A sharp lower bound of index of the cacti with perfect matchings

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Abstract

The Randić index of an organic molecule whose molecular graph is G is the sum of the weights $(d(u)d(v))^{-\frac{1}{2}}$ of all edges uv of G, where $d(u)$ and $d(v)$ are the degrees of the vertices u and v in G. In this paper, we give a sharp lower bound on the Randić index of cacti with perfect matchings.

Keywords: Cactus; Randić index; Perfect matching

1 Introduction

A single number that can be used to characterize some property of the graph of a molecule is called a topological index. One of the most important topological indices is the well-known branching index introduced by Randić [1] which is defined as the sum of certain bond contributions calculated from the vertex degree of the hydrogen suppressed molecular graphs.

Let $G = (V, E)$ be a simple connected graph with the vertex set V and the edge set E. The Randić index (or connectivity index) of G was defined as

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

where $d(u)$ and $d(v)$ denote the degree of the vertices u and v. Randić demonstrated that his index is well correlated with a variety of physic-chemical properties of various classes of organic compounds. Recently, the

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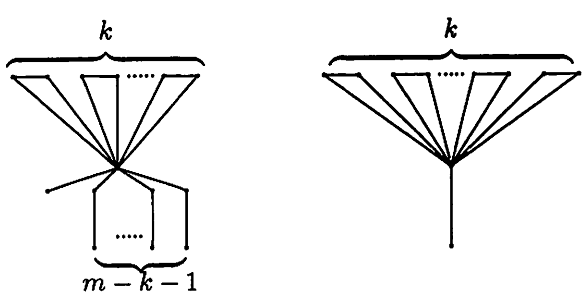
Randić index attracted the attention of many researchers and many results were obtained. In particular, for general graphs, Bollobaás and Erdős gave the sharp lower bound of $R(G) \geq \sqrt{n-1}$. Lu etal [3] gave a sharp lower bound on $R(G)$ of cacti with given number of cycles. In [6, 7], sharp lower bounds on $R(G)$ of trees and unicycle graphs with a given size of matching was given respectively. In this paper, we will investigate a type graph, namely that of conjugated cacti with perfect matchings.

All graphs that we considered is only finite, undirected and connected simple graphs. Let $d_G(x,y)$ denote the length of a shortest (x,y)-path in G. C_n denotes the cycle on n vertices, we by $N(v)$ and $d(v)$ denote the neighbors and the degree of v respectively. A pendant vertex of a graph is a vertex with degree 1. Denote by PV the set of pendant vertices of G. $G-x$ denote the graph that arises from G by deleting the vertex $x \in V(G)$ together with its incident edges, and $\delta(G)$ =min$\{d(v) : v \in V(G)\}$. A subset $M \subseteq E$ is called a matching in G if its elements are edges and no two are adjacent in G. A matching M saturates a vertex v, and v is said to be M-saturated, if a edge of M is incident with v. If every vertex of G is M-saturated, the matching M is perfect.



$G_{m,k}$ $\qquad$ $G_{k+1,k}$

Figure 1. two graphs $G_{m,k}$ and $G_{k+1,k}$

2 Some Lemmas

A graph G is called a cactus if each block of G is either a cycle or an edge. Denote $\mathscr{G}_{m,k}$ the set of cacti with k cycles and perfect matchings on $2m$ vertices. $G_{m,k}$ and $G_{k+1,k}$ are the cacti depicted in Figure 1.

In the following, we give some Lemmas that will be used in the proof of our results.

Lemma 2.1([8]). Let $G \in \mathscr{G}_{m,k}, m \geq 3$, and T 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.

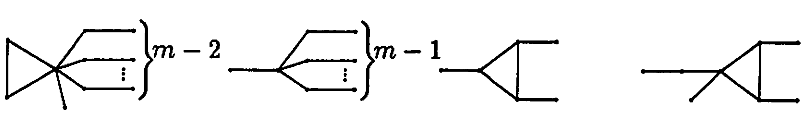
Lemma 2.2([9]). Let $G \in \mathscr{G}_{m,k}, m \geq 3$. If $PV \neq \phi$, then for any vertex $u \in V(G)$, $\mid N(u) \bigcap PV \mid \leq 1$.

Lemma 2.3([9]). The function $f(x) - f(x+1)$ is monotonously increasing in $x \geq 1$, where

$$f(x) = \frac{1}{\sqrt{x+1}} + \frac{x}{\sqrt{2(x+1)}} \quad x \geq 1, \tag{1}$$

and x is a positive integer.

Now we displayed four graphs $U_{2m,m}, T^0(2m,m), H_6, H_8$ in Figure 2.



$U_{2m,m}$ $T^0(2m,m)$ H_6 H_8

Figure 2. The graphs $U_{2m,m}, T^0(2m,m), H_6, H_8$.

Lemma 2.4([6]). Let T be an n-vertex ($n = 2m$) tree with a perfect matching, then $R(T) \geq \phi(2m,m)$ with the equality holds if and only if $T \cong T^0(2m,m)$, where

$$\phi(n,\ m) = \frac{n-2m+1}{\sqrt{n-m}} + \frac{m-1}{\sqrt{2(n-m)}} + \frac{m-1}{\sqrt{2}}.$$

Let $G \in \mathscr{U}_{2m,m} = \{G : G$ is a unicyclic graph with $2m$ vertices and an m-matchings $\}$.

Lemma 2.5([7]). Let $G \in \mathscr{U}_{2m,m} \setminus \{H_6, H_8\}$, $m \geq 2$. Then $R(G) \geq \psi(2m, m)$ with the equality holds if and only if $G \cong U_{2m,m}$, where

$$\psi(n,\ m) = \frac{n-2m+1}{\sqrt{n-m+1}} + \frac{m}{\sqrt{2(n-m+1)}} + \frac{m}{\sqrt{2}} + \frac{1-2\sqrt{2}}{2}.$$

Remark. In [7], it showed that $R(H_6) = 2.7321 < \psi(6,3) = 2.7678$ and $R(H_8) = 3.6260 < \psi(8,4) = 3.6263$, where H_6 and H_8 are shown in Figure 2. Thus H_6 and H_8 are the graphs with the minimum Randić index in $\mathscr{U}_{6,3}$ and $\mathscr{U}_{8,4}$, respectively.

Let

$$\varphi(m,k) = \frac{m+k-1}{\sqrt{2(m+k)}} + \frac{1}{\sqrt{m+k}} + \frac{m-1}{\sqrt{2}} + \frac{(1-\sqrt{2})k}{2}$$

where m and k are positive integers. We have the following result.

Lemma 2.6. If $m \geq 4, k \geq 2$, then $\varphi(m-1,k) + \frac{1}{\sqrt{3}} + \frac{1}{3} > \varphi(m,k)$, $\varphi(m-1,k) + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{1}{2} > \varphi(m,k)$.

Proof.

$$\begin{aligned}
&\varphi(m-1,k) - \varphi(m,k) + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{1}{2} \\
= \ & \frac{m+k-2}{\sqrt{2(m+k-1)}} + \frac{1}{\sqrt{m+k-1}} - \frac{m+k-1}{\sqrt{2(m+k)}} - \frac{1}{\sqrt{m+k}} \\
&+ \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} - \frac{1}{2} \\
= \ & f(m+k-2) - f(m+k-1) + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} - \frac{1}{2} \\
> \ & f(4) - f(5) + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} - \frac{1}{2} \qquad \text{(by Lemma 2.3)} \\
= \ & \frac{4}{\sqrt{10}} + \frac{1}{\sqrt{5}} - \frac{5}{\sqrt{12}} - \frac{1}{\sqrt{6}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} - \frac{1}{2} \\
> \ & 0
\end{aligned}$$

and $\varphi(m-1,k) - \varphi(m,k) + \frac{1}{\sqrt{3}} + \frac{1}{3} > \varphi(m-1,k) - \varphi(m,k) + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{1}{2} > 0$.

Hence the Lemma holds.

3 Main result

In this section, we will give a sharp lower bound of the Randić index of cacti with perfect matchings.

Theorem 3.1. Let $G \in \mathscr{G}_{m,k} \setminus \{H_6, H_8\}$, $m \geq 2$. Then $R(G) \geq \varphi(m,k)$ with the equality if and only if $G \cong G_{m,k}$.

Proof. We prove the result by induction on m and k. The result holds for $k = 0, 1$ by Lemmas 2.4 and 2.5.

We now assume that $k \geq 2$. Then $m \geq 3$. If $m = 3$, there are only four graphs in $\mathscr{G}_{m,k}$, see Figure 3. It can be seen that $G_{3,2}$ is the graph with the minimum Randić index in $\mathscr{G}_{3,2}$, and the result holds.

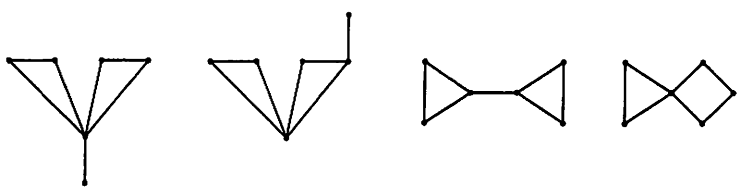


Figure 3. The graphs in $\mathscr{G}_{3,2}$ and their Randić indices.

So we can assume $m \geq 4$. Let $G \in \mathscr{G}_{m,k}$ with a perfect matching M.

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

Assume a graph $G \in \mathscr{G}_{m,k}$, then the maximum degree of a vertex in G is $m + k$ if and only if the vertex is the common vertex of all cycles in the graph $G_{m,k}$. And since each block of G is either a cycle or an edge, G has a cycle $C = u_1u_2 \cdots u_tu_1$ with $2 \leq d(u_1) = d \leq m + k$ and $d(u_i) = 2$ for $i = 2, \cdots, t$. Let $N(u_1) = \{u_2, u_t, x_1, x_2, \cdots, x_{d-2}\}$. Obviously, at least one of the edges u_1u_2 and u_1u_t doesn't belong to the perfect matching M. Without loss of generality, we assume $u_1u_2 \notin M$.

Let $G' = G - u_1u_2$. Then $G' \in \mathcal{G}_{m,k-1} \setminus \{H_6, H_8\}$. By the inductive hypothesis, we have $R(G') \geq \varphi(m, k-1)$.

$$\begin{aligned}
R(G) &= R(G') + \frac{1}{\sqrt{2d}} + (\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}})\sum_{i=1}^{d-1}\frac{1}{\sqrt{d(x_i)}} + \frac{1}{2} - \frac{1}{\sqrt{2}} \\
&\geq \varphi(m,k-1) + \frac{1}{\sqrt{2d}} + (\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}})\sum_{i=1}^{d-1}\frac{1}{\sqrt{d(x_i)}} + \frac{1}{2} - \frac{1}{\sqrt{2}} \\
&= \varphi(m,k) + \frac{m+k-2}{\sqrt{2(m+k-1)}} + \frac{1}{\sqrt{m+k-1}} - \frac{m+k-1}{\sqrt{2(m+k)}} \\
&\quad - \frac{1}{\sqrt{m+k}} + \frac{1}{\sqrt{2d}} + (\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}})\sum_{i=1}^{d-1}\frac{1}{\sqrt{d(x_i)}} \\
&\geq \varphi(m,k) + \frac{m+k-2}{\sqrt{2(m+k-1)}} + \frac{1}{\sqrt{m+k-1}} - \frac{m+k-1}{\sqrt{2(m+k)}} \\
&\quad - \frac{1}{\sqrt{m+k}} + \frac{1}{\sqrt{2d}} + (\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}})\frac{d-1}{\sqrt{2}} \\
&= \varphi(m,k) + (1 - \frac{1}{\sqrt{2}})(\frac{1}{\sqrt{m+k-1}} - \frac{1}{\sqrt{m+k}}) \\
&\quad + \frac{\sqrt{m+k-1} - \sqrt{m+k}}{\sqrt{2}} + \frac{\sqrt{d} - \sqrt{d-1}}{\sqrt{2}} \\
&\geq \varphi(m,k) + (1 - \frac{1}{\sqrt{2}})(\frac{1}{\sqrt{m+k-1}} - \frac{1}{\sqrt{m+k}}) \\
&\quad + \frac{\sqrt{m+k-1} - \sqrt{m+k}}{\sqrt{2}} + \frac{\sqrt{m+k} - \sqrt{m+k-1}}{\sqrt{2}} \\
&= \varphi(m,k) + (1 - \frac{1}{\sqrt{2}})(\frac{1}{\sqrt{m+k-1}} - \frac{1}{\sqrt{m+k}}) \\
&> \varphi(m,k).
\end{aligned}$$

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

Subcase 1. G has at least pendant vertex v which is adjacent to a vertex u of degree 2. Then there is a unique vertex $w \neq v$ such that $uw \in E(G)$. Let $|N(w) \bigcap PV| = r \leq 1$, $d(w) = d \leq m+k$, $d(x_1) = d(x_2) = \cdots = d(x_r) = 1$, $N(w) \setminus PV = \{x_{r+1}, x_{r+2}, \cdots, x_{d-1}, x_d = u\}$ and $d(x_i) = d_i \geq 2$, $i = r+1, r+2, \cdots, d$.

If $G' = G - u - v$, then $G' \in \mathcal{G}_{m-1,k} \setminus \{H_6, H_8\}$ by $k \geq 2$. By the inductive hypothesis, we have $R(G') \geq \varphi(m-1,k)$.

$$
\begin{aligned}
& R(G) \\
= \ & R(G') + r\left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d}}\right) + \left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}}\right)\sum_{i=r+1}^{d-1} \frac{1}{\sqrt{d(x_i)}} \\
& + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2d}} \\
\geq \ & R(G') + r\left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}}\right) + (d-r-1)\left(\frac{1}{\sqrt{2d}} - \frac{1}{\sqrt{2(d-1)}}\right) \\
& + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2d}} \\
\geq \ & \varphi(m-1,k) + r\left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}}\right) + (d-r-1)\left(\frac{1}{\sqrt{2d}} - \frac{1}{\sqrt{2(d-1)}}\right) \\
& + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2d}} \\
= \ & \varphi(m,k) + \frac{m+k-2}{\sqrt{2(m+k-1)}} + \frac{1}{\sqrt{m+k-1}} + \frac{m-2}{\sqrt{2}} + \frac{(1-\sqrt{2})k}{2} \\
& - \frac{m+k-1}{\sqrt{2(m+k)}} - \frac{1}{\sqrt{m+k}} - \frac{m-1}{\sqrt{2}} - \frac{(1-\sqrt{2})k}{2} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2d}} \\
& + r\left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}}\right) + (d-r-1)\left(\frac{1}{\sqrt{2d}} - \frac{1}{\sqrt{2(d-1)}}\right) \\
= \ & \varphi(m,k) + \frac{m+k-2}{\sqrt{2(m+k-1)}} + \frac{1}{\sqrt{m+k-1}} - \frac{m+k-1}{\sqrt{2(m+k)}} - \frac{1}{\sqrt{m+k}} \\
& + \frac{1}{\sqrt{2d}} + r\left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}}\right) + (d-r-1)\left(\frac{1}{\sqrt{2d}} - \frac{1}{\sqrt{2(d-1)}}\right) \qquad (2)
\end{aligned}
$$

Note that $r \leq 1$ by Lemma 2.2. If $r = 0$, then by (2)

$$
\begin{aligned}
& R(G) \\
\geq \ & \varphi(m,k) + \frac{m+k-2}{\sqrt{2(m+k-1)}} + \frac{1}{\sqrt{m+k-1}} - \frac{m+k-1}{\sqrt{2(m+k)}} - \frac{1}{\sqrt{m+k}} \\
& + \frac{1}{\sqrt{2d}} + (d-1)\left(\frac{1}{\sqrt{2d}} - \frac{1}{\sqrt{2(d-1)}}\right) \\
= \ & \varphi(m,k) + [f(m+k-2) - f(m+k-1)] - [f(d-2) - f(d-1)] \\
& + \left(\frac{1}{\sqrt{2}} - 1\right)\left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}}\right) \\
> \ & \varphi(m,k). \qquad \text{(by Lemma 2.3)}
\end{aligned}
$$

If $r = 1$, then by (2)

$$
\begin{aligned}
& R(G) \\
\geq\ & \varphi(m,k) + \frac{m+k-2}{\sqrt{2(m+k-1)}} + \frac{1}{\sqrt{m+k-1}} - \frac{m+k-1}{\sqrt{2(m+k)}} - \frac{1}{\sqrt{m+k}} \\
& + \frac{1}{\sqrt{2d}} + \frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}} + (d-2)\left(\frac{1}{\sqrt{2d}} - \frac{1}{\sqrt{2(d-1)}}\right) \\
=\ & \varphi(m,k) + \frac{m+k-2}{\sqrt{2(m+k-1)}} + \frac{1}{\sqrt{m+k-1}} - \frac{m+k-1}{\sqrt{2(m+k)}} - \frac{1}{\sqrt{m+k}} \\
& + \frac{d-1}{\sqrt{2d}} + \frac{1}{\sqrt{d}} - \frac{d-2}{\sqrt{2(d-1)}} - \frac{1}{\sqrt{d-1}} \\
=\ & \varphi(m,k) + [f(m+k-2) - f(m+k-1)] - [f(d-2) - f(d-1)] \\
\geq\ & \varphi(m,k) \qquad\qquad \text{(by Lemma 2.3)}
\end{aligned}
$$

The equality $R(G) = \varphi(m,k)$ holds if and only if equalities hold throughout the above inequalities, that is, if and only if $R(G') = \varphi(m-1,k)$, $d = m+k, d(x_1) = 1, d(x_2) = \cdots = d(x_{d-1}) = 2$. By the induction hypothesis, $G' \cong G_{m-1,k}$. Note that $G_{m-1,k}$ had a unique vertex of degree greater than 2, and hence $G \cong G_{m,k}$.

Subcase 2. Each pendant vertex in G is adjacent to a vertex with degree more than 2.

Let G_0 be the cactus obtained by deleting all pendant vertices of the cactus G. Since each pendant vertex in G is adjacent to a vertex with degree more than 2, then $\delta(G_0) \geq 2$. And each block of G_0 is either a cycle or an edge, G_0 has a cycle $C = u_1u_2\cdots u_tu_1$ with $2 \leq d(u_1) \leq m+k$ and $d(u_i) = 2$ for $i = 2, 3, \cdots, t$. So, we can find a cycle $C = u_1u_2\cdots u_tu_1$ in G with $2 \leq d(u_1) \leq m+k$ and $2 \leq d(u_i) \leq 3, i = 2, \cdots, t$.

Let t be the length of the cycle C and without loss of generality, assume the edge $u_1u_2 \notin M$.

Subcase 2.1. $t = 3$. Then $C = u_1u_2u_3u_1$.

Let $d(u_1) = d \leq m+k$, $N(u_1) = \{u_2, u_3, x_1, x_2, \cdots, x_{d-2}\}$, and $d(x_1) = d(x_2) = \cdots = d(x_r) = 1$, $d(x_i) \geq 2$, $i = r+1, \cdots, d-2$. $r \leq 1$.

Subcase 2.1.1. $d(u_2) = d(u_3) = 2$, then $u_2u_3 \in M$.

Let $G' = G - u_2 - u_3$, then $G' \in \mathscr{G}_{m-1,k-1}$.

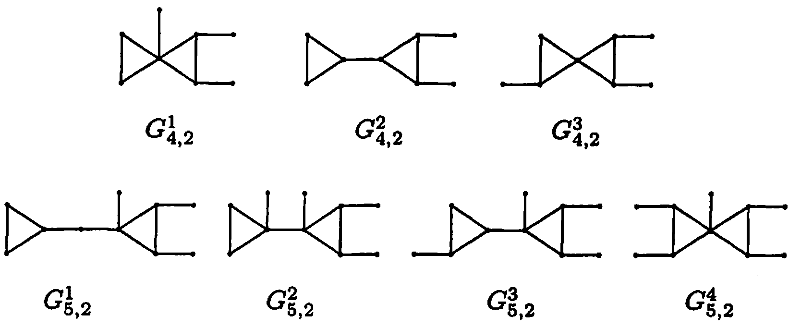


Figure 4. The graphs $G^1_{4,2}, G^2_{4,2}, G^1_{5,2}, G^2_{5,2}$.

If $G' = H_6$, then $m = 4$, $k = 2$ and $G \cong G^1_{4,2}$ or $G \cong G^2_{4,2}$. And $R(G^1_{4,2}) = 3.5841 > \varphi(4,2) = 3.5587$, $R(G^2_{4,2}) = 3.8045 > \varphi(4,2) = 3.5587$.

If $G' = H_8$, then $m = 5$, $k = 2$ and $G \cong G^1_{5,2}$ or $G \cong G^2_{5,2}$. And $R(G^1_{5,2}) = 4.5736 > \varphi(5,2) = 4.3958$, $R(G^2_{5,2}) = 4.5522 > \varphi(5,2) = 4.3958$, where $G^1_{4,2}, G^2_{4,2}, G^1_{5,2}, G^2_{5,2}$ are illustrated in Figure 4.

Otherwise, $G' \in \mathscr{G}_{m-1,k-1} \setminus \{H_6, H_8\}$. By the induction hypothesis, we have $R(G') \geq \varphi(m-1, k-1)$.

$$
\begin{aligned}
& R(G) \\
= \;& R(G') + \left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-2}}\right)\sum_{i=1}^{d-2}\frac{1}{\sqrt{d(x_i)}} + \frac{2}{\sqrt{2d}} + \frac{1}{2} \\
= \;& R(G') + r\left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-2}}\right) + \left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-2}}\right)\sum_{i=r+1}^{d-r-2}\frac{1}{\sqrt{d(x_i)}} \\
& + \frac{2}{\sqrt{2d}} + \frac{1}{2} \\
\geq \;& \varphi(m-1, k-1) + r\left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-2}}\right) + \left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-2}}\right)\sum_{i=r+1}^{d-r-2}\frac{1}{\sqrt{d(x_i)}}
\end{aligned}
$$

$$+\frac{2}{\sqrt{2d}}+\frac{1}{2}$$

$$= \varphi(m,k)+\frac{m+k-3}{\sqrt{2(m+k-2)}}+\frac{1}{\sqrt{m+k-2}}-\frac{m+k-1}{\sqrt{2(m+k)}}-\frac{1}{\sqrt{m+k}}$$

$$+r(\frac{1}{\sqrt{d}}-\frac{1}{\sqrt{d-2}})+(\frac{1}{\sqrt{d}}-\frac{1}{\sqrt{d-2}})\sum_{i=r+1}^{d-r-2}\frac{1}{\sqrt{d(x_i)}}+\frac{2}{\sqrt{2d}} \qquad (3)$$

If $r=0$, then by (3)

$$R(G)$$

$$\geq \varphi(m,k)+\frac{m+k-3}{\sqrt{2(m+k-2)}}+\frac{1}{\sqrt{m+k-2}}-\frac{m+k-1}{\sqrt{2(m+k)}}-\frac{1}{\sqrt{m+k}}$$

$$+(d-2)(\frac{1}{\sqrt{2d}}-\frac{1}{\sqrt{2(d-2)}})+\frac{2}{\sqrt{2d}}$$

$$= \varphi(m,k)+\frac{m+k-3}{\sqrt{2(m+k-2)}}+\frac{1}{\sqrt{m+k-2}}-\frac{m+k-1}{\sqrt{2(m+k)}}-\frac{1}{\sqrt{m+k}}$$

$$+\frac{\sqrt{d}-\sqrt{d-2}}{\sqrt{2}}$$

$$\geq \varphi(m,k)+\frac{m+k-3}{\sqrt{2(m+k-2)}}+\frac{1}{\sqrt{m+k-2}}-\frac{m+k-1}{\sqrt{2(m+k)}}-\frac{1}{\sqrt{m+k}}$$

$$+\frac{\sqrt{m+k}-\sqrt{m+k-2}}{\sqrt{2}}$$

$$= \varphi(m,k)+(1-\frac{1}{\sqrt{2}})(\frac{1}{\sqrt{m+k-2}}-\frac{1}{\sqrt{m+k}})$$

$$> \varphi(m,k).$$

If $r=1$, then by (3)

$$R(G)$$

$$\geq \varphi(m,k)+\frac{m+k-3}{\sqrt{2(m+k-2)}}+\frac{1}{\sqrt{m+k-2}}-\frac{m+k-1}{\sqrt{2(m+k)}}-\frac{1}{\sqrt{m+k}}$$

$$+(d-3)(\frac{1}{\sqrt{2d}}-\frac{1}{\sqrt{2(d-2)}})+\frac{1}{\sqrt{d}}-\frac{1}{\sqrt{d-2}}+\frac{2}{\sqrt{2d}}$$

$$= \varphi(m,k)+\frac{m+k-3}{\sqrt{2(m+k-2)}}+\frac{1}{\sqrt{m+k-2}}-\frac{m+k-1}{\sqrt{2(m+k)}}-\frac{1}{\sqrt{m+k}}$$

$$+\frac{d-1}{\sqrt{2d}}+\frac{1}{\sqrt{d}}-\frac{d-3}{\sqrt{2(d-2)}}+\frac{1}{\sqrt{d-2}}$$

$$= \varphi(m,k) + f(m+k-3) - f(m+k-1) - [f(d-3) - f(d-1)]$$
$$\geq \varphi(m,k).$$

The equality $R(G) = \varphi(m,k)$ holds if and only if equalities hold throughout the above inequalities, that is, if and only if $R(G') = \varphi(m-1,k-1)$, $d = m+k, d(x_1) = 1, d(x_2) = d(x_3) = \cdots = d(x_{d-2}) = 2$. Since $d(u_2) = d(u_3) = 2$, and each pendant vertex in G is adjacent to a vertex of degree more than 2. Thus we have that $G' \cong G_{k,k-1}$. And $R(G) = \varphi(k+1,k)$ if and only if $G \cong G_{k+1,k}$.

Subcase 2.1.2. $d(u_2) = d(u_3) = 3$, then G has two pendant vertices u_2', u_3' such that $u_2u_2' \in M, u_3u_3' \in M$.

Let $G' = G - u_2' - u_3'$. Then $G' \in \mathscr{G}_{m-1,k} \setminus \{H_6, H_8\}$ with a perfect matching $(M \cup \{u_2u_3\}) \setminus \{u_2u_2', u_3u_3'\}$.

$$\begin{aligned}
&R(G)\\
=\ & R(G') + 2(\frac{1}{\sqrt{3d}} - \frac{1}{\sqrt{2d}}) + \frac{1}{3} + \frac{2}{\sqrt{3}} - \frac{1}{2}\\
\geq\ & \varphi(m-1,k) + 2(\frac{1}{\sqrt{3d}} - \frac{1}{\sqrt{2d}}) + \frac{1}{3} + \frac{2}{\sqrt{3}} - \frac{1}{2}\\
=\ & \varphi(m,k) + \frac{m+k-2}{\sqrt{2(m+k-1)}} + \frac{1}{\sqrt{m+k-1}} - \frac{m+k-1}{\sqrt{2(m+k)}} - \frac{1}{\sqrt{m+k}}\\
& +(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}})\frac{2}{\sqrt{d}} + \frac{1}{3} + \frac{2}{\sqrt{3}} - \frac{1}{2} - \frac{1}{\sqrt{2}} \qquad (4)
\end{aligned}$$

If $d \geq 4$, then by (4)

$$\begin{aligned}
&R(G)\\
\geq\ & \varphi(m,k) + \frac{m+k-2}{\sqrt{2(m+k-1)}} + \frac{1}{\sqrt{m+k-1}} - \frac{m+k-1}{\sqrt{2(m+k)}} - \frac{1}{\sqrt{m+k}}\\
& +(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}})\frac{2}{\sqrt{4}} + \frac{1}{3} + \frac{2}{\sqrt{3}} - \frac{1}{2} - \frac{1}{\sqrt{2}}\\
=\ & \varphi(m,k) + \frac{m+k-2}{\sqrt{2(m+k-1)}} + \frac{1}{\sqrt{m+k-1}} - \frac{m+k-1}{\sqrt{2(m+k)}} - \frac{1}{\sqrt{m+k}}\\
& +\frac{1}{3} + \sqrt{3} - \frac{1}{2} - \sqrt{2}
\end{aligned}$$

$$
\begin{aligned}
&= \varphi(m,k) + [f(m+k-2) - f(m+k-1)] + \frac{1}{3} + \sqrt{3} - \frac{1}{2} - \sqrt{2} \\
&\geq \varphi(m,k) + \frac{4}{\sqrt{10}} + \frac{1}{\sqrt{5}} - \frac{5}{\sqrt{12}} - \frac{1}{\sqrt{6}} + \frac{1}{3} + \sqrt{3} - \frac{1}{2} - \frac{1}{\sqrt{2}} \\
&\qquad \text{(by Lemma 2.3 and } m+k \geq 6\text{)} \\
&> \varphi(m,k).
\end{aligned}
$$

If $d = 3$ and $m + k \geq 7$, then by (4),

$$
\begin{aligned}
&R(G) \\
&\geq \varphi(m,k) + \frac{m+k-2}{\sqrt{2(m+k-1)}} + \frac{1}{\sqrt{m+k-1}} - \frac{m+k-1}{\sqrt{2(m+k)}} - \frac{1}{\sqrt{m+k}} \\
&\quad +(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}})\frac{2}{\sqrt{3}} + \frac{1}{3} + \frac{2}{\sqrt{3}} - \frac{1}{2} - \frac{1}{\sqrt{2}} \\
&= \varphi(m,k) + [f(m+k-2) - f(m+k-1)] + (\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}})\frac{2}{\sqrt{3}} \\
&\quad +\frac{1}{3} + \frac{2}{\sqrt{3}} - \frac{1}{2} - \frac{1}{\sqrt{2}} \\
&\geq \varphi(m,k) + \frac{5}{\sqrt{12}} + \frac{1}{\sqrt{6}} - \frac{6}{\sqrt{14}} - \frac{1}{\sqrt{7}} + (\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}})\frac{2}{\sqrt{3}} + \frac{1}{3} + \frac{2}{\sqrt{3}} \\
&\quad -\frac{1}{2} - \frac{1}{\sqrt{2}} \qquad \text{(by Lemma 2.3 and } m+k \geq 7\text{)} \\
&> \varphi(m,k).
\end{aligned}
$$

If $d = 3$ and $m + k = 6$, then there exists the unique graph $G^2_{4,2}$, and $R(G^2_{4,2}) > \varphi(4,2)$ by subcase 2.1.1.

Subcase 2.1.3. $d(u_2) = 3$, $d(u_3) = 2$ or $d(u_2) = 2$, $d(u_3) = 3$, without loss of generality, we may assume that $d(u_2) = 3$, $d(u_3) = 2$. Then there is a pendant vertex u_2' such that $u_2u_2' \in M$. And $u_1u_3 \in M$, then $N(u_1) = \{u_2, u_3, x_1, x_2, \cdots, x_{d-2}\}$, $d(x_i) \geq 2, i = 1, 2, \cdots, d-2$.

Let $G' = G - u_2 - u_2'$, then $G' \in \mathscr{G}_{m-1,k-1}$.

If $G' = H_6$, then $m = 4$, $k = 2$, and $G \cong G^3_{4,2}$. $R(G^3_{4,2}) = 3.6931 > \varphi(4,2) = 3.5587$.

If $G' = H_8$, then $m = 5, k = 2$, and $G \cong G^3_{5,2}$ or $G \cong G^4_{5,2}$. $R(G^3_{5,2}) = 4.3958 > \varphi(5,2) = 4.3958$, $R(G^4_{5,2}) = 4.4561 > \varphi(5,2) = 4.3958$, where

$G^3_{4,2}, G^3_{5,2}, G^4_{5,2}$ are illustrated in Figure 4.

Otherwise, $G' \in \mathcal{G}_{m-1,k-1} \setminus \{H_6, H_8\}$. By the induction hypothesis, we have

$$\begin{aligned}
& R(G) \\
= \; & R(G') + (\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}})\sum_{i=1}^{d-2}\frac{1}{\sqrt{d(x_i)}} + (\frac{1}{\sqrt{3}} + \frac{1}{\sqrt{2}})\frac{1}{\sqrt{d}} + \frac{1}{\sqrt{6}} \\
& + \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{d-1}} \\
\geq \; & \varphi(m-1, k-1) + (\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}})\sum_{i=1}^{d-2}\frac{1}{\sqrt{d(x_i)}} + (\frac{1}{\sqrt{3}} + \frac{1}{\sqrt{2}})\frac{1}{\sqrt{d}} \\
& + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{d-1}} \\
= \; & \varphi(m,k) + \frac{m+k-3}{\sqrt{2(m+k-2)}} + \frac{1}{\sqrt{m+k-2}} - \frac{m+k-1}{\sqrt{2(m+k)}} - \frac{1}{\sqrt{m+k}} \\
& + (d-2)(\frac{1}{\sqrt{2d}} - \frac{1}{\sqrt{2(d-1)}}) + (\frac{1}{\sqrt{3}} + \frac{1}{\sqrt{2}})\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}} \\
& + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} - \frac{1-\sqrt{2}}{2} \\
= \; & \varphi(m,k) + [f(m+k-3) - f(m+k-1)] - [f(d-2) - f(d-1)] \\
& + (\frac{1}{\sqrt{3}} - 1)\frac{1}{\sqrt{d}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{1}{2} \\
= \; & \varphi(m,k) + [f(m+k-2) - f(m+k-1)] - [f(d-2) - f(d-1)] \\
& + [f(m+k-3) - f(m+k-2)] + (\frac{1}{\sqrt{3}} - 1)\frac{1}{\sqrt{d}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{1}{2} \\
> \; & \varphi(m,k) + \frac{3}{\sqrt{8}} + \frac{1}{\sqrt{4}} - 4\frac{1}{\sqrt{10}} - \frac{1}{\sqrt{5}} + \frac{1}{3} + \frac{1}{\sqrt{6}} - \frac{1}{2}
\end{aligned}$$

(If $d \geq 3$, then the inequality holds by Lemma 2.3 and $m+k \geq 6$; If $d = 2$, the graph $G \cong G_{2,1}$, then it is not difficult to check that the inequality holds.)

$$> \varphi(m,k).$$

Subcase 2.2. $t \geq 4$.

Let the cycle $C = u_1u_2 \cdots u_tu_1$. Without loss of generality, we may assume $u_1u_2 \notin M$.

Subcase 2.2.1. $d(u_2) = 3$. Then there exists a pendant vertex u_2' such that the edge $u_2u_2' \in M$, u_3 is another neighbor of the vertex u_2, and $d(u_3) = 2$ or $d(u_3) = 3$.

Let $G' = G - u_2 - u_2' + u_1u_3$. Then $G' \in \mathscr{G}_{m-1,k} \setminus \{H_6, H_8\}$ by $k \geq 2$. By the induction hypothesis, we have

$$
\begin{aligned}
& R(G) \\
= \;& R(G') + \frac{1}{\sqrt{3d}} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{3d(u_3)}} - \frac{1}{\sqrt{dd(u_3)}} \\
\geq \;& \varphi(m-1,k) + \frac{1}{\sqrt{3d}} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{3d(u_3)}} - \frac{1}{\sqrt{dd(u_3)}} \\
= \;& \varphi(m,k) + \frac{m+k-2}{\sqrt{2(m+k-1)}} + \frac{1}{\sqrt{m+k-1}} - \frac{m+k-1}{\sqrt{2(m+k)}} - \frac{1}{\sqrt{m+k}} \\
& + \frac{1}{\sqrt{3d}} + \frac{1}{\sqrt{3d(u_3)}} - \frac{1}{\sqrt{dd(u_3)}} + \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \qquad (5)
\end{aligned}
$$

If $d(u_3) = 3$, then by (5),

$$
\begin{aligned}
& R(G) \\
\geq \;& \varphi(m,k) + \frac{m+k-2}{\sqrt{2(m+k-1)}} + \frac{1}{\sqrt{m+k-1}} - \frac{m+k-1}{\sqrt{2(m+k)}} - \frac{1}{\sqrt{m+k}} \\
& + \frac{1}{\sqrt{3}} + \frac{1}{3} - \frac{1}{\sqrt{2}} \\
= \;& \varphi(m-1,k) + \frac{1}{\sqrt{3}} + \frac{1}{3} \\
> \;& \varphi(m,k) \qquad \text{(by Lemma 2.6)}
\end{aligned}
$$

If $d(u_3) = 2$, then by (5),

$$
\begin{aligned}
& R(G) \\
\geq \;& \varphi(m,k) + \frac{m+k-2}{\sqrt{2(m+k-1)}} + \frac{1}{\sqrt{m+k-1}} - \frac{m+k-1}{\sqrt{2(m+k)}} - \frac{1}{\sqrt{m+k}} \\
& + \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}}\right)\frac{1}{\sqrt{d}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \\
\geq \;& \varphi(m,k) + \frac{m+k-2}{\sqrt{2(m+k-1)}} + \frac{1}{\sqrt{m+k-1}} - \frac{m+k-1}{\sqrt{2(m+k)}} - \frac{1}{\sqrt{m+k}}
\end{aligned}
$$

$$\begin{aligned} & +(\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{2}})\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{6}}+\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{2}} \\ = & \ \varphi(m-1,k)+\frac{2}{\sqrt{6}}+\frac{1}{\sqrt{3}}-\frac{1}{2} \\ > & \ \varphi(m,k) \qquad \text{(by Lemma 2.6)} \end{aligned}$$

Subcase 2.1.2. $d(u_2)=2$. Since $u_1u_2 \notin M$, then $u_2u_3 \in M$. Let $G' = G - u_3u_4 + u_2u_4$. Then $G' \in \mathscr{G}_{m,k} \setminus \{H_6, H_8\}$ and

$$\begin{aligned} R(G)-R(G') &= (\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}})\frac{1}{\sqrt{d}}+1-\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{3d(u_4)}} \\ &\geq (\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}})\frac{1}{\sqrt{d}}+1-\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{6}} \\ &> 0 \end{aligned}$$

If $t-1 \geq 4$, then $R(G') > \varphi(m,k)$ by subcase 2.2.1, and $R(G) > \varphi(m,k)$; If $t-1=3$, then $R(G') > \varphi(m,k)$ by subcase 2.1.3, and $R(G) > \varphi(m,k)$.

So the proof is completed.

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