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On the Harary Index of Cacti

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Abstract. The Harary index is defined as the sum of reciprocals of distances between all pairs of vertices of a connected graph. A connected graph G is a cactus if any two of its cycles have at most one common vertex. Let $\mathscr{G}(n,r)$ be the set of cacti of order n and with r cycles, $\xi(2n,r)$ the set of cacti of order $2n$ with a perfect matching and r cycles. In this paper, we give the sharp upper bounds of the Harary index of cacti among $\mathscr{G}(n,r)$ and $\xi(2n,r)$, respectively, and characterize the corresponding extremal cactus.

1. Introduction

Let $G=(V,E)$ be a simple connected graph. For any $u,v\in V(G)$, the distance $d_G(u,v)$ is defined as the length of the shortest path between u and v in G. The diameter d of a graph is the maximum distance between any two vertices of G. The reciprocal distance matrix $RD(G)$ of G, also called the Harary matrix [11], is an $n\times n$ matrix $(RD_{u,v}(G))$ such that

$$RD_{u,v}(G)=\begin{cases}\frac{1}{d_G(u,v)}, & if \quad u\neq v,\\ 0, & if \quad u=v.\end{cases}$$

The Harary index $H(G)$ of G is defined as the half-sum of the elements in the reciprocal distance matrix, that is,

$$H(G)=\sum_{u,v\in V(G),u\neq v}RD_{u,v}(G)=\sum_{u,v\in V(G),u\neq v}\frac{1}{d_G(u,v)},$$

where the summation goes over all pairs of vertices of G. Let $\gamma(G,k)$ be the number of vertex pairs of the graph G that are at distance k, then

$$H(G)=\sum_{k=1}^{d}\frac{1}{k}\gamma(G,k) \tag{1}$$

This topological index, which was introduced independently by Plavšić et al. [13] and by Ivanciuc et al. [10] in 1993 and named in honor of Professor Frank Harary on the occasion of his 70th birthday, has a number of

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interesting chemical-physics properties, it and its related molecular descriptors have shown some success in structure-property correlations [5–7, 12, 16]. Up to now, many results were obtained concerning the Harary index of a graph. In [16], B. Zhou et al. presented some lower and upper bounds for the Harary index of connected graphs, triangle-free and quadrangle-free graphs. Feng and Ilić [7] established sharp upper bound for the Harary index of graphs with a given matching number. In [8], Gutman attained the trees with the maximum and the minimum Harary index. Xu and Ch. Das [14] determined the extremal (maximal and minimal) unicyclic and bicyclic graphs with respect to Harary index. In this paper, we will consider the Harary index of cacti.

In order to state our results, we introduce some notation and terminology. For other undefined notation we refer to Bollobás [4]. For a vertex v of G, denote the degree of v by $d_G(v)$. Set $N_G(v) = \{u|uv \in E(G)\}$, $N_G[v] = N_G(v) \cup \{v\}$. If $W \subset V(G)$, we denote by $G - W$ the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, if $E \subset E(G)$, we denote by $G - E$ the subgraph of G obtained by deleting the edges of E. If $W = \{v\}$ and $E = \{xy\}$, we write $G - v$ and $G - xy$ instead of $G - \{v\}$ and $G - \{xy\}$, respectively. We call G a cactus if it is connected and all of blocks of G are either edges or cycles, i.e., any two of its cycles have at most one common vertex. Denote $\mathscr{G}(n, r)$ the set of cacti of order n and with r cycles, and $\xi(2n, r)$ the set of cacti of order $2n$ with a perfect matching and r cycles. Specifically, $G(n, 0)$ is the set of trees of order n and $G(n, 1)$ is the set of unicyclic graphs of order n.

Now we give some lemmas that will be used in the proof of our main results.

Lemma 1.1. *[8] Let T be a tree on n vertices. Then*

$$1 + n\sum_{k=2}^{n-1}\frac{1}{k} \le H(T) \le \frac{(n+2)(n-1)}{4}.$$

The right equality holds if and only if $T \cong S_n$, while the left equality holds if and only if $T \cong P_n$.

Denote by $C_{k,n-k}$ the graph obtained by attaching $n - k$ pendent edges to one vertex of C_k.

Lemma 1.2. *[14] For any unicyclic graph G, $H(G) \le \frac{1}{4}(n^2 + n)$ with equality holding if and only if $G \cong C_{3,n-3}$ for $n \ge 6$ and $G \cong C_n$ or $G \cong C_{3,n-3}$ for $n = 5$.*

Let ∞ be the graph obtained by adding two nonadjacent edges to a star S_5. Denote B_n^2 the graph attained by attaching $n - 5$ pendent edges to the unique vertex in ∞ of degree 4.

Lemma 1.3. *[15] For any bicyclic graph G with two edge disjoint cycles, $H(G) \le \frac{1}{4}(n^2+n+2)$ with equality holding if and only if $G \cong B_n^2$.*

For a connected graph G with $u \in V(G)$, we define

$$Q_G(u) = \sum_{w \in V(G)} \frac{d_G(u,w)}{d_G(u,w)+1}.$$

Lemma 1.4. *[14] Let G be a graph of order n and v be a pendent vertex of G with $uv \in E(G)$. Then*

$$H(G) = H(G - v) + n - 1 - Q_{G-v}(u).$$

Lemma 1.5. *[9] Let T be a tree of order n with perfect matching. Then*

$$H(T) \le \frac{1}{4}(17n^2 + 58n - 88).$$

The right equality holds if and only if $T \cong A_{n,\frac{n}{2}}$, where $A_{n,\frac{n}{2}}$ is obtained from the star $S_{\frac{n}{2}+1}$ by attaching a pendent edge to each of certain $\frac{n}{2} - 1$ non-central vertices of $S_{\frac{n}{2}+1}$.

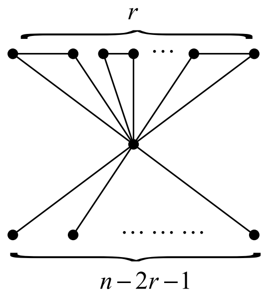

Figure 1: The graph $G^0(n,r)$

2. The maximum Harary index of cacti

In the section, we will study a sharp upper bound on the Harary index of cacti. First, we give some lemmas that will be used.

Lemma 2.1. *Let $G^0(n,r)$ be the graph shown in Figure 1, then*

$$H(G^0(n,r)) = \frac{1}{2}C^2_{n-2r-1} - r^2 + (n-1)r + (n-1).$$

Proof. Obviously, the diameter of $G^0(n,r)$ is 2, by (1), we have

$$\begin{aligned} H(G^0(n,r)) &= \sum_{l=1}^{2}\frac{1}{l}\gamma(G,l) = \gamma(G,1) + \frac{1}{2}\gamma(G,2) \\ &= n+r-1+\frac{1}{2}[C^2_{n-2r-1} + 2r\cdot(n-2r-1) + 2\cdot(2r-2) + 2\cdot(2r-4) + \cdots + 2\cdot 2] \\ &= n+r-1+\frac{1}{2}C^2_{n-2r-1} + r(n-2r-1) + r(r-1) \\ &= \frac{1}{2}C^2_{n-2r-1} - r^2 + (n-1)r + (n-1). \end{aligned}$$

□

Lemma 2.2. *Let $G \in \mathscr{G}(n,r)$ and v be a pendent vertex of G with $uv \in E(G)$, then $Q_{G-v}(u) \geq \frac{n}{2} - 1$. The equality holds if and only if $G \cong G^0(n,r)$.*

Proof. Note that the function $f(x) = \frac{x}{x+1}$ is strictly increasing for $x \geq 1$. Then

$$\begin{aligned} Q_{G-v}(u) &= \sum_{w\in V(G-v)}\frac{d(u,w)}{d(u,w)+1} = \sum_{w\in V(G-v-u)}\frac{d(u,w)}{d(u,w)+1} \\ &\geq \sum_{w\in V(G-v-u)}\frac{1}{1+1} = \frac{n}{2} - 1. \end{aligned}$$

The equality holds if and only if $d(u,w) = 1$ for any $w \in V(G-v-u)$. By the definition of cactus, we have $G \cong G^0(n,r)$. □

Lemma 2.3. *If $n \geq 6$, then $H(C_n) < H(C_{1,n-1})$.*

Proof. Note that $H(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} RD_{i,j}(G)$. If $n = 2l$, $l \geq 3$, we have

$$\begin{aligned} H(C_n) &= l[2(1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{l-1})+\frac{1}{l}] = 2l(1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{l-1})+1, \\ H(C_{1,n-1}) &= (2l-1)(1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{l-1})+1+2(\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{l}) \\ &= 2l(1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{l-1})+1+(\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{l})+\frac{1}{l}-1. \end{aligned}$$

Then

$$H(C_{1,n-1}) - H(C_n) = (\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{l})+\frac{1}{l}-1 > 0.$$

If $n = 2l+1$, $l \geq 3$, we have

$$\begin{aligned} H(C_n) &= (2l+1)(1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{l}), \\ H(C_{1,n-1}) &= 2l(1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{l-1})+1+[2(\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{l})+1+\frac{1}{l+1}] \\ &= (2l+1)(1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{l})+(\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{l+1})-1. \end{aligned}$$

It is easy to see that

$$H(C_{1,n-1}) - H(C_n) = (\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{l+1})-1 > 0.$$

Then we obtain the desired results. □

Theorem 2.4. *Let $G \in \mathscr{G}(n,r)$, then $H(G) \leq \frac{1}{2}C_{n-2r-1}^2 - r^2 + (n-1)r + (n-1)$. The equality holds if and only if $G \cong G^0(n,r)$.*

Proof. By induction on $n+r$. If $r = 0, 1$ or 2, then the theorem holds clearly by lemmas 1.1-1.3. Now, we assume that $r \geq 2$ and $n \geq 5$. If $n = 5$, then the theorem holds clearly by the facts that there is only one graph in $\mathscr{G}(5,2)$. Let $G \in \mathscr{G}(n,r)$, $n \geq 6$ and $r \geq 2$ in the following.

Case 1. $\delta(G) = 1$.

Let $v \in V(G)$ with $d_G(v) = 1$ and $uv \in E(G)$. Note that $G - v \in \mathscr{G}(n-1,r)$. By Lemma 1.4, we have

$$\begin{aligned} H(G) &= H(G-v)+n-1-Q_{G-v}(u) \\ &\leq [\frac{1}{2}C_{n-2r-2}^2 - r^2 + (n-2)r + (n-2)] + n - 1 - Q_{G-v}(u) \\ &\leq [\frac{1}{2}C_{n-2r-2}^2 - r^2 + (n-2)r + (n-2)] + n - 1 - (\frac{n}{2}-1) \quad (by \;\; Lemma \;\; 2.2) \\ &= \frac{1}{2}C_{n-2r-1}^2 - r^2 + (n-1)r + (n-1). \end{aligned}$$

The equality holds if and only if $G \cong G^0(n,r)$.

Case 2. $\delta(G) \geq 2$.

By the definition of cactus, $\delta(G) \geq 2$ and $r \geq 2$, we can choose a cycle $C_k = u_1u_2\ldots u_ku_1$ of G such that $d_G(u_1) = \cdots = d_G(u_{k-1}) = 2$ and $d_G(u_k) \geq 3$. We will finish the proof by considering four subcases.

Subcase 2.1. If $k = 3$, let $G' = G - u_1 - u_2$, then $G' \in \mathscr{G}(n-2, r-1)$.

$$\begin{aligned}
H(G) &= \sum_{u,v\in V(G),u\neq v} \frac{1}{d(u,v)} \\
&= \sum_{u,v\in V(G'),u\neq v} \frac{1}{d(u,v)} + \sum_{u\in V(G')} \frac{1}{d(u,u_1)} + \sum_{u\in V(G')} \frac{1}{d(u,u_2)} + 1 \\
&= H(G') + \sum_{u\in V(G')} \frac{1}{d(u,u_3)+1} + \sum_{u\in V(G')} \frac{1}{d(u,u_3)+1} + 1 \\
&= H(G') + 2\sum_{u\in V(G')} (1 - \frac{d(u,u_3)}{d(u,u_3)+1}) + 1 \\
&= H(G') + 2[n-2-Q_{G'}(u_3)] + 1 \\
&\leq \frac{1}{2}C^2_{n-2-2(r-1)-1} - (r-1)^2 + [(n-2)-1](r-1)) + [(n-2)-1] + 2[n-2-Q_{G'}(u_3)] + 1 \\
&\leq (\frac{1}{2}C^2_{n-2-2(r-1)-1} - (r-1)^2 + [(n-2)-1](r-1)) + [(n-2)-1] \\
&\quad +2[n-2-\frac{n-3}{2}] + 1 \quad (\textit{by Lemma 2.2 } Q_{G'}(u_3) \geq \frac{n-3}{2}) \\
&= \frac{1}{2}C^2_{n-2r-1} - r^2 + (n-1)r + (n-1).
\end{aligned}$$

The equality holds if and only if $G' \cong G^0(n-2, r-1)$, then $G \cong G^0(n, r)$.

Subcase 2.2. If $k = 4$, let $G' = G - u_1 - u_2 - u_3$, then $G' \in \mathscr{G}(n-3, r-1)$.

$$\begin{aligned}
H(G) &= \sum_{u,v\in V(G),u\neq v} \frac{1}{d(u,v)} \\
&= \sum_{u,v\in V(G'),u\neq v} \frac{1}{d(u,v)} + \sum_{u\in V(G')} \frac{1}{d(u,u_1)} + \sum_{u\in V(G')} \frac{1}{d(u,u_2)} + \sum_{u\in V(G')} \frac{1}{d(u,u_3)} \\
&\quad +(\frac{1}{d(u_1,u_2)} + \frac{1}{d(u_1,u_3)} + \frac{1}{d(u_2,u_3)}) \\
&= H(G') + \sum_{u\in V(G')} \frac{1}{d(u,u_4)+1} + \sum_{u\in V(G')} \frac{1}{d(u,u_4)+2} + \sum_{u\in V(G')} \frac{1}{d(u,u_4)+1} + \frac{5}{2} \\
&= H(G') + 2\sum_{u\in V(G')} [1 - \frac{d(u,u_4)}{d(u,u_4)+1}] + \sum_{u\in V(G')} [1 - \frac{d(u,u_4)+1}{d(u,u_4)+2}] + \frac{5}{2} \\
&= H(G') + 2[(n-3) - \sum_{u\in V(G')} \frac{d(u,u_4)}{d(u,u_4)+1}] + [(n-3) - \sum_{u\in V(G')} \frac{d(u,u_4)+1}{d(u,u_4)+2}] + \frac{5}{2} \\
&\leq H(G') + 2[(n-3) - \frac{n-4}{2}] + [(n-3) - \frac{2}{3}(n-4) - \frac{1}{2}] + \frac{5}{2} \\
&= H(G') + \frac{4n}{3} - \frac{1}{3} \\
&\leq \frac{1}{2}C^2_{n-2r-2} - (r-1)^2 + [(n-3)-1](r-1) + [(n-3)-1] + \frac{4n}{3} - \frac{1}{3} \\
&= \frac{1}{2}C^2_{n-2r-2} - r^2 + (n-1)r + (n-1) + \frac{1}{3}(n-3r-1).
\end{aligned}$$

Since $n \geq 6$, then

$$\frac{1}{2}C^2_{n-2r-1} - [\frac{1}{2}C^2_{n-2r-2} + \frac{1}{3}(n-3r-1)] \quad = \quad \frac{n-4}{6} > 0.$$

Hence $H(G) < \frac{1}{2}C^2_{n-2r-1} - r^2 + (n-1)r + (n-1)$.

Subcase 2.3. If $k = 5$, let $G' = G - u_1 - u_2 - u_3 - u_4$, then $G' \in \mathscr{G}(n-4, r-1)$.

$$\begin{aligned}
H(G) &= \sum_{u,v\in V(G),u\neq v} \frac{1}{d(u,v)} \\
&= \sum_{u,v\in V(G'),u\neq v} \frac{1}{d(u,v)} + \sum_{u\in V(G')} \frac{1}{d(u,u_1)} + \sum_{u\in V(G')} \frac{1}{d(u,u_2)} + \sum_{u\in V(G')} \frac{1}{d(u,u_3)} + \sum_{u\in V(G')} \frac{1}{d(u,u_4)} \\
&\quad +(\frac{1}{d(u_1,u_2)} + \frac{1}{d(u_1,u_3)} + \frac{1}{d(u_1,u_4)} + \frac{1}{d(u_2,u_3)} + \frac{1}{d(u_2,u_4)} + \frac{1}{d(u_3,u_4)}) \\
&= H(G') + 2\sum_{u\in V(G')} \frac{1}{d(u,u_5)+1} + 2\sum_{u\in V(G')} \frac{1}{d(u,u_5)+2} + \frac{9}{2} \\
&= H(G') + 2\sum_{u\in V(G')} [1 - \frac{d(u,u_5)}{d(u,u_5)+1}] + 2\sum_{u\in V(G')} [1 - \frac{d(u,u_5)+1}{d(u,u_5)+2}] + \frac{9}{2} \\
&= H(G') + 2[(n-4) - \sum_{u\in V(G')} \frac{d(u,u_4)}{d(u,u_4)+1}] + 2[(n-4) - \sum_{u\in V(G')} \frac{d(u,u_4)+1}{d(u,u_4)+2}] + \frac{9}{2} \\
&\leq H(G') + 2[(n-4) - \frac{n-5}{2}] + 2[(n-4) - \frac{2}{3}(n-5) - \frac{1}{2}] + \frac{9}{2} \\
&= H(G') + \frac{5n}{3} - \frac{5}{6} \\
&\leq (n-4) + (r-1) - 1 + \frac{1}{2}C^2_{n-2r-3} + (r-1)(n-2r-3) + (r-1)(r-2) + \frac{5n}{3} - \frac{5}{6} \\
&= \frac{1}{2}C^2_{n-2r-3} - r^2 + (n-1)r + (n-1) + \frac{1}{6}(4n - 12r - 5).
\end{aligned}$$

Note that $n \geq 6$, we have

$$\frac{1}{2}C^2_{n-2r-1} - [\frac{1}{2}C^2_{n-2r-3} + \frac{1}{6}(4n-12r-5)] = \frac{n-5}{3} > 0.$$

Then $H(G) < \frac{1}{2}C^2_{n-2r-1} - r^2 + (n-1)r + (n-1)$.

Subcase 2.4. If $k \geq 6$, then $G' = G - u_1u_2 + u_2u_k \in \mathscr{G}(n,r)$. Let $V_1 = \{u_1, u_2, \ldots, u_k\}, V_2 = V(G) - V_1$.

$$\begin{aligned}
H(G) &= \sum_{u,v\in V(G),u\neq v} \frac{1}{d_G(u,v)} \\
&= \sum_{u,v\in V_2,u\neq v} \frac{1}{d_G(u,v)} + \sum_{u\in V_2} \frac{1}{d_G(u,u_1)} + \cdots + \sum_{u\in V_2} \frac{1}{d_G(u,u_{k-1})} + \sum_{u\in V_2} \frac{1}{d_G(u,u_k)} \\
&\quad + \sum_{u,v\in V_1,u\neq v} \frac{1}{d_G(u,v)} \\
&= \sum_{u,v\in V_2,u\neq v} \frac{1}{d_G(u,v)} + \sum_{u\in V_2} \frac{1}{d_G(u,u_1)} + \cdots + \sum_{u\in V_2} \frac{1}{d_G(u,u_{k-1})} + \sum_{u\in V_2} \frac{1}{d_G(u,u_k)} + H(C_k), \\
H(G') &= \sum_{u,v\in V(G'),u\neq v} \frac{1}{d_{G'}(u,v)} \\
&= \sum_{u,v\in V_2,u\neq v} \frac{1}{d_{G'}(u,v)} + \sum_{u\in V_2} \frac{1}{d_{G'}(u,u_1)} + \cdots + \sum_{u\in V_2} \frac{1}{d_{G'}(u,u_{k-1})} + \sum_{u\in V_2} \frac{1}{d_{G'}(u,u_k)}
\end{aligned}$$

$$+\sum_{u,v\in V_1,u\neq v}\frac{1}{d_{G'}(u,v)}$$
$$=\sum_{u,v\in V_2,u\neq v}\frac{1}{d_{G'}(u,v)}+\sum_{u\in V_2}\frac{1}{d_{G'}(u,u_1)}+\cdots+\sum_{u\in V_2}\frac{1}{d_{G'}(u,u_{k-1})}+\sum_{u\in V_2}\frac{1}{d_{G'}(u,u_k)}$$
$$+H(C_{k-1}(1^1)).$$

Note that $d_G(u,u_i)\geq d_{G'}(u,u_i)$ for $i=1,2,\ldots,k$, then

$$H(G')-H(G) = \sum_{u\in V_2}[\frac{1}{d_{G'}(u,u_1)}-\frac{1}{d_G(u,u_1)}]+\cdots+\sum_{u\in V_2}[\frac{1}{d_{G'}(u,u_{k-1})}-\frac{1}{d_G(u,u_{k-1})}]$$
$$+\sum_{u\in V_2}[\frac{1}{d_{G'}(u,u_k)}-\frac{1}{d_G(u,u_k)}]+H(C_{k-1}(1^1))-H(C_k)$$
$$\geq H(C_{k-1}(1^1))-H(C_k)>0 \quad (\textit{by Lemma } 2.3).$$

Hence $H(G')>H(G)$. Note that $\delta(G')=1$, by case 1, we have

$$H(G')\leq\frac{1}{2}C^2_{n-2r-1}-r^2+(n-1)r+(n-1).$$

This completes the proof. □

3. The maximum Harary index of cacti with a perfect matching

Now, we will study a sharp upper bound on the Harary index of cacti with a perfect matching. The following Lemma 3.1 can be proved easily.

Lemma 3.1. *If $G\in\xi(2n,r)$, $n\geq 3$, then each vertex of G is adjacent to at most one pendent vertex.*

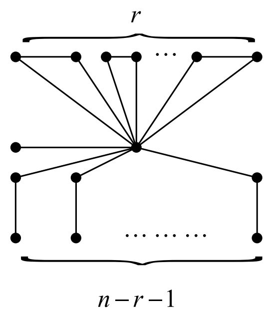

Figure 2: The graph $G(2n,r)$

Lemma 3.2. *Let $G(2n,r)$ be the graph as shown in Figure 2, then*

$$H(G(2n,r)) = \frac{1}{24}(n-r-1)(23n+17r-2)+2n+r^2+r-1.$$

Proof. It is easy to see that

$$\begin{aligned}\gamma(G,1) &= 2n+r-1,\\ \gamma(G,2) &= (n+r+1)(n-r-1)+2r^2,\\ \gamma(G,3) &= (n+r-1)(n-r-1),\\ \gamma(G,4) &= \frac{1}{2}(n-r-1)(n-r-2).\end{aligned}$$

Then

$$\begin{aligned}H(G(2n,r) &= \sum_{l=1}^{4}\frac{1}{l}\gamma(G,l)\\ &= (2n+r-1)+\frac{1}{2}[(n+r+1)(n-r-1)+2r^2]+\frac{1}{3}(n+r-1)(n-r-1)\\ &\quad +\frac{1}{8}(n-r-1)(n-r-2)\\ &= \frac{1}{24}(n-r-1)(23n+17r-2)+2n+r^2+r-1.\end{aligned}$$

□

Let C_k $(k\geq 4)$ be a cycle with vertex set $V(C_k)=\{u_1,u_2,\ldots,u_k\}$. Let G_1 be a graph of order n, which is obtained from C_k $(n-k\leq k)$ by attaching a pendent edge to each of certain $n-k$ vertices of C_k. Then $2\leq d_{G_1}(u_i)\leq 3$ for $i=1,2,\ldots,k$. Let

$$\delta_i=\begin{cases}1, & if\ \ d_{G_1}(u_i)=3,\\ 0, & if\ \ d_{G_1}(u_i)=2.\end{cases} \tag{2}$$

Denote the pendent vertex adjacent to u_i by $u_i'(\delta_i)$. In fact, if $\delta_i=0$, there does not exist such pendent vertex adjacent to u_i, for convenience, we name $u_i'(\delta_i)$ as a pseudo-pendent vertex adjacent to u_i. If there exist adjacent 3−degree vertices in G_1, without loss of generality, let $d_{G_1}(u_1)=d_{G_1}(u_2)=3$; If there does not exist adjacent 3−degree vertices in G_1, let $d_{G_1}(u_1)=2, d_{G_1}(u_2)=3$ and $d_{G_1}(u_3)=2$.

Lemma 3.3. *Let G_1 be the graph as described above, $G_2=G_1-u_2u_3+u_1u_3$.*

(i) *If $d_{G_1}(u_1)=d_{G_1}(u_2)=3$, then $H(G_1)\leq H(G_2)$.*

(ii) *If $d_{G_1}(u_1)=2, d_{G_1}(u_2)=3$ and $d_{G_1}(u_3)=2$ and $k\geq 8$, then $H(G_1)\leq H(G_2)$.*

Proof. Let PV be the set of pendent vertices of G_1. Obviously, G_2 has the same set of pendent vertices as G_1. By the definition of δ_i and pseudo-pendent vertex, we can set $PV=\{u_i'(\delta_i)|i=1,2,\ldots,k\}$. Then

$$\begin{aligned}H(G_1) &= \sum_{u,v\in V(G_1),u\neq v}\frac{1}{d_{G_1}(u,v)}\\ &= \sum_{u,v\in V(C_k),u\neq v}\frac{1}{d_{G_1}(u,v)}+\sum_{u\in V(C_k)}\sum_{i=1}^{k}\frac{\delta_i}{d_{G_1}(u,u_i'(\delta_i))}+\sum_{i=1}^{k}\sum_{i<j\leq k}\frac{\delta_i\delta_j}{d_{G_1}(u_i'(\delta_i),u_j'(\delta_j))},\\ H(G_2) &= \sum_{u,v\in V(C_k),u\neq v}\frac{1}{d_{G_2}(u,v)}+\sum_{u\in V(C_k)}\sum_{i=1}^{k}\frac{\delta_i}{d_{G_2}(u,u_i'(\delta_i))}+\sum_{i=1}^{k}\sum_{i<j\leq k}\frac{\delta_i\delta_j}{d_{G_2}(u_i'(\delta_i),u_j'(\delta_j))}.\end{aligned}$$

The proof need not distinguish two cases that k is even or not. However for convenience, we prefer to given only the proof for even $k=2l$. Let

$$A_{G_1}(u_j)=\sum_{i=1}^{k}\frac{\delta_i}{d_{G_1}(u_j,u_i'(\delta_i))},\quad A_{G_2}(u_j)=\sum_{i=1}^{k}\frac{\delta_i}{d_{G_2}(u_j,u_i'(\delta_i))}\quad (j=1,\ldots,k);$$

$$B_{G_1}(u'_i(\delta_i)) = \sum_{i<j\le k} \frac{\delta_i\delta_j}{d_{G_1}(u'_j(\delta_j), u'_i(\delta_i))}, \quad B_{G_2}(u'_i(\delta_i)) = \sum_{i<j\le k} \frac{\delta_i\delta_j}{d_{G_2}(u'_j(\delta_j), u'_i(\delta_i))} \quad (i = 1, \ldots, k).$$

Note that as we pass from G_1 to G_2, the distance of u_1 from a vertex in $\{u_3, \ldots, u_{l+1}\}$ is decreased by 1 and the distance of u_2 from a vertex in $\{u_3, \ldots, u_{l+1}\}$ is increased by 1, whereas the distances of u_1, u_2 from a vertex in $V(C_k) - \{u_3, \ldots, u_{l+1}\}$ are unchanged. Then

$$\begin{aligned}
A_{G_2}(u_1) - A_{G_1}(u_1) &= (\frac{\delta_3}{1+\delta_3} + \frac{\delta_4}{2+\delta_4} + \cdots + \frac{\delta_{l+1}}{l-1+\delta_{l+1}}) - (\frac{\delta_3}{2+\delta_3} + \frac{\delta_4}{3+\delta_4} + \cdots + \frac{\delta_{l+1}}{l+\delta_{l+1}}),\\
A_{G_2}(u_2) - A_{G_1}(u_2) &= (\frac{\delta_3}{2+\delta_3} + \frac{\delta_4}{3+\delta_4} + \cdots + \frac{\delta_{l+1}}{l+\delta_{l+1}}) - (\frac{\delta_3}{1+\delta_3} + \frac{\delta_4}{2+\delta_4} + \cdots + \frac{\delta_{l+1}}{l-1+\delta_{l+1}}).
\end{aligned}$$

Similarly, it is easy to see that the distance of u_3 from a vertex in $\{u_1, u_2, u_{2l} \ldots, u_{l+3}\}$ is changed, and the distances of u_3 from a vertex in $V(C_k) - \{u_1, u_2, u_{2l} \ldots, u_{l+3}\}$ is unchanged; the distance of u_4 from a vertex in $\{u_1, u_2, u_{2l} \ldots, u_{l+4}\}$ is changed, and the distances of u_4 from a vertex in $V(C_k) - \{u_1, u_2, u_{2l} \ldots, u_{l+4}\}$ is unchanged; $\cdots$; the distance of u_{l+1} from a vertex in $\{u_1, u_2\}$ is changed, and the distances of u_{l+1} from a vertex in $V(C_k) - \{u_1, u_2\}$ is unchanged; the distances of u_{l+2} from a vertex in $V(C_k)$ is unchanged; the distance of u_{l+2} from u_3 is changed, and the distances of u_{l+2} from a vertex in $V(C_k) - \{u_3\}$ is unchanged; $\cdots$; the distance of u_{2l} from a vertex in $\{u_3, u_4, \ldots, u_l\}$ is changed, whereas the distances of u_{2l} from a vertex in $V(C_k) - \{u_3, u_4, \ldots, u_l\}$ is unchanged. Then

$$\begin{aligned}
A_{G_2}(u_3) - A_{G_1}(u_3) &= (\frac{\delta_1}{1+\delta_1} + \frac{\delta_2}{2+\delta_2} + \frac{\delta_{2l}}{2+\delta_{2l}} + \cdots + \frac{\delta_{l+3}}{l-1+\delta_{l+3}}) -\\
&\quad (\frac{\delta_1}{2+\delta_1} + \frac{\delta_2}{1+\delta_2} + \frac{\delta_{2l}}{3+\delta_{2l}} + \cdots + \frac{\delta_{l+3}}{l+\delta_{l+3}}),\\
A_{G_2}(u_4) - A_{G_1}(u_4) &= (\frac{\delta_1}{2+\delta_1} + \frac{\delta_2}{3+\delta_2} + \frac{\delta_{2l}}{3+\delta_{2l}} + \cdots + \frac{\delta_{l+4}}{l-1+\delta_{l+4}}) -\\
&\quad (\frac{\delta_1}{3+\delta_1} + \frac{\delta_2}{2+\delta_2} + \frac{\delta_{2l}}{4+\delta_{2l}} + \cdots + \frac{\delta_{l+4}}{l+\delta_{l+4}}),\\
&\quad \vdots\\
A_{G_2}(u_{l+1}) - A_{G_1}(u_{l+1}) &= (\frac{\delta_1}{l-1+\delta_1} + \frac{\delta_2}{l+\delta_2}) - (\frac{\delta_1}{l+\delta_1} + \frac{\delta_2}{l-1+\delta_2}),\\
A_{G_2}(u_{l+2}) - A_{G_1}(u_{l+2}) &= 0,\\
A_{G_2}(u_{l+3}) - A_{G_1}(u_{l+3}) &= \frac{\delta_3}{l-1+\delta_3} - \frac{\delta_3}{l+\delta_3},\\
&\quad \vdots\\
A_{G_2}(u_{2l}) - A_{G_1}(u_{2l}) &= (\frac{\delta_3}{2+\delta_3} + \frac{\delta_4}{3+\delta_4} + \cdots + \frac{\delta_l}{l-1+\delta_l}) - (\frac{\delta_3}{3+\delta_3} + \frac{\delta_4}{4+\delta_4} + \cdots + \frac{\delta_l}{l+\delta_l}).
\end{aligned}$$

Similarly, it is easy to know that the distance of $u'_1(\delta_1)$ from a vertex in $\{u'_3(\delta_3), \ldots, u'_{l+1}(\delta_{l+1})\}$ is changed, and the distances of $u'_1(\delta_1)$ from a vertex in $PV - \{u'_3(\delta_3), \ldots, u'_{l+1}(\delta_{l+1})\}$ is unchanged; the distance of $u'_2(\delta_2)$ from a vertex in $\{u'_3(\delta_3), \ldots, u'_{l+1}(\delta_{l+1})\}$ is changed, and the distances of $u'_2(\delta_2)$ from a vertex in $PV - \{u'_3(\delta_3), \ldots, u'_{l+1}(\delta_{l+1})\}$ is unchanged; the distance of $u'_3(\delta_3)$ from a vertex $u'_j(\delta_j)$ for $j \ge 4$, if $j = 2l, 2l-1, \ldots, l+3$, the distance is changed, and the others are unchanged; $\cdots$; the distance of $u'_l(\delta_l)$ from a vertex $u'_j(\delta_j)$ for $j \ge l+1$, if $j = 2l$, the distance is changed, and the others are unchanged; the distance of $u'_i(\delta_i)$ from a vertex $u'_j(\delta_j)$ for $j > i$ and $i \geq l+1$, the distance is unchanged. Then

$$\begin{aligned}
B_{G_2}(u'_1(\delta_1)) - B_{G_1}(u'_1(\delta_1)) &= (\frac{\delta_1\delta_3}{1+\delta_1+\delta_3} + \frac{\delta_1\delta_4}{2+\delta_1+\delta_4} + \cdots + \frac{\delta_1\delta_{l+1}}{l-1+\delta_1+\delta_{l+1}}) - \\
&\quad (\frac{\delta_1\delta_3}{2+\delta_1+\delta_3} + \frac{\delta_1\delta_4}{3+\delta_1+\delta_4} + \cdots + \frac{\delta_1\delta_{l+1}}{l+\delta_1+\delta_{l+1}}), \\
B_{G_2}(u'_2(\delta_2)) - B_{G_1}(u'_2(\delta_2)) &= (\frac{\delta_2\delta_3}{2+\delta_2+\delta_3} + \frac{\delta_2\delta_4}{3+\delta_2+\delta_4} + \cdots + \frac{\delta_2\delta_{l+1}}{l+\delta_2+\delta_{l+1}}) - \\
&\quad (\frac{\delta_2\delta_3}{1+\delta_2+\delta_3} + \frac{\delta_2\delta_4}{2+\delta_2+\delta_4} + \cdots + \frac{\delta_2\delta_{l+1}}{l-1+\delta_2+\delta_{l+1}}), \\
B_{G_2}(u'_3(\delta_3)) - B_{G_1}(u'_3(\delta_3)) &= (\frac{\delta_3\delta_{2l}}{2+\delta_3+\delta_{2l}} + \cdots + \frac{\delta_3\delta_{l+3}}{l-1+\delta_3+\delta_{l+3}}) - \\
&\quad (\frac{\delta_3\delta_{2l}}{3+\delta_3+\delta_{2l}} + \cdots + \frac{\delta_3\delta_{l+3}}{l+\delta_3+\delta_{l+3}}), \\
B_{G_2}(u'_4(\delta_4)) - B_{G_1}(u'_4(\delta_4)) &= (\frac{\delta_4\delta_{2l}}{3+\delta_4+\delta_{2l}} + \cdots + \frac{\delta_4\delta_{l+4}}{l-1+\delta_4+\delta_{l+4}}) - \\
&\quad (\frac{\delta_4\delta_{2l}}{4+\delta_4+\delta_{2l}} + \cdots + \frac{\delta_4\delta_{l+4}}{l+\delta_4+\delta_{l+4}}), \\
&\ \ \vdots \\
B_{G_2}(u'_l(\delta_l)) - B_{G_1}(u'_l(\delta_l)) &= \frac{\delta_l\delta_{2l}}{l-1+\delta_l+\delta_{2l}} - \frac{\delta_l\delta_{2l}}{l+\delta_l+\delta_{2l}},
\end{aligned}$$

and $B_{G_2}(u'_i(\delta_i)) - B_{G_1}(u'_i(\delta_i)) = 0$ for $i = l+1,\ \ldots,\ 2l$.

By Lemma 2.3, if $l \geq 2$, we have

$$\sum_{u,v\in V(C_k),u\neq v}\frac{1}{d_{G_2}(u,v)} - \sum_{u,v\in V(C_k),u\neq v}\frac{1}{d_{G_1}(u,v)} = (\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{l}) + \frac{1}{l} - 1 \geq 0.$$

(i) If $d_{u_1} = d_{u_2} = 3$, then $\delta_1 = \delta_2 = 1$. By the above discussion, it is easy to see that

$$\sum_{j=1}^{2l}(A_{G_2}(u_j) - A_{G_1}(u_j)) = \sum_{u\in V(C_k)}\sum_{i=1}^{k}\frac{\delta_i}{d_{G_2}(u,u'_i(\delta_i))} - \sum_{u\in V(C_k)}\sum_{i=1}^{k}\frac{\delta_i}{d_{G_1}(u,u'_i(\delta_i))} \geq 0,$$

$$\sum_{j=1}^{2l}(B_{G_2}(u'_j(\delta_j)) - B_{G_1}(u'_j(\delta_j))) = \sum_{i=1}^{k}\sum_{i<j\leq k}\frac{\delta_i\delta_j}{d_{G_2}(u'_i(\delta_i),u'_j(\delta_j))} - \sum_{i=1}^{k}\sum_{i<j\leq k}\frac{\delta_i\delta_j}{d_{G_1}(u'_i(\delta_i),u'_j(\delta_j))} \geq 0.$$

Then $H(G_1) \leq H(G_2)$.

(ii) If $d_{u_1} = 2, d_{u_2} = 3$, then $\delta_1 = 0, \delta_2 = 1$ and $\delta_3 = 0$. By the above discussion, we have

$$\begin{aligned}
\sum_{j=1}^{2l}(A_{G_2}(u_j) - A_{G_1}(u_j)) &\geq \frac{1}{l+1} - \frac{1}{2} + (\frac{\delta_4}{3+\delta_4} + \cdots + \frac{\delta_l}{l-1+\delta_l}) - (\frac{\delta_4}{4+\delta_4} + \cdots + \frac{\delta_l}{l+\delta_l}), \\
\sum_{j=1}^{2l}(B_{G_2}(u'_j(\delta_j)) - B_{G_1}(u'_j(\delta_j))) &\geq (\frac{\delta_4}{4+\delta_4} + \cdots + \frac{\delta_{l+1}}{l+1+\delta_{l+1}}) - (\frac{\delta_4}{3+\delta_4} + \cdots + \frac{\delta_{l+1}}{l+\delta_{l+1}}).
\end{aligned}$$

Hence

$$H(G_2) - H(G_1) = (\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{l}) + \frac{1}{l} - 1 + \frac{1}{l+1} - \frac{1}{2} + \frac{\delta_{l+1}}{l+1+\delta_{l+1}} - \frac{\delta_{l+1}}{l+\delta_{l+1}}$$

Note that $k = 2l \geq 8$, then $l \geq 4$. If $\delta_{l+1} = 0$, it is easy to see that

$$H(G_2) - H(G_1) = (\frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{l}) + \frac{1}{l} - 1 + \frac{1}{l+1} - \frac{1}{2} > 0.$$

If $\delta_{l+1} = 1$, obviously

$$H(G_2) - H(G_1) = (\frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{l}) + \frac{1}{l} - 1 + \frac{1}{l+1} - \frac{1}{2} + \frac{1}{l+2} - \frac{1}{l+1} \geq 0.$$

Then $H(G_1) \leq H(G_2)$. □

Theorem 3.4. *Let $G \in \xi(2n, r)$, $n \geq 3$, then $H(G) \leq \frac{1}{24}(n - r - 1)(23n + 17r - 2) + 2n + r^2 + r - 1$. The equality holds if and only if $G \cong G(2n, r)$.*

Proof. By induction on $n + r$. If $r = 0$, then the theorem holds clearly by Lemmas 1.5. Now, we assume that $r \geq 1$ and $n \geq 2$.

Case 1. $\delta(G) = 1$.

Subcase 1.1. There exists a vertex u of degree 2 which is adjacent to a pendent vertex v in G. Let $G' = G - u - v$, we have $G' \in \mathscr{G}(2n - 2, r)$. By the inductive assumption, we have

$$\begin{aligned} H(G') &\leq \frac{1}{24}[(n - r - 1) - 1][(23n + 17r - 2) - 23] + (2n - 2) + r^2 + r - 1 \\ &= H(G(2n, r) - \frac{23}{12}n + \frac{1}{4}r. \end{aligned}$$

Note that $2n \geq 2r + 2$, then

$$\begin{aligned} H(G) &= H(G') + \sum_{x \in V(G-v-u)} \frac{1}{d(x, w) + 1} + \sum_{x \in V(G-v-u)} \frac{1}{d(x, w) + 2} + 1 \\ &\leq H(G') + (\frac{n + r - 1}{2} + \frac{n - r - 2}{3} + 1) + (\frac{n + r - 1}{3} + \frac{n - r - 2}{4} + \frac{1}{2}) + 1 \\ &\leq H(G(2n, r) - \frac{23}{12}n + \frac{1}{4}r + (\frac{n + r - 1}{2} + \frac{n - r - 2}{3} + 1) + (\frac{n + r - 1}{3} + \frac{n - r - 2}{4} + \frac{1}{2}) + 1 \\ &= H(G(2n, r) - \frac{1}{2}(n - r - 1) \leq H(G(2n, r). \end{aligned}$$

Subcase 1.2. The degree of any vertex which is adjacent to a pendent vertex in G is at least 3. We can choose a cycle $C = u_1u_2 \ldots u_ku_1$ of G such that u_i $(i = 2, 3, \ldots, k)$ does not appear on other cycles of G and there at least exists one of u_i adjacent to a pendent vertex for $i = 1, 2, \ldots, k$. Then $d_{u_i} = 3$ if u_i is adjacent to a pendent vertex, otherwise $d_{u_i} = 2$; and $3 \leq d_{u_1} = d \leq n + r$. Note that at most one of u_1u_2, u_1u_k belongs to the perfect matching M of G. Without loss of generality, we assume that $u_1u_2 \notin M$.

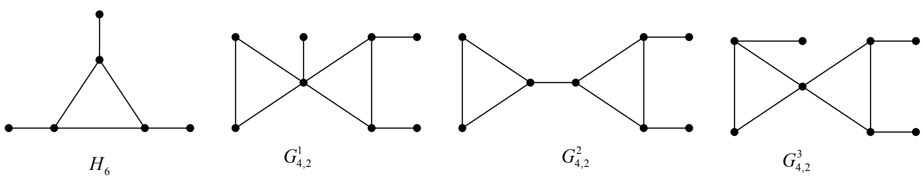

Figure 3: The graphs $H_6, G^1_{4,2}, G^2_{4,2}$ and $G^3_{4,2}$.

Subcase 1.2.1. $k = 3$.

(i) If $d_{u_2} = d_{u_3} = 2$, then $u_2u_3 \in M$ and there is a pendent vertex u'_1 adjacent to u_1. Let $G' = G - u_2 - u_3$, obviously $G' \in \mathscr{G}(2n - 2, r - 1)$.

If $G' \cong H_6$, then $n = 4, r = 2$. We have $G \cong G^1_{4,2}$ (as shown in Figure 3) and $H(G^1_{4,2}) = 17.3333$. By Lemma 3.1, $H(G(8, 2)) = 18.1516$. Then the result holds.

If $G' \ncong H_6$, then $G' \in \mathscr{G}(2n-2, r-1) \setminus H_6$. By the inductive assumption, we have

$$\begin{aligned} H(G') &\leq \frac{1}{24}[(n-1)-(r-1)-1][(23n+17r-2)-40]+(2n-2)+(r-1)^2+(r-1)-1 \\ &= \frac{1}{24}(n-r-1)(23n+17r-2)+2n+r^2+r-1-\frac{1}{3}(5n+r+1) \\ &= H(G(2n,r)-\frac{1}{3}(5n+r+1). \end{aligned}$$

Then

$$\begin{aligned} H(G) &= H(G')+\sum_{x\in V(G-u_2-u_3)}\frac{1}{d(x,u_1)+1}+\sum_{x\in V(G-v-u)}\frac{1}{d(x,u_1)+1}+1 \\ &\leq H(G')+2(\frac{n+r-2}{2}+\frac{n-r-1}{3}+1)+1 \end{aligned}$$

$$\leq H(G(2n,r)-\frac{1}{3}(5n+r+1)+2(\frac{n+r-2}{2}+\frac{n-r-1}{3}+1)+1=H(G(2n,r).$$

The equality holds if and only if $G-u_2-u_3 \cong G(2n-2,r-1)$, then $G \cong G(2n,r)$.

(ii) If $d_{u_2}=d_{u_3}=3$, then there exist two pendent vertices u_2', u_3' adjacent to u_2, u_3, respectively, and $u_2u_2' \in M, u_3u_3' \in M$. Let $G' = G-u_2'-u_3'$. Then $M \cup \{u_2u_3\} \setminus \{u_2u_2', u_3u_3'\}$ is a perfect matching of G' and $G' \in \mathscr{G}(2n-2, r) \setminus H_6$.

By the inductive assumption, we have

$$\begin{aligned} H(G') &\leq \frac{1}{24}[(n-1)-r-1][(23n+17r-2)-23]+(2n-2)+r^2+r-1 \\ &= H(G(2n,r)-\frac{23}{12}n+\frac{1}{4}r. \end{aligned}$$

Then

$$\begin{aligned} H(G) &= H(G')+(\sum_{x\in V_2}\frac{1}{d(x,u_1)+2}+1+\frac{1}{2})+(\sum_{x\in V_2}\frac{1}{d(x,u_1)+2}+1+\frac{1}{2})+\frac{1}{3} \\ &\leq H(G')+2(\frac{n+r-3}{3}+\frac{1}{2}+\frac{n-r-2}{4}+1+\frac{1}{2})+\frac{1}{3} \\ &\leq H(G(2n,r)-\frac{23}{12}n+\frac{1}{4}r+2(\frac{n+r-3}{3}+\frac{1}{2}+\frac{n-r-2}{4}+1+\frac{1}{2})+\frac{1}{3} \\ &= H(G(2n,r)-\frac{1}{12}(9n-r-16), \end{aligned}$$

since $n \geq r+1, r \geq 1$, then $9n-r-16 \geq 8r-7 > 0$. Hence $H(G) < H(G(2n,r)$.

(iii) If $d_{u_2}=2, d_{u_3}=3$ or $d_{u_2}=3, d_{u_3}=2$, without loss of generality, let $d_{u_2}=3, d_{u_3}=2$. Then there exists a pendent vertex u_2' adjacent to u_2, and $u_2u_2', u_1u_3 \in M$. Let $G' = G-u_2-u_2'$.

If $G' \cong H_6$, then $n=4, r=2$. We have $G \cong G^3_{4,2}$ (as shown in Figure 3) and $H(G^3_{4,2}) = 16.8333$. Note that $H(G(8,2)) = 18.1516$. Then the result holds.

If $G' \ncong H_6$, then $G' \in \mathscr{G}(2n-2, r-1) \setminus H_6$. By the inductive assumption, we have

$$\begin{aligned} H(G') &\leq \frac{1}{24}[(n-1)-(r-1)-1][(23n+17r-2)-40]+(2n-2)+(r-1)^2+(r-1)-1 \\ &= \frac{1}{24}(n-r-1)(23n+17r-2)+2n+r^2+r-1-\frac{1}{3}(5n+r+1) \\ &= H(G(2n,r)-\frac{1}{3}(5n+r+1). \end{aligned}$$

Let $V_1 = \{u_2, u_2', u_3\}$, $V_2 = V(G) - V_1$. Then

$$\begin{aligned} H(G) &= H(G') + (\sum_{x\in V_2} \frac{1}{d(x,u_1)+1} + 1) + (\sum_{x\in V_2} \frac{1}{d(x,u_1)+2} + \frac{1}{2}) + 1 \\ &\leq H(G') + (1 + \frac{n+r-3}{2} + \frac{n-r-1}{3} + 1) + (\frac{1}{2} + \frac{n+r-3}{3} + \frac{n-r-1}{4} + \frac{1}{2}) + 1 \\ &\leq H(G(2n,r) - \frac{1}{3}(5n+r+1) + \frac{17}{12}n + \frac{1}{4}r + \frac{5}{12} \\ &= H(G(2n,r) - \frac{1}{12}(3n+r-1) < H(G(2n,r). \end{aligned}$$

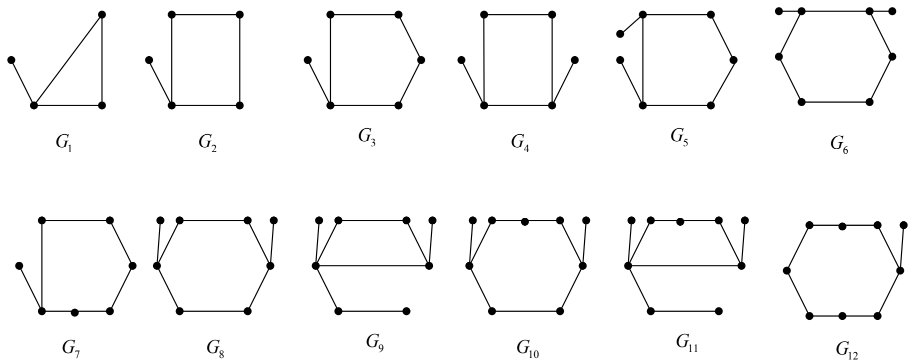

Figure 4: The graphs $G_1, G_2, \ldots, G_{12}$.

Subcase 1.2.2. $k \geq 4$. Let $V_1 = \{u_1, u_1'(\delta_1), u_2, u_2'(\delta_2), \ldots, u_k, u_k'(\delta_k)\}$ (note that if $\delta_i = 0$, $u_i'(\delta_i)$ isn't an element of V_1), $V_2 = V(G) - V_1$. Let $i + l \equiv (i + l) \mod k$. Then

$$\begin{aligned} H(G) &= \sum_{u,v\in V(G),u\neq v} \frac{1}{d_G(u,v)} \\ &= \sum_{u,v\in V_2,u\neq v} \frac{1}{d_G(u,v)} + \sum_{u\in V_2}\sum_{i=1}^{k} \frac{1}{d_G(u,u_i)} + \sum_{u\in V_2}\sum_{i=1}^{k} \frac{\delta_i}{d_G(u,u_i'(\delta_i))} + \sum_{u,v\in V_1,u\neq v} \frac{1}{d_G(u,v)}. \end{aligned}$$

Subcase 1.2.2.1. There exist two adjacent vertices $u_i, u_{i+1} \in V(C_k)$ with $\delta_i = \delta_{i+1} = 1$. Note that if $k = 4$, it must coincide with this case. Let $G' = G - u_{i+1}u_{i+2} + u_iu_{i+2}$, obviously $G' \in \mathscr{G}(2n,r)$. Then

$$\begin{aligned} H(G') &= \sum_{u,v\in V(G'),u\neq v} \frac{1}{d_{G'}(u,v)} \\ &= \sum_{u,v\in V_2,u\neq v} \frac{1}{d_{G'}(u,v)} + \sum_{u\in V_2}\sum_{i=1}^{k} \frac{1}{d_{G'}(u,u_i)} + \sum_{u\in V_2}\sum_{i=1}^{k} \frac{\delta_i}{d_{G'}(u,u_i'(\delta_i))} + \sum_{u,v\in V_1,u\neq v} \frac{1}{d_{G'}(u,v)}. \end{aligned}$$

Note that if $u, v \in V_2, u \neq v$, $d_G(u,v) = d_{G'}(u,v)$; if $u \in V_2$, $d_G(u,u_i) \geq d_{G'}(u,u_i)$ and $d_G(u,u_i'(\delta_i)) \geq d_{G'}(u,u_i'(\delta_i))$. Hence

$$\begin{aligned} H(G') - H(G) &= \sum_{u\in V_2}\sum_{i=1}^{k}(\frac{1}{d_{G'}(u,u_i)} - \frac{1}{d_G(u,u_i)}) + \sum_{u,v\in V_1,u\neq v} \frac{1}{d_{G'}(u,v)} - \sum_{u,v\in V_1,u\neq v} \frac{1}{d_G(u,v)} \\ &\geq \sum_{u,v\in V_1,u\neq v} \frac{1}{d_{G'}(u,v)} - \sum_{u,v\in V_1,u\neq v} \frac{1}{d_G(u,v)}. \end{aligned}$$

By Lemma 3.3 (i), we have $H(G') \geq H(G)$. Further by Subcase 1.1, $H(G(2n,r) \geq H(G')$.

Subcase 1.2.2.2. There do not exist two adjacent vertices $u_i, u_{i+1} \in V(C_k)$ with $\delta_i = \delta_{i+1} = 1$. Without loss of generality, let $\delta_i = \delta_{i+2} = 0, \delta_{i+1} = 1$.

If $k \geq 8$, let $G' = G - u_{i+1}u_{i+2} + u_iu_{i+2}$, similar to Subcase 1.2.2.1, we have

$$H(G') - H(G) \geq \sum_{u,v \in V_1, u \neq v} \frac{1}{d_{G'}(u,v)} - \sum_{u,v \in V_1, u \neq v} \frac{1}{d_G(u,v)}.$$

By Lemma 3.3 (ii), we have $H(G') \geq H(G)$. Further by Subcase 1.1, $H(G(2n,r) \geq H(G')$.

Now we only need to consider the cases of $5 \leq k \leq 7$, let $G' = G - u_{i+1}u_{i+2} + u_iu_{i+2}$, or $G' = G - u_{i+3}u_{i+4} + u_iu_{i+2}$. By direct calculation, we have

$$\begin{aligned} H(G_1) = 5, \quad H(G_2) = 8.3333, \quad H(G_3) = 10.1667, \quad H(G_4) = 10.3333; \\ H(G_5) = 13.5, \quad H(G_6) = 16.5, \quad H(G_7) = 12.9167, \quad H(G_8) = 16.2333; \\ H(G_9) = 18.1667, \quad H(G_{10}) = 19.5667, \quad H(G_{11}) = 21.6667, \quad H(G_{12}) = 16.25. \end{aligned} \tag{3}$$

By (3.3), it is easy to see the following results:

(i) If $k = 5$, $H(G_3) < H(G_4)$;

(ii) If $k = 6$, $H(G_7) < H(G_5)$ and $H(G_8) < H(G_9)$;

(iii) If $k = 7$, $H(G_{12}) < H(G_6)$ and $H(G_{10}) < H(G_{11})$.

So $H(G') > H(G)$. Now either G' exists a vertex of degree 2 which is adjacent to a pendent vertex, or G' has two adjacent vertices u_i, u_{i+1} with $\delta_i = \delta_{i+1} = 1$. At the same time, it is easy to see that the other cases of G must have two adjacent vertices u_i, u_{i+1} with $\delta_i = \delta_{i+1} = 1$. Further by Subcase 1.1 and Subcase 1.2.2.1, we have $H(G(2n,r) \geq H(G')$.

Case 2. $\delta(G) = 2$. We can choose a cycle $C_k = u_1u_2 \dots u_ku_1$ of G such that $d_G(u_2) = \cdots = d_G(u_k) = 2$ and $d_G(u_1) \geq 3$.

If $k = 3$, let $G' = G - u_2u_3$. If $G' \cong H_6$, then $n = 4, r = 2$. We have $G \cong G^2_{4,2}$ (as shown in Figure 3) and $H(G^2_{4,2}) = 14$. By Lemma 3.1, $H(G(8,2)) = 18.1516$. Then the result holds. If $G' \ncong H_6$, similar to Subcase 1.2.1, we have the desired result.

If $k = 4, 5$, let $G' = G - u_1u_2 + u_1u_3$, note that $H(C_4) = 5 = H(G_1)$, $H(C_5) = 7.5 < H(G_2)$. Then we have $H(G') \geq H(G)$, by Case 1, we have $H(G(2n,r) \geq H(G')$.

If $k \geq 6$, Let $G' = G - u_1u_2 + u_1u_3$. Similar to the proof of Subcase 2.4 in Theorem 2.4, we have $H(G') \geq H(G)$. Further by Case 1 in Theorem 3.4, we obtain the desired result. □

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