

THE HARMONIC INDEX OF UNICYCLIC GRAPHS WITH GIVEN MATCHING NUMBER

JIAN-BO LV¹, JIANXI LI¹, AND WAI CHEE SHIU²

ABSTRACT. The harmonic index of a graph G is defined as the sum of weights $\frac{2}{d(u)+d(v)}$ of all edges uv of G , where $d(u)$ and $d(v)$ are the degrees of the vertices u and v in G , respectively. In this paper, we determine the graph with minimum harmonic index among all unicyclic graphs with a perfect matching. Moreover, the graph with minimum harmonic index among all unicyclic graphs with a given matching number is also determined.

1. INTRODUCTION

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Its order is $|V(G)|$, denoted by n . For $v \in V(G)$, let $d_G(v)$ (or $d(v)$) and $N_G(v)$ (or $N(v)$) be the degree and the neighborhood of v , respectively.

The Randić index is one of the most successful molecular descriptors in structure-property and structure-activity relationships studies. The Randić index of a graph G is defined in [13] as the sum of the weights $(d(u)d(v))^{-\frac{1}{2}}$ over all edges uv of G . The mathematical properties of this graph invariant have been studied extensively (see recent book [7] and survey [9]). Motivated by the success of Randić index, various generalizations and modifications were introduced, such as the sum-connectivity index [15, 17] and the general sum-connectivity index [2, 3].

Another variant of the Randić index, named the harmonic index $H(G)$, which is defined as

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

where the summation goes over all edges uv of G . This index was first appeared in [5]. Estimating bounds for $H(G)$ is of great interest, and many results have been obtained.

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For example, Favaron *et al.* [6] considered the relationship between the harmonic index and the eigenvalues of graphs; Zhong [18, 19, 20] determined the minimum and maximum values of the harmonic index for simple connected graphs, trees, unicyclic graphs and bicyclic graphs, and characterized the corresponding extremal graphs, respectively. Li and Shiu [10] studied how the harmonic index behaves when the graph is under perturbations and provided a simpler method for determining the unicyclic graphs with maximum and minimum harmonic index among all unicyclic graphs, respectively. Moreover, lower bounds for harmonic index are also obtained in [10] and [14], respectively. Recently, Deng *et al.* [4] studied the relationship between the harmonic index and the chromatic number of a graph G , and obtained the lower bound for $H(G)$ in terms of its chromatic number. Lv and Li [11] studied the relationship between the harmonic index and the matching number for trees, and determined the trees with minimum harmonic index among trees with a perfect matching and among trees with a given matching number, respectively.

In this paper, we further consider the relationship between the harmonic index and the matching number for unicyclic graphs. The graph with minimum harmonic index among all unicyclic graphs with a perfect matching is determined. Moreover, the graph with minimum harmonic index among all unicyclic graphs with a given matching number is also determined.

2. PRELIMINARIES

We first introduce some terminologies and notations of graphs. For a connected graph G , a pendant vertex is a vertex of degree 1 in G . Let PV be the set of all pendant vertices of G . Let $d_G(x, y)$ be the length of a shortest (x, y) -path in G . We 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 $M \subseteq E$ is called a matching in G if its elements are edges and any two of them are not adjacent in G . A matching M saturates a vertex v , and v is said to be M -saturated, if some edge of M is incident with v . If every vertex of G is M -saturated, then the matching M is perfect. A matching M is said to be an m -matching, if $|M| = m$ and for every matching M' in G , $|M'| \leq m$.

Denote by C_n the cycle of order n . Let n and m be positive integers with $n \geq 2m$. Let $\mathcal{U}_{n,m}$ be the set of unicyclic graphs of order n with an m -matching. For any $G \in \mathcal{U}_{n,m} \setminus \{C_n\}$, G consists of a unique cycle, denoted by C_g , and some trees attached to some vertices on the cycle. Those vertices attached to trees, for convenience, are called the roots of the trees attached to them. A root may have more than one tree attached to it. In order to prove our main results, the following lemmas are needed.

Lemma 2.1. [1] *Let $G \in \mathcal{U}_{2m,m}$ ($m \geq 3$), and 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. [12] *Let $G \in \mathcal{U}_{2m,m}$. If $PV \neq \emptyset$, then for any $u \in V(G)$, we have $|N(u) \cap PV| \leq 1$.*

Lemma 2.3. [16] *Let $G \in \mathcal{U}_{n,m}$ ($n > 2m$) and $G \not\cong C_n$. Then there is an m -matching M and a pendant vertex v such that M does not saturate v .*

Lemma 2.4. (1) *For $x \geq 2$, the function $f_1(x) = \frac{2x-2}{x+2} - \frac{2x-6}{x+1} - \frac{2}{x}$ is monotonically decreasing on x .*

(2) *For $x \geq 2$, the function $f_2(x) = \frac{2x}{x+2} - \frac{2x-2}{x+1}$ is monotonically decreasing on x .*

(3) *For $x \geq 2$, the function $f_3(x) = \frac{2x-2}{x+2} - \frac{2x-4}{x+1}$ is monotonically decreasing on x .*

(4) *For $x \geq 3$, the function $f_4(x) = \frac{2}{x+1} + \frac{2x-4}{x+2} - \frac{2x}{x+3}$ is monotonically increasing on x .*

Proof. (1) We consider the derivative of $f_1(x)$. Note that, for $x \geq 2$, we have

$$\begin{aligned} \frac{df_1(x)}{dx} &= \frac{6}{(x+2)^2} - \frac{8}{(x+1)^2} + \frac{2}{x^2} \\ &= \frac{6x^2(x+1)^2 + 2(x+2)^2(x+1)^2 - 8(x+2)^2x^2}{x^2(x+1)^2(x+2)^2} \\ &= \frac{-8x^3 + 24x + 8}{x^2(x+1)^2(x+2)^2} < 0. \end{aligned}$$

Then $f_1(x)$ is monotonically decreasing on x .

(2) The results follows from

$$\frac{df_2(x)}{dx} = \frac{4}{(x+2)^2} - \frac{4}{(x+1)^2} < 0.$$

(3) The results follows from

$$\frac{df_3(x)}{dx} = \frac{6}{(x+2)^2} - \frac{6}{(x+1)^2} < 0.$$

(4) Note that, for $x \geq 3$, we have

$$\begin{aligned} \frac{df_4(x)}{dx} &= \frac{-2}{(x+1)^2} + \frac{8}{(x+2)^2} + \frac{-6}{(x+3)^2} \\ &= \frac{8(x+1)^2(x+3)^2 - 2(x+2)^2(x+3)^2 - 6(x+1)^2(x+2)^2}{(x+1)^2(x+2)^2(x+3)^2} \\ &= \frac{8(x+1)^3 - 24(x+1) - 8}{(x+1)^2(x+2)^2(x+3)^2} > 0. \end{aligned}$$

Thus the result holds. □

Lemma 2.5. *Let x, y be positive integers with $1 \leq y \leq x - 1$. Let*

$$g(x, y) = \frac{2x - 2y}{x + 2} - \frac{2x - 4y}{x + 1} - \frac{2y - 2}{x}.$$

Then $g(x, y)$ is monotonically decreasing on x and y , respectively.

Proof. We consider some partial derivatives of $g(x, y)$. Note that

$$\begin{aligned} \frac{\partial g(x, y)}{\partial y} &= \frac{4}{x+1} - \frac{2}{x+2} - \frac{2}{x} \\ &= \frac{-4}{(x+2)(x+1)x} < 0. \end{aligned}$$

Then $g(x, y)$ is monotonically decreasing on y .

On the other hand,

$$\begin{aligned} \frac{\partial g(x, y)}{\partial x} &= \frac{2y+4}{(x+2)^2} + \frac{2y-2}{x^2} - \frac{4y+2}{(x+1)^2} \\ &= \frac{12x^2y + 24xy + 8y - 12x^3 - 30x^2 - 24x - 8}{(x+2)^2(x+1)^2x^2}. \end{aligned}$$

Note that $y \leq x - 1$. Then we have

$$\begin{aligned} \frac{\partial g(x, y)}{\partial x} &\leq \frac{12x^2(x-1) + 24x(x-1) + 8(x-1) - 12x^3 - 30x^2 - 24x - 8}{(x+2)^2(x+1)^2x^2} \\ &= \frac{-18x^2 - 40x - 16}{(x+2)^2(x+1)^2x^2} < 0. \end{aligned}$$

Thus $g(x, y)$ is monotonically decreasing on x . □

Let $U_{n,m}$ (Shown in Figure 1) be a graph of order n obtained from C_3 by attaching $n - 2m + 1$ pendent edges and $m - 2$ paths of length 2 to one vertex of C_3 . Let $H(U_{n,m}) = \Psi(n, m)$, where

$$\Psi(n, m) = \frac{2m}{n-m+3} + \frac{2(n-2m+1)}{n-m+2} + \frac{2m}{3} - \frac{5}{6}.$$

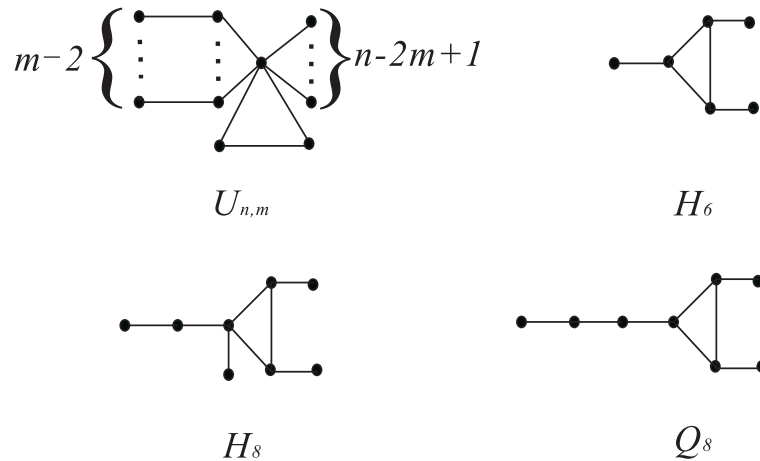


FIGURE 1. Graphs $U_{n,m}$, H_6 , H_8 and Q_8

Lemma 2.6. For $m \geq 3$, then we have

$$\Psi(2(m-1), m-1) + \frac{4}{5} > \Psi(2m, m).$$

Proof. By Lemma 2.4(4), we have

$$\begin{aligned} & \Psi(2(m-1), m-1) + \frac{4}{5} - \Psi(2m, m) \\ &= \frac{2}{m+1} + \frac{2m-4}{m+2} - \frac{2m}{m+3} + \frac{2}{15} \\ &\geq \frac{1}{2} + \frac{2}{5} - 1 + \frac{2}{15} > 0. \end{aligned}$$

Hence the result holds. □

Lemma 2.7 ([19]). Let $\mathcal{U}(n)$ be the set of unicyclic graphs of order $n \geq 4$. Then for any $G \in \mathcal{U}(n)$, $H(G) \leq \frac{n}{2}$, and the equality holds if and only if $G \cong C_n$.

3. MAIN RESULTS

Now, we give the main results of this section.

Theorem 3.1. Let $G \in \mathcal{U}_{2m,m} \setminus \{H_6, H_8\}$, where $m \geq 2$. Then $H(G) \geq \Psi(2m, m)$, and the equality holds if and only if $G \cong U_{2m,m}$.

Proof. Note that if $m = 2$, then either $G \cong C_4$ or $G \cong U_{4,2}$. Then the result follows since $H(C_4) = 2 > H(U_{4,2}) = \frac{9}{5}$.

So, we suppose that $m \geq 3$. We now prove the assertion by the induction on m . If $G \cong C_{2m}$, then Lemma 2.7 implies that $H(C_{2m}) > \Psi(2m, m)$. The result follows. In what follows, we assume that $G \not\cong C_{2m}$. From Lemmas 2.1 and 2.2, we need only consider the following two cases.

Case 1 G has a pendant vertex v such that $N(v) = \{w\}$ and $d(w) = 2$.

In this case, there is a unique vertex $u \neq v$ such that $uw \in E(G)$. Let $N(u) \cap PV = \{v_1, v_2, \dots, v_{r-1}, v_r\}$ and $N(u) \setminus PV = \{x_1, \dots, x_{t-r-1}, x_{t-r} = w\}$. Then $t \leq m+1$, $d(x_j) \geq 2$ for each $j = 1, \dots, t-r-1$ and $d(x_{t-r}) = d(w) = 2$. Let $G' = G - v - w$. Clearly, $G' \in \mathcal{U}_{2(m-1), m-1}$.

If $G' \cong H_6$, then $G \cong Q_8$, where H_6 and Q_8 are shown in Figure 1. Hence the result follows since $H(Q_8) = 3.5666 > \Psi(8, 4) = 3.3095$.

If $G' \cong H_8$ (shown in Figure 1), then $G \in \{G_i | 1 \leq i \leq 6\}$, where $G_i (1 \leq i \leq 6)$ and their harmonic indices are shown in Figure 2, respectively. Hence the result follows since $H(G_i) > \Psi(10, 5) = 4.0357$ for $1 \leq i \leq 6$.

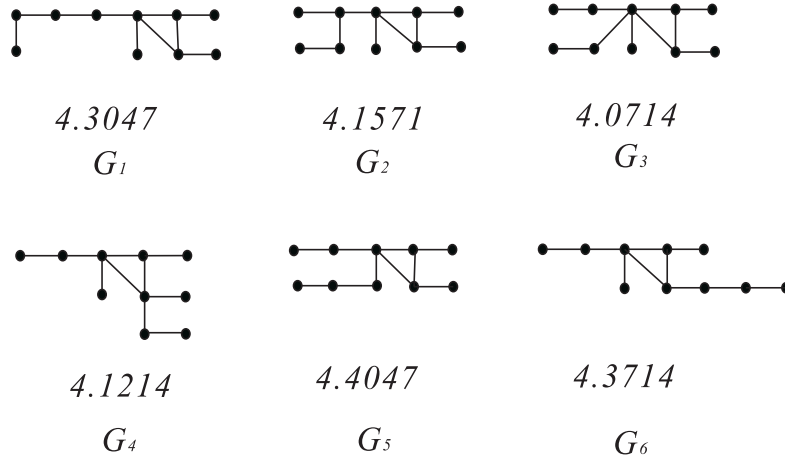


FIGURE 2. Graphs G_1, \dots, G_6 and their harmonic indices

If $G' \notin \{H_6, H_8\}$, then by the induction hypothesis, we have

$$\begin{aligned}
 H(G) &= H(G') + \frac{2}{3} + \frac{2}{t+2} + r \left(\frac{2}{t+1} - \frac{2}{t} \right) \\
 &\quad + \sum_{i=1}^{t-r-1} \left(\frac{2}{t+d(x_i)} - \frac{2}{t+d(x_i)-1} \right) \\
 &\geq H(G') + \frac{2}{3} + \frac{2}{t+2} + r \left(\frac{2}{t+1} - \frac{2}{t} \right) \\
 &\quad + (t-r-1) \left(\frac{2}{t+2} - \frac{2}{t+1} \right) \\
 &\geq \Psi(2m-2, m-1) + \frac{2}{3} + \frac{2}{t+2} + r \left(\frac{2}{t+1} - \frac{2}{t} \right) \\
 &\quad + (t-r-1) \left(\frac{2}{t+2} - \frac{2}{t+1} \right) \\
 &= \Psi(2m, m) + \frac{2}{m+1} + \frac{2m-4}{m+2} - \frac{2m}{m+3} \\
 &\quad + \frac{2}{t+2} + r \left(\frac{2}{t+1} - \frac{2}{t} \right) + (t-r-1) \left(\frac{2}{t+2} - \frac{2}{t+1} \right).
 \end{aligned}$$

Note that by Lemma 2.2, we have $r \leq 1$. Recall that $t \leq m+1$.
 If $r = 1$, then by Lemma 2.4(1), we have

$$\begin{aligned}
 H(G) &\geq \Psi(2m, m) + \frac{2}{m+1} + \frac{2m-4}{m+2} - \frac{2m}{m+3} \\
 &\quad + \frac{2t-2}{t+2} - \frac{2t-6}{t+1} - \frac{2}{t} \\
 &\geq \Psi(2m, m) + \frac{2}{m+1} + \frac{2m-4}{m+2} - \frac{2m}{m+3} \\
 &\quad + \frac{2m}{m+3} - \frac{2m-4}{m+2} - \frac{2}{m+1} \\
 &= \Psi(2m, m).
 \end{aligned}$$

Suppose that the equality holds. Then all inequalities in the above argument should be equalities.

Then we have $H(G') = \Psi(2m-2, m-1)$, $t = m+1$ and $d(x_1) = \dots = d(x_{t-r}) = 2$. Thus by the induction hypothesis, we have $G' \cong U_{2m-2, m-1}$. Hence $G \cong U_{2m, m}$.

If $r = 0$, then by Lemma 2.4(2), we have

$$\begin{aligned}
 H(G) &\geq \Psi(2m, m) + \frac{2}{m+1} + \frac{2m-4}{m+2} - \frac{2m}{m+3} \\
 &\quad + \frac{2}{t+2} + (t-1) \left(\frac{2}{t+2} - \frac{2}{t+1} \right) \\
 &= \Psi(2m, m) + \frac{2}{m+1} + \frac{2m-4}{m+2} - \frac{2m}{m+3} \\
 &\quad + \frac{2t}{t+2} - \frac{2t-2}{t+1} \\
 &\geq \Psi(2m, m) + \frac{2}{m+1} - \frac{4}{m+2} + \frac{2}{m+3} \\
 &= \Psi(2m, m) + \frac{4}{(m+1)(m+2)(m+3)} \\
 &> \Psi(2m, m).
 \end{aligned}$$

Case 2 G is a cycle C_g together with some pendant edges attached to some vertices on C_g . For convenience, we label the vertices of C_g with u_1, u_2, \dots, u_g .

Note that $G \not\cong C_n$. If $d_G(u_i) = 3$ for each $i = 1, 2, \dots, g$, then $m \geq 4$ since $G \not\cong H_6$. If $m = 4$, then the result follows since $H(G) = 4 \left(\frac{1}{3} + \frac{1}{2} \right) = 3.3333 > \Psi(8, 4) = 3.3095$. If $m \geq 5$, by the induction hypothesis and Lemma 2.6, then we have

$$\begin{aligned}
 H(G) &= (m-1) \left(\frac{1}{3} + \frac{1}{2} \right) + \frac{1}{3} + \frac{1}{2} > \Psi(2m-2, m-1) + \frac{5}{6} \\
 &> \Psi(2m-2, m-1) + \frac{4}{5} \\
 &> \Psi(2m, m).
 \end{aligned}$$

If there exists some $i \in \{1, 2, \dots, g\}$ such that $d_G(u_i) = 3$ and $d_G(u_{i+1}) = 2$, where $u_{g+1} = u_1$. Without loss of generality, we assume that $d_G(u_2) = 3$ and $d_G(u_3) = 2$. Let v_2 the pendant vertex which adjacent to u_2 . Note that every pair of vertices of degree 3 can not be adjacent to a common vertex of degree 2 since G has a perfect matching. Then each vertex of degree 2 on C_g must be adjacent to another vertex of degree 2. 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. Clearly, $G' \in \mathcal{U}_{n-2, m-1} \setminus \{H_6, H_8\}$. Hence, by the induction hypothesis and Lemma 2.6, if $d_G(u_1) = 3$, then

$$\begin{aligned} H(G) &= H(G') + \frac{1}{3} + \frac{1}{2} + \frac{2}{5} - \frac{2}{5} \geq \Psi(2m-2, m-1) + \frac{1}{3} + \frac{1}{2} \\ &> \Psi(2m, m); \end{aligned}$$

if $d_G(u_1) = 2$, then

$$\begin{aligned} H(G) &= H(G') + \frac{4}{5} + \frac{1}{2} - \frac{1}{2} \geq \Psi(2m-2, m-1) + \frac{4}{5} \\ &> \Psi(2m, m). \end{aligned}$$

Conversely, if $G \cong U_{2m, m}$, then it is easy to check that the equality holds. This completes the proof. \square

Remark 3.1. It is easy to calculate that $H(H_6) = 2.5 < \Psi(6, 3) = 2.5666$ and $H(H_8) = 3.3047 < \Psi(8, 4) = 3.3095$, where H_6 and H_8 are shown in Figure 1. Thus, by Theorem 3.1, H_6 has the minimum harmonic index in $\mathcal{U}_{6, 3}$ and H_8 has the minimum harmonic index in $\mathcal{U}_{8, 4}$.

Theorem 3.2. *Let $G \in \mathcal{U}_{n, m}$, where $n \geq 2m$ and $m \geq 5$. Then $H(G) \geq \Psi(n, m)$, and the equality holds if and only if $G \cong U_{n, m}$.*

Proof. We prove the assertion by the induction on n .

If $n = 2m$, then the result follows from Theorem 3.1. Now, we assume that $n > 2m$. If $G \cong C_n$, then $n = 2m+1$. Lemma 2.7 implies that $H(C_{2m+1}) > \Psi(2m+1, m)$. The result follows. So in what follows, we assume that $G \not\cong C_n$. Then Lemma 2.3 implies that G has an m -matching M and a pendant vertex v such that M does not saturate v . Let $uv \in E(G)$ and $d(u) = t$. Denote $N(u) \cap PV = \{v_1, \dots, v_{r-1}, v_r = v\}$ and $N(u) \setminus PV = \{x_1, \dots, x_{t-r}\}$. Then $d(x_j) \geq 2$ for each $j = 1, \dots, t-r$. Let $G' = G - v$. Then $G' \in \mathcal{U}_{n-1, m}$. Now we consider the following two cases.

Case 1 $r = 1$, that is $v_1 = v$.

Note that $t \leq n - m + 1$. Then by the induction hypothesis and Lemma 2.4(3), we have

$$\begin{aligned}
 H(G) &= H(G') + \frac{2}{t+1} + \sum_{j=1}^{t-1} \left(\frac{2}{d(x_j)+t} - \frac{2}{d(x_j)+t-1} \right) \\
 &\geq \Psi(n-1, m) + \frac{2}{t+1} + (t-1) \left(\frac{2}{2+t} - \frac{2}{1+t} \right) \\
 &= \Psi(n-1, m) + \frac{2t-2}{t+2} - \frac{2t-4}{t+1} \\
 &= \Psi(n, m) + \frac{2n-4m}{n-m+1} - \frac{2n-6m+2}{n-m+2} - \frac{2m}{n-m+3} \\
 &\quad + \frac{2t-2}{t+2} - \frac{2t-4}{t+1} \\
 &\geq \Psi(n, m) + \frac{2n-4m}{n-m+1} - \frac{4n-8m}{n-m+2} + \frac{2n-4m}{n-m+3} \\
 &> \Psi(n, m).
 \end{aligned}$$

Case 2 $r \geq 2$.

Note that $t \leq n - m + 1$ and $r \leq n - 2m + 1$. Then by the induction hypothesis and Lemma 2.5, we have

$$\begin{aligned}
 H(G) &= H(G') + \frac{2}{t+1} + (r-1) \left(\frac{2}{t+1} - \frac{2}{t} \right) \\
 &\quad + \sum_{j=1}^{t-r} \left(\frac{2}{d(x_j)+t} - \frac{2}{d(x_j)+t-1} \right) \\
 &\geq \Psi(n-1, m) + \frac{2r}{t+1} - \frac{2r-2}{t} + \sum_{j=1}^{t-r} \left(\frac{2}{d(x_j)+t} - \frac{2}{d(x_j)+t-1} \right) \\
 &\geq \Psi(n-1, m) + \frac{2r}{t+1} - \frac{2r-2}{t} + (t-r) \left(\frac{2}{2+t} - \frac{2}{1+t} \right) \\
 &= \Psi(n, m) + \frac{2n-4m}{n-m+1} - \frac{2n-6m+2}{n-m+2} - \frac{2m}{n-m+3} \\
 &\quad - \frac{2r-2}{t} - \frac{2t-4r}{t+1} + \frac{2t-2r}{t+2} \\
 &\geq \Psi(n, m) + \frac{2n-4m}{n-m+1} - \frac{2n-6m+2}{n-m+2} - \frac{2m}{n-m+3} \\
 &\quad - \frac{2n-4m}{n-m+1} + \frac{2n-6m+2}{n-m+2} + \frac{2m}{n-m+3} \\
 &= \Psi(n, m).
 \end{aligned}$$

Suppose that the equality holds. Then all inequalities in the above argument should be equalities. Then we have $H(G') = \Psi(n-1, m)$, $t = n - m + 1$, $r = n - 2m + 1$ and

$d(x_1) = \cdots = d(x_{t-r}) = 2$. Thus by the induction hypothesis, we have $G' \cong U_{n-1,m}$. Hence, it is not difficult to see that $G \cong U_{n,m}$.

Conversely, if $G \cong U_{n,m}$, then it is easy to see that the equality holds. This completes the proof. \square

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¹SCHOOL OF MATHEMATICS AND STATISTICS,
MINNAN NORMAL UNIVERSITY, ZHANGZHOU, FUJIAN, P. R. CHINA
E-mail address: ptjxli@hotmail.com (J. Li, Corresponding author)

²DEPARTMENT OF MATHEMATICS,
HONG KONG BAPTIST UNIVERSITY, KOWLOON TONG, HONG KONG, P.R. CHINA.
E-mail address: wcshiu@hkbu.edu.hk