u)$(or $N(u)$ for short) to denote the set of the vertices adjacent to u in G. Let $\delta(G)$ be the minimum degree of G and let $\triangle(G)$ be the maximum degree of G . We use $G-u$ to denote the graph obtained from G by deleting the vertex u and the edges adjacent with u. $G-uv$ is the graph obtained from G by deleting the edge $uv \in E(G)$. $G+uv$ is the graph obtained from G by adding an edge uv between two non-adjacent vertices u and v of G. For an edge $e = uv$ of 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. It is denoted by $H(G)$ and is defined in [2] as

$$H(G) = \sum_{uv\in E(G)} \frac{2}{d(u)+d(v)}. \tag{1}$$

The harmonic index is another variant of the Randić index which is defined in [8].

$$R(G) = \sum_{uv\in E(G)} (d(u)d(v))^{-\frac{1}{2}}. \tag{2}$$

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The Randić index was first proposed by Randić in 1975. It has been found that the Randić index had good connected with the chemical and physical properties, such as boiling point, vapour pressure, surface area, solubility in water and so on, see [8]. The Randić index is one of the most successful molecular variant in structure-property and structure-activity relationships studies, suitable for measuring the extent of branching of the carbonatom skeleton of saturated hydrocarbons. When comparing $H(G)$ to $R(G)$, it is easy to get that $H(G) \leq R(G)$ with equality if and only if G is a regular graph ($\delta(G)=\triangle(G)$). The harmonic index gives better relations with the chemical and physical properties than the Randić index, see [10].

The harmonic index is one of the most important indices in chemical and mathematical fields. New results related to the harmonic index of a graph are constantly being obtained. In [3], Favaron et al. got the relation between the harmonic index and the eigenvalues of graphs. In [5], Liu gave the relationship between the harmonic index and diameter of graphs. In [1], Deng et al. obtained that the connection between the harmonic index and the chromatic number of a graph. In [11], Zhong gave the minimum values of the harmonic index for simple connected graphs and trees, and also characterized the corresponding extremal graphs. He proved that the trees with maximum and minimum harmonic indices were the path P_n and the star S_n, respectively. In [4], Hu and Zhou gave the minimum and maximum values of the harmonic index for unicyclic and bicyclic graphs and described the corresponding extremal graphs. They also showed that the regular or almost regular graphs had the maximum harmonic in connected graphs with n vertices and m edges. In [9], Wu et al. gave the minimum value of the harmonic index of a graph (a triangle-free graph, respectively) with minimum degree at least two and characterized the corresponding extremal graphs. In [6], Liu obtained the minimum value of the harmonic index for any triangle-free graphs with order n and minimum degree $\delta \geq k$ for $k \leq \frac{n}{2}$ and the corresponding extremal graph is the complete bipartite graph $K_{k,n-k}$. In [7], Lv got the minimum values of the harmonic index for the graphs with k vertices of degree $n-1$, and showed the corresponding extremal graph. In this work, we study the minimum value of the harmonic index among the graphs with minimum degree at least three.

2. Main Results

In this section, we get a lower bound for the harmonic index of a graph with minimum degree at least three and describe the corresponding extremal graph.

Lemma 2.1. *([9]) If e is an edge with maximal weight in G, then $H(G-e) < H(G)$.*

Let $K_{a,b}$ be the complete bipartite graphs with a and b vertices in its two partite sets, respectively. For $n \geq 4$, $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$, let $K^*_{k,n-k}$ be the graph obtained from $K_{k,n-k}$ by joining an edge between any two non-adjacent vertices of degree $n-k$.

Lemma 2.2. *([7])* $H(K^*_{k,n-k}) = \frac{2k(n-k)}{k+n-1} + \frac{k(k-1)}{2(n-1)}$.

Proof. $H(K^*_{k,n-k}) = \frac{2k(n-k)}{k+n-1} + \frac{2(k-1+\cdots+2+1)}{n-1+n-1} = \frac{2k(n-k)}{k+n-1} + \frac{k(k-1)}{2(n-1)}$.

Particularly, for $k=3$, it is obtained that $H(K^*_{3,n-3}) = h_1(n) = 6 + \frac{3}{n-1} - \frac{30}{n+2}$.

Theorem 2.3. *Let G be a graph with $n \geq 6$ vertices and $\delta(G) \geq 3$. Then $H(G) \geq H(K^*_{3,n-3}) = h_1(n)$ with equality if and only if $G = K^*_{3,n-3}$.*

Proof. It is easy to check that the conclusion is true for $n = 6$. Assume it holds for $6 \leq k < n$. Next we prove that it holds for $k = n$.

Let G be a graph with $n \geq 6$ vertices. If $\delta(G) \geq 4$, then by Lemma 2.1, the deletion of an edge with maximal weight yields a graph G' of minimal degree at least three such that $H(G') < H(G)$. So, we only need to prove the result is true for G with $\delta(G) = 3$. Next we discuss the following four cases.

Case 1. There is no pair of adjacent vertices of degree three.

Let u be a vertex of degree three of G and let u_1, u_2, u_3 be the neighbors of u, we have $d(u_1), d(u_2), d(u_3) \geq 4$.

Subcase 1.1. If edges $u_1u_2, u_1u_3, u_2u_3 \in E(G)$, let $G_1 = G - \{u\}$, then $H(G_1) \geq h_1(n-1)$ by the induction hypothesis.

Note that

$$f_1(x,y,z) = \frac{2}{3+x} + \frac{2}{3+y} + \frac{2}{3+z} - \frac{4}{(x+y)(x+y-2)} - \frac{4}{(x+z)(x+z-2)} - \frac{4}{(y+z)(y+z-2)} - \frac{2(x-3)}{(x+3)(x+2)} - \frac{2(y-3)}{(y+3)(y+2)} - \frac{2(z-3)}{(z+3)(z+2)},$$

where $4 \leq x, y, z \leq n-1$.

$$\frac{\partial f_1}{\partial x} = \frac{-2}{(x+3)^2} + \frac{8(x+y-1)}{(x+y)^2(x+y-2)^2} + \frac{8(x+z-1)}{(x+z)^2(x+z-2)^2} + \frac{2x^2-12x-42}{(x+3)^2(x+2)^2}$$
$$= \frac{-20x-50}{(x+3)^2(x+2)^2} + \frac{8(x+y-1)}{(x+y)^2(x+y-2)^2} + \frac{8(x+z-1)}{(x+z)^2(x+z-2)^2}.$$

$$\frac{\partial^2 f_1}{\partial x \partial y} = \frac{8[(x+y-2)(x+y) - 4(x+y-1)^2]}{(x+y-2)^3(x+y)^3} < \frac{8[(x+y-1)(x+y) - 4(x+y-1)^2]}{(x+y-2)^3(x+y)^3} < \frac{8(x+y-1)(-3x-3y+4)}{(x+y-2)^3(x+y)^3} < 0.$$

Similarly, we get $\frac{\partial^2 f_1}{\partial x \partial z} < 0$. Since $\frac{\partial^2 f_1}{\partial x \partial y} < 0, \frac{\partial^2 f_1}{\partial x \partial z} < 0$, we have

$$\frac{\partial f_1}{\partial x} \leq \frac{\partial f_1(x,4,4)}{\partial x} = \frac{(-20x-50)(x+4)^2 + 16(x+3)^3}{(x+2)^2(x+3)^2(x+4)^2} < 0.$$

From the symmetry on x, y, z of $f_1(x,y,z)$, it follows that $\frac{\partial f_1}{\partial y} < 0, \frac{\partial f_1}{\partial z} < 0$. Then we get $f_1(x,y,z) \geq f_1(n-1, n-1, n-1) = \frac{6}{n+2} - \frac{3}{(n-1)(n-2)} - \frac{6(n-4)}{(n+2)(n+1)}$.

$$\begin{aligned} H(G) = H(G_1) &+ \frac{2}{3+d(u_1)} + \frac{2}{3+d(u_2)} + \frac{2}{3+d(u_3)} + \frac{2}{d(u_1)+d(u_2)} - \frac{2}{d(u_1)+d(u_2)-2} \\ &+ \frac{2}{d(u_1)+d(u_3)} - \frac{2}{d(u_1)+d(u_3)-2} + \frac{2}{d(u_2)+d(u_3)} - \frac{2}{d(u_2)+d(u_3)-2} \\ &+ \sum_{v \in N(u_1)\backslash\{u,u_2,u_3\}} \left(\frac{2}{d(u_1)+d(v)} - \frac{2}{d(u_1)-1+d(v)}\right) \\ &+ \sum_{v \in N(u_2)\backslash\{u,u_1,u_3\}} \left(\frac{2}{d(u_2)+d(v)} - \frac{2}{d(u_2)-1+d(v)}\right) \\ &+ \sum_{v \in N(u_3)\backslash\{u,u_1,u_2\}} \left(\frac{2}{d(u_3)+d(v)} - \frac{2}{d(u_3)-1+d(v)}\right) \\ \geq H(G_1) &+ \frac{2}{3+d(u_1)} + \frac{2}{3+d(u_2)} + \frac{2}{3+d(u_3)} + \frac{-4}{(d(u_1)+d(u_2))(d(u_1)+d(u_2)-2)} \\ &- \frac{4}{(d(u_1)+d(u_3))(d(u_1)+d(u_3)-2)} - \frac{4}{(d(u_2)+d(u_3))(d(u_2)+d(u_3)-2)} \end{aligned}$$

$$
\begin{aligned}
&- \frac{2(d(u_1)-3)}{(d(u_1)+3)(d(u_1)+2)} - \frac{2(d(u_2)-3)}{(d(u_2)+3)(d(u_2)+2)} - \frac{2(d(u_3)-3)}{(d(u_3)+3)(d(u_3)+2)} \\
&\geq h_1(n-1) + \frac{6}{n+2} - \frac{3}{(n-1)(n-2)} - \frac{6(n-4)}{(n+2)(n+1)} \\
&\quad (\text{with equality if and only if } d(u_1) = d(u_2) = d(u_3) = n-1) \\
&= h_1(n).
\end{aligned}
$$

Then equality $H(G) = h_1(n)$ holds if and only if $G = K^*_{3,n-3}$.

Subcase 1.2. If edges $u_1u_2, u_1u_3 \in E(G)$, edge $u_2u_3 \notin E(G)$, let $G_2 = G - \{u\} + \{u_2u_3\}$, then $H(G_2) \geq h_1(n-1)$ by the induction hypothesis. Note that

$$
\begin{aligned}
f_2(x,y,z) = &\frac{2}{x+3} + \frac{2}{y+3} + \frac{2}{z+3} - \frac{2}{(x+y-1)(x+y)} - \frac{2}{(x+z-1)(x+z)} \\
&- \frac{2(x-3)}{(x+2)(x+3)} - \frac{2}{y+z},
\end{aligned}
$$

where $4 \leq x \leq n-1, 4 \leq y, z \leq n-2$.

$$\frac{\partial f_2}{\partial x} = \frac{-20x-50}{(x+2)^2(x+3)^2} + \frac{4x+4y-2}{(x+y-1)^2(x+y)^2} + \frac{4x+4z-2}{(x+z-1)^2(x+z)^2},$$

$$\frac{\partial^2 f_2}{\partial x \partial y} = \frac{-12(x+y)^2 + 12(x+y) - 4}{(x+y-1)^3(x+y)^3} < 0,$$

$$\frac{\partial^2 f_2}{\partial x \partial z} = \frac{-12(x+z)^2 + 12(x+z) - 4}{(x+z-1)^3(x+z)^3} < 0,$$

so

$$\frac{\partial f_2}{\partial x} \leq \frac{\partial f_2(x,4,4)}{\partial x} = \frac{-20x-50}{(x+2)^2(x+3)^2} + \frac{8x+28}{(x+3)^2(x+4)^2} < 0,$$

$$\frac{\partial f_2}{\partial y} = \frac{-2}{(y+3)^2} + \frac{2(2x+2y-1)}{(x+y-1)^2(x+y)^2} + \frac{2}{(y+z)^2},$$

$$\frac{\partial^2 f_2}{\partial y \partial x} = \frac{-12(x+y)^2 + 12(x+y) - 12}{(x+y-1)^3(x+y)^3} < 0, \frac{\partial^2 f_2}{\partial y \partial z} = -\frac{4}{(y+z)^3} < 0,$$

so

$$\frac{\partial f_2}{\partial y} \leq \frac{\partial f_2(4,y,4)}{\partial y} = \frac{-2}{(y+3)^2} + \frac{14+4y}{(y+3)^2(y+4)^2} + \frac{2}{(y+4)^2} = 0.$$

From the symmetry on y, z of $f_2(x,y,z)$, we get that $\frac{\partial f_2}{\partial z} \leq 0$. Then we have $f_2(x,y,z) \geq f_2(n-1,n-2,n-2) = \frac{2}{n+2} + \frac{4}{n+1} - \frac{2}{(2n-3)(n-2)} - \frac{2(n-4)}{(n+2)(n+3)} - \frac{1}{n-2}$.

$$H(G) = H(G_2) + \frac{2}{3+d(u_1)} + \frac{2}{3+d(u_2)} + \frac{2}{3+d(u_3)} + \frac{2}{d(u_1)+d(u_2)} - \frac{2}{d(u_1)-1+d(u_2)}$$

$$+\frac{2}{d(u_1)+d(u_3)}-\frac{2}{d(u_1)-1+d(u_3)}-\frac{2}{d(u_2)+d(u_3)}$$
$$+\sum_{v\in N(u_1)\setminus\{u,u_2,u_3\}}(\frac{2}{d(u_1)+d(v)}-\frac{2}{d(u_1)-1+d(v)})$$
$$\geq H(G_2)+\frac{2}{3+d(u_1)}+\frac{2}{3+d(u_2)}+\frac{2}{3+d(u_3)}-\frac{2}{(d(u_1)+d(u_2)-1)(d(u_1)+d(u_2))}$$
$$-\frac{2}{(d(u_1)+d(u_3)-1)(d(u_1)+d(u_3))}-\frac{2}{d(u_2)+d(u_3)}-\frac{2(d(u_1)-3)}{(d(u_1)+2)(d(u_1)+3)}$$
$$\geq h_1(n-1)+\frac{2}{n+2}+\frac{4}{n+1}-\frac{2}{(2n-3)(n-2)}-\frac{1}{n-2}-\frac{2(n-4)}{(n+1)(n+2)}>h_1(n).$$

Subcase 1.3. If edge $u_1u_2\in E(G)$, edges $u_1u_3,u_2u_3\notin E(G)$, let $G_3=G-\{u\}+\{u_1u_3,u_2u_3\}$, then $H(G_3)\geq h_1(n-1)$ by the induction hypothesis. Note that

$$f_3(x,y,z)=\frac{2}{3+x}+\frac{2}{3+y}+\frac{2}{3+z}-\frac{2}{x+z+1}-\frac{2}{y+z+1}+\frac{2(z-1)}{(z+n-1)(z+n-2)},$$

where $4\leq x,y\leq n-2, 4\leq z\leq n-3$. $\frac{\partial f_3}{\partial x}=\frac{-2}{(x+3)^2}+\frac{2}{(x+z+1)^2}<0, \frac{\partial f_3}{\partial y}=\frac{-2}{(y+3)^2}+\frac{2}{(y+z+1)^2}<0,$

$$\begin{aligned}\frac{d(\frac{-2z-4n+6}{(z+n-2))(z+n-1)})}{dz} &= \frac{(2z+4n-6)(2z+2n-3)-2(z+n-2)(z+n-1)}{(z+n-2)^2(z+n-1)^2}\\ &> \frac{(2z+4n-6)(2z+2n-4)-2(z+n-2)(z+n-1)}{(z+n-2)^2(z+n-1)^2}\\ &> \frac{2(z+n-2)(z+3n-5)}{(z+n-2)^2(z+n-1)^2}>0.\end{aligned} \tag{3}$$

Then we have $f_3(x,y,z)>\frac{4}{n+1}+\frac{2}{n}-\frac{4n+2}{(n+2)(n+3)}$.

$$H(G)=H(G_3)+\frac{2}{3+d(u_1)}+\frac{2}{3+d(u_2)}+\frac{2}{3+d(u_3)}-\frac{2}{d(u_1)+d(u_3)+1}$$
$$-\frac{2}{d(u_2)+d(u_3)+1}+\sum_{v\in N(u_3)\setminus\{u\}}(\frac{2}{d(u_3)+d(v)}-\frac{2}{d(u_3)+1+d(v)})$$
$$\geq H(G_3)+\frac{2}{3+d(u_1)}+\frac{2}{3+d(u_2)}+\frac{2}{3+d(u_3)}-\frac{2}{d(u_1)+d(u_3)+1}$$
$$-\frac{2}{d(u_2)+d(u_3)+1}+\frac{2(d(u_3)-1)}{(d(u_3)+n-2)(d(u_3)+n-1)}$$
$$\geq h_1(n-1)+\frac{4}{n+1}+\frac{2}{3+d(u_3)}+\frac{-2d(u_3)-4n+6}{(d(u_3)+n-2)(d(u_3)+n-1)}$$
$$(with\ equality\ if\ and\ only\ if\ d(u_1)=d(u_2)=n-2)$$
$$\geq h_1(n-1)+\frac{4}{n+1}+\frac{2}{3+d(u_3)}+\frac{-4n-2}{(n+2)(n+3)}\quad (by\ (3))$$
$$>h_1(n-1)+\frac{4}{n+1}+\frac{2}{n}+\frac{-4n-2}{(n+2)(n+3)}>h_1(n).$$

Subcase 1.4. If edges $u_1u_2,u_1u_3,u_2u_3\notin E(G)$, let $G_4=G-\{u\}+\{u_1u_2,u_2u_3\}$, then $H(G_4)\geq h_1(n-1)$ by the induction hypothesis. Note that

$$f_4(x,y,z)=\frac{2}{3+x}+\frac{2}{3+y}+\frac{2}{3+z}-\frac{2}{x+y+1}-\frac{2}{y+z+1}+\frac{2(y-1)}{(y+n-2)(y+n-1)},$$

where $4 \le x, y, z \le n-3$.

$$\frac{\partial f_4}{\partial x} = \frac{-2}{(x+3)^2} + \frac{2}{(x+y+1)^2} < 0,$$

$$\frac{\partial f_4}{\partial z} = \frac{-2}{(z+3)^2} + \frac{2}{(y+z+1)^2} < 0,$$

$$\frac{d(\frac{-2y-4n+2}{(y+n-2)(y+n-1)})}{dy} = \frac{2-10n+6n^2-4y+8ny+2y^2}{(y+n-2)^2(y+n-1)^2} > 0. \quad (4)$$

Then we get $f_4(x,y,z) > \frac{6}{n} + \frac{-4n+2}{(n+2)(n+3)}$.

$$\begin{aligned}
H(G) &= H(G_4) + \frac{2}{3+d(u_1)} + \frac{2}{3+d(u_2)} + \frac{2}{3+d(u_3)} - \frac{2}{d(u_1)+d(u_2)+1} \\
&\quad - \frac{2}{d(u_2)+d(u_3)+1} + \sum_{v\in N(u_2)\backslash\{u\}} (\frac{2}{d(u_2)+d(v)} - \frac{2}{d(u_2)+1+d(v)}) \\
&\ge H(G_4) + \frac{2}{3+d(u_1)} + \frac{2}{3+d(u_2)} + \frac{2}{3+d(u_3)} - \frac{2}{d(u_1)+d(u_2)+1} \\
&\quad - \frac{2}{d(u_2)+d(u_3)+1} + \frac{2(d(u_2)-1)}{(d(u_2)+n-2)(d(u_2)+n-1)} \\
&\ge h_1(n-1) + \frac{4}{n} + \frac{2}{3+d(u_2)} - \frac{4}{d(u_2)+n-2} + \frac{2(d(u_2)-1)}{(d(u_2)+n-2)(d(u_2)+n-1)} \\
&\quad (with\ equality\ if\ and\ only\ if\ d(u_1) = d(u_3) = n-3) \\
&= h_1(n-1) + \frac{4}{n} + \frac{2}{3+d(u_2)} + \frac{-2d(u_2)-4n+2}{(d(u_2)+n-2)(d(u_2)+n-1)} \\
&\ge h_1(n-1) + \frac{4}{n} + \frac{2}{3+d(u_2)} + \frac{-4n-6}{(n+2)(n+3)} \quad (by\ (4)) \\
&> h_1(n-1) + \frac{6}{n} + \frac{-4n-6}{(n+2)(n+3)} > h_1(n).
\end{aligned}$$

Case 2. There is a pair of adjacent vertices of degree three without common neighbors.

Let u and v be a pair of adjacent vertices with degree three in G which has no common neighbor. Let u_1, u_2 be the neighbors of u different from v, and let v_1, v_2 be the neighbors of v different from u. We know that vu_1, vu_2 are not the edges in G and $3 \le d(u_1), d(u_2), d(v_1), d(v_2) \le n-2$. Let $G_5 = G - \{u\} + \{vu_1, vu_2\}$, then $H(G_5) \ge h_1(n-1)$ by the induction hypothesis.

$$\begin{aligned}
H(G) &= H(G_5) + \frac{2}{3+3} + \frac{2}{3+d(u_1)} + \frac{2}{3+d(u_2)} + \frac{2}{3+d(v_1)} + \frac{2}{3+d(v_2)} - \frac{2}{4+d(u_1)} \\
&\quad - \frac{2}{4+d(u_2)} - \frac{2}{4+d(v_1)} - \frac{2}{4+d(v_2)} \\
&= H(G_5) + \frac{1}{3} + \frac{2}{(3+d(u_1))(4+d(u_1))} + \frac{2}{(3+d(u_2))(4+d(u_2))} \\
&\quad + \frac{2}{(3+d(v_1))(4+d(v_1))} + \frac{2}{(3+d(v_2))(4+d(v_2))} \\
&\ge h_1(n-1) + \frac{1}{3} + \frac{8}{(n+1)(n+2)} > h_1(n).
\end{aligned}$$

Case 3. There is a pair of adjacent vertices of degree three which has one common neighbor.

Let u and v be a pair of adjacent vertices with degree three in G which has one common neighbor w. Let u_1 be the neighbor of u in G different from v, w, and let v_1 be the neighbor of v different from u, w.

Subcase 3.1. $d(w) = 3$.

Subcase 3.1.1. Edge $u_1w \in E(G)$.

Let $G_6 = G - \{u\} + \{vu_1, v_1w\}$, then $H(G_6) \geq h_1(n-1)$ by the induction hypothesis and $3 \leq d(u_1) \leq n-2, 3 \leq d(v_1) \leq n-3$. Suppose that $g_1(x) = \frac{2}{3+x} - \frac{4}{4+x} + \frac{2(x-1)}{(x+n-4)(x+n-3)}$, where $3 \leq x \leq n-3$, $\frac{dg_1}{dx} = \frac{2x^2+8x+4}{(3+x)^2(4+x)^2} + \frac{2(5-5n+n^2+2x-x^2)}{(x+n-4)^2(x+n-3)^2} > 0$. Then we have $g_1(x) \geq g_1(3) = -\frac{5}{21} + \frac{4}{(n-1)n}$.

$$\begin{aligned} H(G) &= H(G_6) + \frac{2\cdot 2}{3+3} + \frac{2}{3+d(u_1)} - \frac{2}{3+d(u_1)} - \frac{2}{3+d(v_1)+1} + \frac{2}{3+d(v_1)} - \frac{2}{3+d(v_1)+1} \\ &\quad + \sum_{z\in N(v_1)\backslash\{v\}} \left(\frac{2}{d(v_1)+d(z)} - \frac{2}{d(v_1)+1+d(z)}\right) \\ &\geq H(G_6) + \frac{2}{3} + \frac{2}{3+d(v_1)} - \frac{4}{4+d(v_1)} + \frac{2(d(v_1)-1)}{(d(v_1)+n-4)(d(v_1)+n-3)} \\ &\geq h_1(n-1) + \frac{3}{7} + \frac{4}{(n-1)n} > h_1(n). \end{aligned}$$

Subcase 3.1.2. Edge $u_1w \notin E(G)$.

Let $G_7 = G - \{u\} + \{vu_1, u_1w\}$, then $H(G_7) \geq h_1(n-1)$ by the induction hypothesis and $3 \leq d(u_1) \leq n-3$. Similarly, suppose that $g_2(x) = \frac{2}{3+x} - \frac{4}{4+x} + \frac{2(x-1)}{(x+n-3)(x+n-2)}$,

$$\frac{dg_2}{dx} = \frac{2x^2+8x+4}{(3+x)^2(4+x)^2} + \frac{2(1-3n+n^2+2x-x^2)}{(x+n-3)^2(x+n-2)^2} > 0.$$

We have $g_2(x) \geq g_2(3) = -\frac{5}{21} + \frac{4}{n(n+1)}$.

$$\begin{aligned} H(G) &= H(G_7) + \frac{2\cdot 2}{3+3} + \frac{2}{3+d(u_1)} - \frac{2\cdot 2}{3+d(u_1)+1} + \sum_{z\in N(u_1)\backslash\{u\}} \left(\frac{2}{d(u_1)+d(z)} - \frac{2}{d(u_1)+1+d(z)}\right) \\ &\geq H(G_7) + \frac{2}{3} + \frac{2}{3+d(u_1)} - \frac{4}{4+d(u_1)} + \frac{2(d(u_1)-1)}{(d(u_1)+n-3)(d(u_1)+n-2)} \\ &\geq h_1(n-1) + \frac{3}{7} + \frac{4}{n(n+1)} > h_1(n). \end{aligned}$$

Subcase 3.2. $d(w) \geq 4$.

Subcase 3.2.1. Edge $u_1w \in E(G)$.

Let $G_8 = G - \{u\} + \{vu_1\}$, then $H(G_8) \geq h_1(n-1)$ by the induction hypothesis and $3 \leq d(u_1) \leq n-2$.

$$\begin{aligned} H(G) &= H(G_8) + \frac{2}{3+3} + \frac{2}{3+d(u_1)} + \frac{2}{3+d(w)} - \frac{2}{3+d(u_1)} + \frac{2}{3+d(w)} - \frac{2}{3+d(w)-1} \\ &\quad + \frac{2}{d(u_1)+d(w)} - \frac{2}{d(u_1)+d(w)-1} + \sum_{z\in N(w)\backslash\{u,v,u_1\}} \left(\frac{2}{d(w)+d(z)} - \frac{2}{d(w)-1+d(z)}\right) \\ &\geq H(G_8) + \frac{1}{3} + \frac{2+2d(w)}{(2+d(w))(3+d(w))} - \frac{2}{(d(u_1)+d(w)-1)(d(u_1)+d(w))} - \frac{2(d(w)-3)}{(d(w)+2)(d(w)+3)} \\ &\geq h_1(n-1) + \frac{1}{3} + \frac{6}{(n+1)(n+2)} \\ &\quad (\textit{with equality if and only if } d(w) = n-1, d(u_1) = 3) \\ &> h_1(n). \end{aligned}$$

Subcase 3.2.2. Edge $u_1w \notin E(G)$.

Let $G_9 = G - \{u\} + \{vu_1\}$, then $H(G_9) \geq h_1(n-1)$ by the induction hypothesis.

$$\begin{aligned}
H(G) &= H(G_9) + \frac{2}{3+3} + \frac{2}{3+d(u_1)} + \frac{2}{3+d(w)} - \frac{2}{3+d(u_1)} + \frac{2}{3+d(w)} - \frac{2}{3+d(w)-1} \\
&\quad + \sum_{z\in N(w)\setminus\{u,v\}} \left(\frac{2}{d(w)+d(z)} - \frac{2}{d(w)-1+d(z)}\right) \\
&\geq H(G_9) + \frac{1}{3} + \frac{2+2d(w)}{(2+d(w))(3+d(w))} - \frac{2(d(w)-2)}{(d(w)+2)(d(w)+3)} \\
&\geq h_1(n-1) + \frac{1}{3} + \frac{6}{(2+d(w))(3+d(w))} \\
&\geq h_1(n-1) + \frac{1}{3} + \frac{6}{n(n+1)} \\
&\quad (\textit{with equality if and only if } d(w) = n-2) \\
&> h_1(n).
\end{aligned}$$

Case 4. There is a pair of adjacent vertices of degree three which has two common neighbors.

Let u_1 and u_2 be a pair of adjacent vertices with degree three in G which has two common neighbors u_3, u_4.

Subcase 4.1. $d(u_3) = 3$.

Subcase 4.1.1. Edge $u_3u_4 \in E(G)$.

(1) If $d(u_4) = 3$, let $G_{10} = G - \{u_1, u_2, u_3, u_4\}$, then $H(G_{10}) \geq h_1(n-4)$ by the induction hypothesis.

$$H(G) = H(G_{10}) + \frac{6\cdot 2}{3+3} \geq h_1(n-4) + 2 > h_1(n).$$

(2) If $d(u_4) \geq 4$, let u_5 be the neighbor of u_4 different from $\{u_1, u_2, u_3\}$. Let $G_{11} = G - \{u_1\} + \{u_2u_5, u_3u_5\}$, then $H(G_{11}) \geq h_1(n-1)$ by the induction hypothesis. Note that $\varphi_1(x,y) = \frac{8}{(2+x)(3+x)} + \frac{2}{(x+y)(x+y+1)} - \frac{4}{5+y} + \frac{4(y-1)}{(y+n-4)(y+n-2)}$, where $4 \leq x \leq n-1, 3 \leq y \leq n-4$. We get

$$\frac{\partial\varphi_1}{\partial x} = -\frac{8}{(x+2)^2(x+3)^2} - \frac{2}{(x+y)^2(x+y+1)^2} < 0,$$

$$\begin{aligned}
\frac{\partial\varphi_1}{\partial y} &= \frac{4}{(5+y)^2} - \frac{2(2x+2y+1)}{(x+y)^2(x+y+1)^2} + \frac{4}{(y+n-4)(y+n-2)} + \frac{-4(y-1)(2y+2n-6)}{(y+n-4)^2(y+n-2)^2} \\
&> \frac{4}{(5+y)^2} - \frac{2(2x+2y+2)}{(x+y)^2(x+y+1)^2} + \frac{4}{(y+n-4)(y+n-2)} + \frac{-4(y-1)(2y+2n-4)}{(y+n-4)^2(y+n-2)^2} \\
&= \frac{4}{(5+y)^2} - \frac{4}{(x+y)^2(x+y+1)} + \frac{4n-4y-8}{(y+n-4)^2(y+n-2)} \\
&> \frac{4}{(5+y)^2} - \frac{4}{(x+y)^2(x+y+1)} > 0.
\end{aligned}$$

Then we get $\varphi_1(x,y) \geq \varphi_1(n-1,3) = \frac{8}{(n+1)(n+2)} + \frac{2}{(n+2)(n+3)} - \frac{1}{2} + \frac{8}{(n-1)(n+1)}$.

$$\begin{aligned}
H(G) &= H(G_{11}) + \frac{2}{3+3} + \frac{2}{3+3} + \frac{2}{3+d(u_4)} + \frac{2}{3+d(u_4)} - \frac{2}{3+d(u_4)-1} + \frac{2}{3+d(u_4)} \\
&- \frac{2}{3+d(u_4)-1} + \frac{2}{d(u_4)+d(u_5)} - \frac{2}{d(u_4)-1+d(u_5)+2} - \frac{2}{3+d(u_5)+2} \\
&- \frac{2}{3+d(u_5)+2} + \sum_{z\in N(u_4)\backslash\{u_1,u_2,u_3,u_5\}} (\frac{2}{d(u_4)+d(z)} - \frac{2}{d(u_4)-1+d(z)}) \\
&+ \sum_{z\in N(u_5)\backslash\{u_4\}} (\frac{2}{d(u_5)+d(z)} - \frac{2}{d(u_5)+2+d(z)}) \\
&\geq H(G_{11}) + \frac{2}{3} + \frac{2d(u_4)}{(2+d(u_4))(3+d(u_4))} + \frac{2}{(d(u_4)+d(u_5))(d(u_4)+d(u_5)+1)} \\
&- \frac{4}{5+d(u_5)} + \frac{-2(d(u_4)-4)}{(2+d(u_4))(3+d(u_4))} + \frac{4(d(u_5)-1)}{(d(u_5)+n-4)(d(u_5)+n-2)} \\
&= H(G_{11}) + \frac{2}{3} + \frac{8}{(2+d(u_4))(3+d(u_4))} + \frac{2}{(d(u_4)+d(u_5))(d(u_4)+d(u_5)+1)} \\
&- \frac{4}{5+d(u_5)} + \frac{4(d(u_5)-1)}{(d(u_5)+n-4)(d(u_5)+n-2)} \\
&\geq h_1(n-1) + \frac{2}{3} + \frac{8}{(n+1)(n+2)} + \frac{2}{(n+2)(n+3)} - \frac{1}{2} + \frac{8}{(n-1)(n+1)} \\
&\quad (\textit{with equality if and only if } d(u_4) = n-1, d(u_5) = 3) \\
&> h_1(n).
\end{aligned}$$

Subcase 4.1.2. If edge $u_3u_4 \notin E(G)$, let u_5 be the neighbor of u_3 different from u_1, u_2. Let $G_{12} = G - \{u_1\} + \{u_2u_5, u_3u_4\}$, then $H(G_{12}) \geq h_1(n-1)$ by the induction hypothesis. Note that $\varphi_2(x) = \frac{2}{x+3} - \frac{4}{x+4} + \frac{2(x-1)}{(x+n-4)(x+n-3)}$, where $3 \leq x \leq n-3$. $\frac{d\varphi_2}{dx} = \frac{2(2+4x+x^2)}{(x+3)^2(x+4)^2} + \frac{2(5-5n+n^2+2x-x^2)}{(x+n-4)^2(x+n-3)^2} > 0$. Then we have $\varphi_2(x) \geq \varphi_2(3) = \frac{2}{3+3} - \frac{4}{7} + \frac{4}{(n-1)n}$.

$$\begin{aligned}
H(G) &= H(G_{12}) + \frac{2}{3+3} + \frac{2}{3+3} + \frac{2}{3+d(u_4)} - \frac{2}{3+d(u_5)+1} - \frac{2}{3+d(u_4)} + \frac{2}{3+d(u_5)} \\
&- \frac{2}{3+d(u_5)+1} + \sum_{z\in N(u_5)\backslash\{u_3\}} (\frac{2}{d(u_5)+d(z)} - \frac{2}{d(u_5)+1+d(z)}) \\
&\geq H(G_{12}) + \frac{2}{3} + \frac{2}{3+d(u_5)} - \frac{4}{4+d(u_5)} + \frac{2(d(u_5)-1)}{(d(u_5)+n-4)(d(u_5)+n-3)} \\
&\geq h_1(n-1) + \frac{2}{3} + \frac{2}{3+3} - \frac{4}{7} + \frac{4}{(n-1)n} \\
&\quad (\textit{with equality if and only if } d(u_5) = 3) \\
&> h_1(n).
\end{aligned}$$

Subcase 4.2. $d(u_3) \geq 4$.

Subcase 4.2.1. If edge $u_3u_4 \in E(G)$, let u_5 be a neighbor of u_3 different from u_1, u_2, u_4.

(1) If $u_4u_5 \in E(G)$, let $G_{13} = G - \{u_1\} + \{u_2u_5\}$, then $H(G_{13}) \geq h_1(n-1)$ by the induction hypothesis. Note that

$$\varphi_3(x,y,z) = \frac{10}{(x+2)(x+3)} + \frac{10}{(y+2)(y+3)} - \frac{4}{(x+y-2)(x+y)} - \frac{2}{4+z} + \frac{2(z-2)}{(z+n-3)(z+n-2)},$$

where $4 \le x, y \le n-1, 3 \le z \le n-3$.

$$\begin{aligned}\frac{\partial \varphi_3}{\partial x} &= \frac{-10(2x+5)}{(x+2)^2(x+3)^2} + \frac{4(2x+2y-2)}{(x+y-2)^2(x+y)^2} < \frac{-10(2x+5)}{(x+2)^2(x+3)^2} + \frac{4(2x+2y)}{(x+y-2)^2(x+y)^2} \\ &= \frac{-10(2x+5)}{(x+2)^2(x+3)^2} + \frac{8}{(x+y-2)^2(x+y)} < \frac{-10(2x+5)}{(x+2)^2(x+3)^2} + \frac{8}{(x+2)^2(x+4)} < 0.\end{aligned}$$

By the symmetry on x,y of $\varphi_3(x,y,z)$, we get $\frac{\partial \varphi_3}{\partial y} < 0$. $\frac{\partial \varphi_3}{\partial z} = \frac{2}{(4+z)^2} + \frac{2(n^2-n-4+4z-z^2)}{(z+n-3)^2(z+n-2)^2} > 0$. Then we have $\varphi_3(x,y,z) \ge \varphi_3(n-1,n-1,3) = \frac{20}{(n+1)(n+2)} - \frac{4}{(2n-4)(2n-2)} - \frac{2}{7} + \frac{2}{n(n+1)}$.

$$\begin{aligned}H(G) &= H(G_{13}) + \frac{2}{3+3} + \frac{2}{3+d(u_3)} + \frac{2}{3+d(u_4)} - \frac{2}{3+d(u_5)+1} + \frac{2}{3+d(u_3)} \\ &\quad + \frac{2}{3+d(u_4)} + \frac{2}{d(u_3)+d(u_4)} - \frac{2}{3+d(u_3)-1} - \frac{2}{3+d(u_4)-1} - \frac{2}{d(u_3)-1+d(u_4)-1} \\ &\quad + \sum_{z\in N(u_3)\setminus\{u_1,u_2,u_4,u_5\}} \left(\frac{2}{d(u_3)+d(z)} - \frac{2}{d(u_3)-1+d(z)}\right) \\ &\quad + \sum_{z\in N(u_4)\setminus\{u_1,u_2,u_3,u_5\}} \left(\frac{2}{d(u_4)+d(z)} - \frac{2}{d(u_4)-1+d(z)}\right) \\ &\quad + \sum_{z\in N(u_5)\setminus\{u_3,u_4\}} \left(\frac{2}{d(u_5)+d(z)} - \frac{2}{d(u_5)+1+d(z)}\right) \\ &\ge H(G_{13}) + \frac{1}{3} + \frac{2+2d(u_3)}{(2+d(u_3))(3+d(u_3))} + \frac{2+2d(u_4)}{(2+d(u_4))(3+d(u_4))} + \frac{2}{d(u_3)+d(u_4)} \\ &\quad - \frac{2}{d(u_3)+d(u_4)-2} - \frac{2}{4+d(u_5)} + \frac{-2(d(u_3)-4)}{(d(u_3)+2)(d(u_3)+3)} \\ &\quad + \frac{-2(d(u_4)-4)}{(d(u_4)+2)(d(u_4)+3)} + \frac{2(d(u_5)-2)}{(d(u_5)+n-3)(d(u_5)+n-2)} \\ &= H(G_{13}) + \frac{1}{3} + \frac{10}{(d(u_3)+2)(d(u_3)+3)} + \frac{10}{(d(u_4)+2)(d(u_4)+3)} \\ &\quad - \frac{4}{(d(u_3)+d(u_4)-2)(d(u_3)+d(u_4))} - \frac{2}{4+d(u_5)} + \frac{2(d(u_5)-2)}{(d(u_5)+n-3)(d(u_5)+n-2)} \\ &\ge h_1(n-1) + \frac{1}{3} + \frac{20}{(n+1)(n+2)} - \frac{4}{(2n-4)(2n-2)} - \frac{2}{7} + \frac{2}{n(n+1)} \\ &\quad (with\ equality\ if\ and\ only\ if\ d(u_3)=n-1, d(u_4)=n-1, d(u_5)=3) \\ &> h_1(n).\end{aligned}$$

(2)If $u_4u_5 \notin E(G)$, let $G_{14} = G - \{u_1\} + \{u_2u_5\}$, then $H(G_{14}) \ge h_1(n-1)$ by the induction hypothesis. Note that

$$\varphi_4(x,y,z) = \frac{10}{(x+2)(x+3)} + \frac{8}{(y+2)(y+3)} - \frac{4}{(x+y-2)(x+y)} - \frac{2}{4+z} + \frac{2(z-1)}{(z+n-3)(z+n-2)},$$

where $4 \le x \le n-1, 4 \le y \le n-2, 3 \le z \le n-4$.

$$\frac{\partial \varphi_4}{\partial x} = -\frac{10}{(x+2)^2(x+3)^2} + \frac{8(x+y-1)}{(x+y-2)^2(x+y)^2} < 0,$$

$$\frac{\partial \varphi_4}{\partial y} = -\frac{8}{(y+2)^2(y+3)^2} + \frac{8(x+y-1)}{(x+y-2)^2(x+y)^2} < 0,$$

$$\frac{\partial \varphi_4}{\partial z} = \frac{2}{(4+z)^2} + \frac{2(1-3n+n^2+2z-z^2)}{(z+n-3)^2(z+n-2)^2} > 0.$$

Then we get that $\varphi_4(x,y,z)\varphi_4(n-1,n-2,3) = \frac{10}{(n+1)(n+2)} + \frac{8}{n(n+1)} - \frac{4}{(2n-5)(2n-3)} - \frac{2}{7} + \frac{4}{n(n+1)}$.

$$\begin{aligned}
H(G) &= H(G_{14}) + \frac{2}{3+3} + \frac{2}{3+d(u_3)} + \frac{2}{3+d(u_4)} - \frac{2}{3+d(u_5)+1} + \frac{2}{3+d(u_3)} + \frac{2}{3+d(u_4)} \\
&+ \frac{2}{d(u_3)+d(u_4)} - \frac{2}{3+d(u_3)-1} - \frac{2}{3+d(u_4)-1} - \frac{2}{d(u_3)-1+d(u_4)-1} \\
&+ \sum_{z\in N(u_3)\setminus\{u_1,u_2,u_4,u_5\}} \left(\frac{2}{d(u_3)+d(z)} - \frac{2}{d(u_3)-1+d(z)}\right) \\
&+ \sum_{z\in N(u_4)\setminus\{u_1,u_2,u_3\}} \left(\frac{2}{d(u_4)+d(z)} - \frac{2}{d(u_4)-1+d(z)}\right) \\
&+ \sum_{z\in N(u_5)\setminus\{u_3\}} \left(\frac{2}{d(u_5)+d(z)} - \frac{2}{d(u_5)+1+d(z)}\right) \\
&\geq H(G_{14}) + \frac{1}{3} + \frac{2+2d(u_3)}{(2+d(u_3))(3+d(u_3))} + \frac{2+2d(u_4)}{(2+d(u_4))(3+d(u_3))} \\
&- \frac{4}{(d(u_3)+d(u_4)-2)(d(u_3)+d(u_4))} - \frac{2}{4+d(u_5)} + \frac{-2(d(u_3)-4)}{(d(u_3)+2)(d(u_3)+3)} \\
&+ \frac{-2(d(u_4)-3)}{(d(u_4)+2)(d(u_4)+3)} + \frac{2(d(u_5)-1)}{(d(u_5)+n-3)(d(u_5)+n-2)} \\
&= H(G_{14}) + \frac{1}{3} + \frac{10}{(d(u_3)+2)(d(u_3)+3)} + \frac{8}{(d(u_4)+2)(d(u_4)+3)} \\
&- \frac{4}{(d(u_3)+d(u_4)-2)(d(u_3)+d(u_4))} - \frac{2}{4+d(u_5)} + \frac{2(d(u_5)-1)}{(d(u_5)+n-3)(d(u_5)+n-2)} \\
&\geq H(G_{13}) + \frac{1}{3} + \frac{10}{(n+1)(n+2)} + \frac{8}{n(n+1)} - \frac{4}{(2n-5)(2n-3)} - \frac{2}{7} + \frac{4}{n(n+1)} \\
&\quad (with\ equality\ if\ and\ only\ if\ d(u_3)=n-1, d(u_4)=n-2, d(u_5)=3) \\
&\geq h_1(n-1) + \frac{1}{21} + \frac{10}{(n+1)(n+2)} - \frac{4}{(2n-5)(2n-3)} + \frac{12}{n(n+1)} > h_1(n).
\end{aligned}$$

Subcase 4.2.2. If edge $u_3u_4 \notin E(G)$, let u_5 be the neighbor of u_3 different from $\{u_1,u_2\}$. Let $G_{15} = G - \{u_1\} + \{u_2u_5, u_3u_4\}$, then $H(G_{15}) \geq h_1(n-1)$ by the induction hypothesis. Note that

$$\varphi_5(x,y,z) = \frac{2}{x+3} + \frac{2}{y+3} - \frac{2}{x+y} + \frac{2}{x+z} - \frac{2}{x+z+1} - \frac{2}{4+z} + \frac{2(z-1)}{(z+n-3)(z+n-2)},$$

where $4 \leq x, y \leq n-2, 3 \leq z \leq n-3$. We get

$$\frac{\partial \varphi_5}{\partial x} = -\frac{2}{(x+3)^2} + \frac{2}{(x+y)^2} - \frac{2}{(x+z)^2} + \frac{2}{(x+z+1)^2} < 0,$$

$$\frac{\partial \varphi_5}{\partial y} = -\frac{2}{(y+3)^2} + \frac{2}{(x+y)^2} < 0,$$

$$\frac{\partial \varphi_5}{\partial z} = \frac{2}{(z+4)^2} + \frac{2(1-3n+n^2+2z-z^2)}{(z+n-3)^2(z+n-2)^2} - \frac{2}{(x+z)^2} + \frac{2}{(x+z+1)^2} > 0.$$

Then we have $\varphi_5(x,y,z) \geq \varphi_5(n-2,n-2,3) = \frac{2}{n+1} + \frac{2}{n+1} - \frac{2}{2n-4} + \frac{2}{n+1} - \frac{2}{n+2} - \frac{2}{7} + \frac{4}{n(n+1)}$.

$$\begin{aligned}
H(G) &= H(G_{15}) + \frac{2}{3+3} + \frac{2}{3+d(u_3)} + \frac{2}{3+d(u_4)} - \frac{2}{d(u_3)+d(u_4)} + \frac{2}{d(u_3)+d(u_5)} \\
&\quad - \frac{2}{d(u_3)+d(u_5)+1} - \frac{2}{3+d(u_5)+1} + \sum_{z\in N(u_5)\backslash\{u_3\}} \left(\frac{2}{d(u_5)+d(z)} - \frac{2}{d(u_5)+1+d(z)}\right) \\
&\geq H(G_{15}) + \frac{1}{3} + \frac{2}{3+d(u_3)} + \frac{2}{3+d(u_4)} - \frac{2}{d(u_3)+d(u_4)} + \frac{2}{d(u_3)+d(u_5)} \\
&\quad - \frac{2}{d(u_3)+d(u_5)+1} - \frac{2}{4+d(u_5)} + \frac{2(d(u_5)-1)}{(d(u_5)+n-3)(d(u_5)+n-2)} \\
&\geq H(G_{15}) + \frac{1}{3} + \frac{2}{n+1} + \frac{2}{n+1} - \frac{2}{2n-4} + \frac{2}{n+1} - \frac{2}{n+2} - \frac{2}{7} + \frac{4}{n(n+1)} \\
&\quad (\textit{with equality if and only if } d(u_3) = n-2, d(u_4) = n-2, d(u_5) = 3) \\
&\geq h_1(n-1) + \frac{1}{21} + \frac{6}{n+1} - \frac{1}{n-2} - \frac{2}{n+2} + \frac{4}{n(n+1)} > h_1(n).
\end{aligned}$$

The proof of our theorem is completed.

We have the following conjecture.

Conjecture 2.4. *Let G be a graph with $n \geq 4$ vertices and $\delta(G) \geq k$, where $1 \leq k \leq \lfloor \frac{n}{2} \rfloor + 1$. Then $H(G) \geq H(K^*_{k,n-k})$ with equality if and only if $G = K^*_{k,n-k}$.*

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