A sharp lower bound of the Randić index of cacti with \( r \) pendants

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Abstract

The Randić index of a simple connected graph \( G \) is defined as \( \sum_{uv \in E(G)} (d(u)d(v))^{-1/2} \). In this paper, we present a sharp lower bound on the Randić index of cacti with \( r \) pendants.

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1. Introduction

A single number that can be used to characterize some property of the graph of a molecule is called a topological index. For quite some time there has been rising interest in the field of computational chemistry in topological indices that capture the structural essence of compounds. The interest in topological indices is mainly related to their use in nonempirical quantitative structure–property relationships and quantitative structure–activity relationships. One of the most important topological indices is the well-known branching index introduced by Randić [9] which is defined as the sum of certain bond contributions calculated from the vertex degree of the hydrogen suppressed molecular graphs.

For a molecular graph \( G = (V(G), E(G)) \) where \( V(G) \) and \( E(G) \) denote the set of vertices and the set of edges of \( G \) respectively, the Randić index of \( G \) is defined as

\[
R(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-1/2},
\]

where \( d(\cdot) \) denotes the degree of the corresponding vertex. The Randić index and some of its variants have received intensive attention recently. Much effort has been spent to derive nontrivial bounds for the Randić index of molecular graphs. For general graphs, a lower bound of \( R(G) \) was given by Bollobás and Erdös [1], while an upper bound was recently presented in [5]. In [8], Pavlović gave an upper bound of the zeroth-order Randić index for general graphs. Also an interesting linear programming approach was proposed in [2] to find the lower bounds of certain generalized Randić index for general graphs. A lot of research focused on special classes of graphs. For example, trees with the

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largest and the smallest Randić index were considered in [4,10,11]. In [3], Lu et al. gave a sharp lower bound for the Randić index of trees with \( n \) vertices and \( k \) pendants where \( 2 \leq k \leq n - 1 \). An upper bound of the Randić index of trees with \( n \) vertices and \( k \) pendants where \( n \geq 3k - 2 \) was given in [12]. Gao and Lu [3] obtained sharp lower and upper bounds for the Randić index of unicyclic graphs. Pan et al. [7] gave a sharp lower bound for unicyclic graphs with \( k \) pendants.

A graph \( G \) is called a cactus if each block of \( G \) is either an edge or a cycle. Lu et al. [6] gave a sharp lower bound on the Randić index of cacti with given number of cycles. In this paper we will investigate the Randić index of connected cacti with \( r \) pendants and obtain a sharp lower bound on the Randić index of such graphs.

Before proceeding, we introduce some notations. The maximum degree of \( G \) is denoted by \( \Delta(G) \). An \( i \)-vertex of \( G \) means a vertex with degree \( i \). As usual, \( C_n \) denotes the cycle on \( n \) vertices, \( P_n \) denotes the path on \( n \) vertices, and \( S_n \) denotes the star on \( n \) vertices. A pendant of a graph is a vertex with degree 1. We use \( L(n, r) \) to denote the set of connected cacti with \( r \) pendants.

It is straightforward to compute

\[
R(G(n, r)) = \begin{cases} 
\frac{n - 1 - r}{4} + \frac{n - 1 - r}{\sqrt{2(n - 1)}} + \frac{r}{\sqrt{n - 1}} & \text{if } n - r \text{ is odd,} \\
\frac{n - r}{4} + \frac{n - 2 - r}{\sqrt{2(n - 2)}} + \frac{r}{\sqrt{n - 2}} & \text{if } n - r \text{ is even,}
\end{cases}
\]

when \( r \leq n - 3 \). In this paper, we are going to show that \( G(n, r) \) has the minimum Randić index in the family \( L(n, r) \).

\section{Lemma}

Let

\[
f(n, r) = \begin{cases} 
\frac{n - 1 - r}{4} + \frac{n - 1 - r}{\sqrt{2(n - 1)}} + \frac{r}{\sqrt{n - 1}} & \text{if } n - r \text{ is odd,} \\
\frac{n - r}{4} + \frac{n - 2 - r}{\sqrt{2(n - 2)}} + \frac{r}{\sqrt{n - 2}} & \text{if } n - r \text{ is even.}
\end{cases}
\]

\begin{lemma}
\[ f(n - 1, r) + \frac{1}{2} \geq f(n, r), \]
\end{lemma}

with equality if and only if \( n - r \) is even.
Proof. By the definition of \( f(n, r) \), we have

\[
f(n - 1, r) + \frac{1}{2} = \begin{cases} 
\frac{n - 2 - r}{4} + \frac{n - 2 - r}{\sqrt{2(n - 2)}} + \frac{r}{\sqrt{n - 2}} + \frac{1}{2} & \text{if } n - 1 - r \text{ is odd}, \\
\frac{n - 1 - r}{4} + \frac{n - 3 - r}{\sqrt{2(n - 3)}} + \frac{r}{\sqrt{n - 3}} + \frac{1}{2} & \text{if } n - 1 - r \text{ is even.}
\end{cases}
\]

If \( n - r \) is even, then \( n - 1 - r \) is odd. Hence we have

\[
f(n - 1, r) + \frac{1}{2} = \frac{n - 2 - r}{4} + \frac{n - 2 - r}{\sqrt{2(n - 2)}} + \frac{r}{\sqrt{n - 2}} + \frac{1}{2} = \frac{n - r}{4} + \frac{n - 2 - r}{\sqrt{2(n - 2)}} + \frac{r}{\sqrt{n - 2}} = f(n, r).
\]

If \( n - r \) is odd, then \( n - 1 - r \) is even and we have

\[
f(n - 1, r) + \frac{1}{2} = \frac{n - 1 - r}{4} + \frac{n - 3 - r}{\sqrt{2(n - 3)}} + \frac{r}{\sqrt{n - 3}} + \frac{1}{2} = f(n, r) + \frac{1}{2} \left( \sqrt{n - 3} - \sqrt{n - 1} \right) + 1 \]

\[
+ r \left( 1 - \frac{1}{\sqrt{2}} \right) \left( \frac{1}{\sqrt{n - 3}} - \frac{1}{\sqrt{n - 1}} \right)
\]

\[
\geq f(n, r) + \frac{1}{2} - \frac{\sqrt{2}}{\sqrt{n - 3} + \sqrt{n - 1}} > f(n, r) \quad (\text{since } n \geq 5). \quad \square
\]

Lemma 2.2. Let \( n, r \) be two integers with \( 1 \leq r \leq n - 3 \) and \( d \) be an integer with \( 2 \leq d \leq n - 3 \). We have the following two inequalities:

\[
(1) \quad A = \frac{n - 1 - r}{\sqrt{2(n - 2)}} - \frac{n - 1 - r}{\sqrt{2(n - 1)}} + \frac{r - 1}{\sqrt{n - 2}} - \frac{r}{\sqrt{n - 1}}
\]

\[
+ \frac{1}{\sqrt{d}} - \frac{\sqrt{d - 1}}{\sqrt{2\sqrt{d} + \sqrt{d - 1}}} > 0.
\]

\[
(2) \quad B = \frac{n - 2 - r}{\sqrt{2(n - 3)}} - \frac{n - 2 - r}{\sqrt{2(n - 2)}} + \frac{r - 1}{\sqrt{n - 3}} - \frac{r}{\sqrt{n - 2}}
\]

\[
+ \frac{1}{\sqrt{d}} - \frac{\sqrt{d - 1}}{\sqrt{2\sqrt{d} + \sqrt{d - 1}}} > 0.
\]
Proof.

\[
\frac{1}{\sqrt{d}} - \frac{\sqrt{d - 1}}{\sqrt{2}\sqrt{d}(\sqrt{d} + \sqrt{d - 1})} = \frac{1}{\sqrt{d}} - \frac{1}{\sqrt{2}\sqrt{d}} \frac{1}{\sqrt{d - 1} + 1} \\
\geq \frac{1}{\sqrt{d}} - \frac{1}{\sqrt{2}\sqrt{d}} \frac{1}{2} \\
= \left(1 - \frac{1}{\sqrt{2}}\right) \frac{1}{\sqrt{d}} \\
\geq \left(1 - \frac{1}{\sqrt{2}}\right) \frac{1}{\sqrt{n - 3}} \\
> \left(1 - \frac{1}{\sqrt{2}}\right) \frac{1}{\sqrt{n - 2}}.
\]

Hence

\[
A = \left(\frac{n - 1 - r}{\sqrt{2}} + r\right) \frac{1}{\sqrt{n - 2}\sqrt{n - 1}(\sqrt{n - 2} + \sqrt{n - 1})} - \frac{1}{\sqrt{n - 2}} \\
+ \frac{1}{\sqrt{d}} - \frac{\sqrt{d - 1}}{\sqrt{2}\sqrt{d}(\sqrt{d} + \sqrt{d - 1})} \\
\geq \frac{n - 1}{\sqrt{2}} \frac{1}{\sqrt{n - 2}\sqrt{n - 1}(\sqrt{n - 2} + \sqrt{n - 1})} \\
- \frac{1}{\sqrt{n - 2}} + \left(1 - \frac{1}{\sqrt{2}}\right) \frac{1}{\sqrt{n - 2}} \\
= \frac{1}{\sqrt{2}} \frac{1}{\sqrt{n - 2}} \left(\frac{n - 2}{n - 1} + 1\right) - \frac{1}{2\sqrt{2}} \frac{1}{\sqrt{n - 2}} \\
\geq \frac{1}{\sqrt{2}} [2\sqrt{n - 2} \frac{1}{\sqrt{n - 2}} - \frac{1}{2\sqrt{2}} \frac{1}{\sqrt{n - 2}} = 0.
\]

\[
B = \left(\frac{n - 2 - r}{\sqrt{2}} + r\right) \frac{1}{\sqrt{n - 3}\sqrt{n - 2}(\sqrt{n - 3} + \sqrt{n - 2})} \\
- \frac{1}{\sqrt{n - 3}} + \frac{1}{\sqrt{d}} - \frac{\sqrt{d - 1}}{\sqrt{2}\sqrt{d}(\sqrt{d} + \sqrt{d - 1})} \\
\geq \frac{n - 2}{\sqrt{2}} \frac{1}{\sqrt{n - 3}\sqrt{n - 2}(\sqrt{n - 3} + \sqrt{n - 2})} - \frac{1}{\sqrt{n - 3}} + \left(1 - \frac{1}{\sqrt{2}}\right) \frac{1}{\sqrt{n - 3}} \\
= \frac{1}{\sqrt{2}} \frac{1}{\sqrt{n - 3}} \left(\frac{n - 2}{n - 1} + 1\right) - \frac{1}{2\sqrt{2}} \frac{1}{\sqrt{n - 3}} \\
\geq \frac{1}{\sqrt{2}} [2\sqrt{n - 3} \frac{1}{\sqrt{n - 3}} - \frac{1}{2\sqrt{2}} \frac{1}{\sqrt{n - 3}} = 0. \quad \Box
\]

Lemma 2.3. Let $a, b$ be two integers with $3 \leq a \leq b$. Let $g(a, b) = (\sqrt{a} + \sqrt{b} + 1)(1 - \frac{1}{\sqrt{ab}}) + 1$. Then $g(a, b) > g(2, a + b - 2)$.

Proof. It suffices to show $g(a, b) > g(a - 1, b + 1)$.

Notice that $(a - 1)(b + 1) < ab$ since $(a - 1)(b + 1) = ab - (a + b) < 0$. Hence

$$1 - \frac{1}{\sqrt{(a - 1)(b + 1)}} < 1 - \frac{1}{\sqrt{ab}}$$

(1)

Since $(\sqrt{a - 1} + \sqrt{b + 1})^2 - (\sqrt{a} + \sqrt{b})^2 = 2(\sqrt{(a - 1)(b + 1)} - \sqrt{ab}) < 0$, we have

$$\sqrt{a - 1} + \sqrt{b + 1} < a + \sqrt{b}.$$ 

(2)

Therefore, by Eqs. (1) and (2), we have

$$(\sqrt{a} + \sqrt{b} + 1) \left(1 - \frac{1}{\sqrt{ab}}\right) + 1$$

$$> (\sqrt{a - 1} + \sqrt{b + 1} + 1) \left(1 - \frac{1}{\sqrt{(a - 1)(b + 1)}}\right) + 1.$$ 

That is $g(a, b) > g(a - 1, b + 1)$.

3. A sharp lower bound

Our main result is the following:

Theorem 3.1. Let $G$ be a connected cactus on $n \geq 3$ vertices with $r$ pendants. Then

1. $R(G) \geq \sqrt{n - 1}$ if $r = n - 1$ with equality if and only if $G = S_n$;
2. $R(G) \geq (n - 3)/\sqrt{n - 2} + 1/2\sqrt{n - 2} + 1/\sqrt{2}$ if $r = n - 2$ with equality if and only if $G$ is the graph obtained by inserting one degree two vertex in one edge of the start $S_{n-1}$;
3. $R(G) \geq f(n, r)$ if $r \leq n - 3$ with equality if and only if $G = G(n, r)$.

Theorem 3.1(1) is obvious since if $r = n - 1$, then $G = S_n$. Now we prove (2).

Proof of Theorem 3.1(2). Since $G$ has $n - 2$ pendants, it has exactly two vertices, say $x, y$, of degree at least 2 and $G$ is a tree. Since $G$ is connected and all vertices other than $x, y$ are of degree 1, we have $n \geq 4$, and $x$ and $y$ are adjacent, and each vertex $z \in V(G) \setminus \{x, y\}$ is either adjacent to $x$ or adjacent to $y$ but not both. Let $a = d(x)$ and $b = d(y)$. Then $a + b = n$. Without loss of generality, assume $a \leq b$. If $a = 2$, then $G$ is the graph obtained by inserting a degree 2 vertex in one edge of the star $S_{n-1}$. Hence $R(G) = n - 3/\sqrt{2(n - 2)} + 1/\sqrt{2(n - 3)} + 1/\sqrt{2} = g(2, n - 2)$. If $a > 3$, then

$$R(G) = \frac{a - 1}{\sqrt{a}} + \frac{b - 1}{\sqrt{b}} + \frac{1}{\sqrt{ab}}$$

$$= (\sqrt{a} + \sqrt{b} - 1)(1 - \frac{1}{\sqrt{ab}}) + 1$$

$$= g(a, b) \quad \text{(Here $(a, b)$ is the function defined in Lemma 2.3)}$$

$$> g(2, a + b - 2) = g(2, n - 2) \quad \text{(by Lemma 2.3)}.$$ 

This proves (2) of Theorem 3.1.
Theorem 3.1(3) is equivalent to the following theorem.

**Theorem 3.2.** Let $G$ be a connected cactus on $n \geq 3$ vertices with $0 \leq r \leq n - 3$ pendants. If $G \neq G(n, r)$, then

$$R(G) > R(G, r) = f(n, r)$$

$$= \begin{cases} \frac{n - 1 - r}{4} + \frac{n - 1 - r}{\sqrt{2(n - 1)}} + \frac{r}{\sqrt{n - 1}} & \text{if } n - r \text{ is odd}, \\ \frac{n - r}{4} + \frac{n - 2 - r}{\sqrt{2(n - 2)}} + \frac{r}{\sqrt{n - 2}} & \text{if } n - r \text{ is even.} \end{cases}$$

**Proof.** We prove by contradiction. Let $G$ be a counterexample such that

1. $n$ is as small as possible.
2. subject to (1), $r$ is as small as possible.
3. subject to (1) and (2), $R(G)$ is as small as possible.

Then $r \leq n - 3$ and $R(G) \leq f(n, r)$.

**Claim 1.** $n \geq 5$ and $\Delta(G) \leq n - 2$.

If $n = 3$, then $G = G(3, 0)$ since $r \leq n - 3 = 0$, a contradiction to the assumption. If $n = 4$, then $r \leq n - 3 = 1$. Then either $G = C_4 = G(4, 0)$ or $G = G(4, 1)$, a contradiction again to the assumption that $G \neq G(n, r)$. Hence $n \geq 5$.

If $\Delta(G) = n - 1$, then $G = G(n, r)$, a contradiction. Hence $\Delta(G) \leq n - 2$.

**Claim 2.** No vertex in $G$ is adjacent to two or more 1-vertices.

Suppose the contrary that $u$ is adjacent to two 1-vertices, say $v, w$. Let $d = d(u)$ and $G' = G + vw$. Then $G' \in \mathcal{L}(n, r - 2)$ and

$$R(G) = R(G') - \frac{1}{2} + \frac{2}{\sqrt{d}} - \frac{2}{\sqrt{2d}}.$$  

By the choice of $G$, we have $R(G') \geq f(n, r - 2)$ with equality if and only if $G' = G(n, r - 2)$. Note that $n - r$ and $n - (r - 2)$ have the same parity. Hence $R(G) \geq f(n, r - 2) - \frac{1}{2} + 2/\sqrt{d} - 2/\sqrt{2d}$. That is,

$$R(G) \geq \begin{cases} \frac{n - 1 - (r - 2)}{4} + \frac{n - 1 - (r - 2)}{\sqrt{2(n - 1)}} \\ + \frac{r - 2}{\sqrt{n - 1}} - \frac{1}{2} + \frac{2}{\sqrt{d}} - \frac{2}{\sqrt{2d}} & \text{if } n - r \text{ is odd,} \\ \frac{n - (r - 2)}{4} + \frac{n - 2 - (r - 2)}{\sqrt{2(n - 2)}} \\ + \frac{r - 2}{\sqrt{n - 2}} - \frac{1}{2} + \frac{2}{\sqrt{d}} - \frac{2}{\sqrt{2d}} & \text{if } n - r \text{ is even.} \end{cases}$$
adjacent to two 1-vertices and is adjacent to at least two 1-vertices, a contradiction to Claim 2. Hence, Claim 3.

Therefore, \( R(G) > f(n, r) \). Hence \( R(G) = f(n, r) \). In order for this to happen, we must have \( d = n - 2 \), \( n - r \) is even, and \( G' = G(n, r - 2) \). But this clearly leads to \( G = G(n, r) \), a contradiction. This proves Claim 2.

Claim 3. \( r \leq n - 4 \).

Otherwise, assume \( r = n - 3 \). If \( n \geq 7 \), then \( n - 3 \geq 4 > 3 \). By the pigeon hole principle, there must be a vertex which is adjacent to at least two 1-vertices, a contradiction to Claim 2. Hence \( n \leq 6 \). If \( n = 5 \), then \( r = 2 \). Since no vertex is adjacent to two 1-vertices and \( G \) has exactly two 1-vertices, we have either \( G \) is a path \( P = x_1x_2x_3x_4x_5 \) on five vertices or \( G = P + x_2x_4 \). It is easy to check that and \( R(P) > f(5, 2) \) and \( R(P + x_2x_4) > f(5, 2) \). If \( n = 6 \), then \( r = 3 \). Then by Claim 2, \( G \) must be one of the two graphs in Fig. 2 and \( R(G) > f(6, 3) \). This proves Claim 3.

Claim 4. \( G \) does not contain a path \( P = x_1x_2x_3x_4 \) with \( d(x_2) = d(x_3) = 2 \).

Otherwise, assume \( G \) contains a path \( P = x_1x_2x_3x_4 \) with \( d(x_2) = d(x_3) = 2 \). Let \( G' = G - x_3 + x_2x_4 \in \mathcal{G}(n - 1, r) \). Then \( R(G) = R(G') + \frac{1}{2} \). Since \( r \leq n - 4 = (n - 1) - 3 \), by the choice of \( G \), we have \( R(G') > f(n - 1, r) \) with equality if and only if \( G' = G(n - 1, r) \).

If \( R(G') > f(n - 1, r) \), then \( R(G) > f(n - 1, r) + \frac{1}{2} \geq f(n, r) \) by Lemma 2.1, a contradiction. Thus \( R(G') = f(n - 1, r) \) and \( G' = G(n - 1, r) \). By Lemma 2.1, \( n - r \) is even otherwise \( R(G) = f(n - 1, r) + \frac{1}{2} > f(n, r) \). Since \( n - r \) and \( n - r - 2 \) have the same parity and \( G' = G(n - 1, r) \), each block of \( G' \) is either a triangle or an edge. Since
Hence we have that the three vertices \( x_1, x_3, x_4 \) induces a triangle in \( G' \). Thus \( x_1x_2x_3x_4 \) is a 4-cycle of \( G \). Since \( G' = G(n - 1, r) \) and \( (n - 1) - r \) is odd, we have \( G = G(n, r) \), a contradiction. This completes the proof of Claim 4.

**Claim 5.** Each vertex of degree one is adjacent to a \((\geq n - 2)\)-vertex.

Otherwise, assume there is a 1-vertex, say \( x \), which is adjacent to a vertex, say \( y \), of degree \( d \leq n - 3 \). Consider \( G - x \). If \( d = 2 \), let \( z \) be the other neighbor of \( y \). Then \( G - x \in G(n - 1, r) \) and by Claim 4 \( d(z) \geq 3 \). By Claim 3, \( r \leq (n - 1) - 3 \).

Hence

\[
R(G) = R(G - x) + \frac{1}{\sqrt{d}} + \frac{1}{\sqrt{2d(z)}} - \frac{1}{\sqrt{d(z)}} \\
\geq f(n - 1, r) + \frac{1}{\sqrt{2} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}}} - \frac{1}{2}.
\]

Since \( \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{3}} - \frac{1}{2} > 0 \), by Lemma 2.1, we have \( R(G) > f(n, r) \), a contradiction.

Now assume \( d \geq 3 \). Then \( G - x \in G(n - 1, r - 1) \). Denote \( N(y) = \{ x, y_2, \ldots, y_d \} \). By Claim 2, \( d(y_i) \geq 2 \) for each \( 2 \leq i \leq d \).

Hence

\[
R(G) = R(G - x) + \frac{1}{\sqrt{d}} + \sum_{i=2}^{d} \left( \frac{1}{\sqrt{d(y_i)}} - \frac{1}{\sqrt{d(y_i)(d - 1)}} \right) \\
\geq f(n - 1, r - 1) + \frac{1}{\sqrt{d}} - \frac{\sqrt{d - 1}}{\sqrt{2}\sqrt{d}(\sqrt{d} + \sqrt{d - 1})}.
\]

Hence we have

\[
R(G) \geq \begin{cases} 
\frac{n - r}{4} + \frac{n - 1 - r}{\sqrt{2(n - 2)}} + \frac{r - 1}{\sqrt{n - 2}} & \text{if } n - r \text{ is odd}, \\
\frac{n - r}{4} + \frac{n - 2 - r}{\sqrt{2(n - 3)}} + \frac{r - 1}{\sqrt{n - 3}} & \text{if } n - r \text{ is even}, \\
\frac{n - r}{4} + \frac{n - 1 - r}{\sqrt{2(n - 2)}} + \frac{r - 1}{\sqrt{n - 2}} & \text{if } n - r \text{ is odd}, \\
\frac{n - r}{4} + \frac{n - 2 - r}{\sqrt{2(n - 3)}} + \frac{r - 1}{\sqrt{n - 3}} & \text{if } n - r \text{ is even}.
\end{cases}
\]

\[
\geq \begin{cases} 
\begin{cases} 
f(n, r) + A & \text{if } n - r \text{ is odd}, \\
f(n, r) + B & \text{if } n - r \text{ is even},
\end{cases}
\end{cases}
\]

...
where $A$, $B$ are defined in Lemma 2.2. Since $d \leq n - 3$, by Lemma 2.2, we have $R(G) > f(n, r)$, a contradiction. This proves Claim 5.

**Claim 6.** $\delta(G) \geq 2$, where $\delta(G)$ is the minimum degree of $G$.

We prove by contradiction. Suppose $G$ has a vertex of degree 1. By Claim 1 that $A(G) \leq n - 2$ and Claim 5 that each 1-vertex is adjacent to a $(\geq n - 2)$-vertex, we have $A(G) = n - 2$. Let $x$ be a vertex of degree $A(G) = n - 2$ and $N(x) = \{x_1, \ldots, x_{n-2}\}$. Let $y \neq x$ be the only vertex not adjacent to $x$.

Since each block of $G$ is either a cycle or an edge, each $x_i$ is adjacent to at most one vertex in $N(x)$. Hence, each neighbor of $y$ is of degree at most three. By Claim 5, $d(y) \geq 2$. Let $N(y) = \{y_1, y_2, \ldots, y_s\}$ where $s = d(y)$.

If $s \geq 3$, let $y_1, y_2, y_3$ be three distinct neighbors of $y$. Then the subgraph induced by $y, y_1, y_2, y_3, x$ is 2-connected and is not a cycle. This is a contradiction to the fact that each block of $G$ is either a cycle or an edge. Therefore $s = d(y) = 2$. Similarly we can show that $d(y_1) = d(y_2) = 2$. Hence we have a path $xy_1y_2y_3$ with $d(y_1) = d(y) = 2$, a contradiction to Claim 4. This contradiction completes the proof of Claim 6.

**Claim 7.** $G$ has a triangle $C = x_1x_2x_3x_1$ with $d(x_1) = 3$ and $d(x_2) = d(x_3) = 2$.

Since $r = 0$ by Claim 6 and each block of $G$ is either a cycle or an edge, $G$ has a cycle $C = x_1x_2\ldots x_t x_1$ with $d(x_1) \geq 2$ and $d(x_i) = 2$ for each $i = 2, \ldots, t$. By Claim 4, we have $t \leq 3$. It implies $t = 3$ and $d(x_2) = d(x_3) = 2$. Now we prove that $d(x_1) = 3$. Since $G$ is connected and $n \geq 5$, $d(x_1) \geq 3$. So, it suffices to show that $d(x_1) \leq 3$. Suppose the contrary that $d(x_1) > 4$. By Claim 1, $d(x_1) \leq n - 2$. If $d(x_1) = n - 2$. Then $x_1$ is adjacent to all vertices in $G$ except one, say $y$ and by Claim 6 $d(y) \geq 2$. Similar to the argument in Claim 6, we can obtain an contradiction. Now we can assume that $d = d(x_1) \leq n - 3$. Let $N(x_1) = \{x_2, x_3, u_3, \ldots, u_d\}$ and $G' = G - x_2 - x_3$. Then $G' \in \mathcal{P}(n - 2, 0)$. Then

$$R(G) = R(G') + \frac{1}{2} + \frac{2}{\sqrt{2d}} + \sum_{i=3}^{d} \left( \frac{1}{\sqrt{d(u_i)d}} - \frac{1}{\sqrt{d(u_i)(d-2)}} \right).$$

Since $n$ and $n - 2$ have the same parity, we have

$$R(G) \geq f(n, 0) + \left\{ \begin{array}{ll}
\frac{2}{\sqrt{2d}} + \frac{d-2}{\sqrt{2}} \left( \frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-2}} \right) + \frac{\sqrt{n-3}}{\sqrt{2}} - \frac{\sqrt{n-1}}{\sqrt{2}} & \text{if } n \text{ is odd}, \\
\frac{2}{\sqrt{2d}} + \frac{d-2}{\sqrt{2}} \left( \frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-2}} \right) + \frac{\sqrt{n-4}}{\sqrt{2}} - \frac{\sqrt{n-2}}{\sqrt{2}} & \text{if } n \text{ is even}.
\end{array} \right.$$  

So, it suffices to prove

$$\frac{2}{\sqrt{2d}} + \frac{d-2}{\sqrt{2}} \left( \frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-2}} \right) + \frac{\sqrt{n-3}}{\sqrt{2}} - \frac{\sqrt{n-1}}{\sqrt{2}} > 0,$$

$$\frac{2}{\sqrt{2d}} + \frac{d-2}{\sqrt{2}} \left( \frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-2}} \right) + \frac{\sqrt{n-4}}{\sqrt{2}} - \frac{\sqrt{n-2}}{\sqrt{2}} > 0.$$

Since $\sqrt{n-3}/\sqrt{2} - \sqrt{n-1}/\sqrt{2} > \sqrt{n-4}/\sqrt{2} - \sqrt{n-2}/\sqrt{2}$, we only need to show the second inequality. Define $g(x) = 2/\sqrt{x} + (x - 2)/(\sqrt{x} - 1/\sqrt{x} - 4/\sqrt{x} - \sqrt{n-4} - \sqrt{n-2})$ where $3 \leq x \leq n - 3$. Then

$$g(x) = (\sqrt{x} - \sqrt{n-2}) - (\sqrt{n-2} - \sqrt{n-4}) > 0 \text{ since } x \leq n - 3.$$

Therefore, $R(G) \geq f(n, 0) + g(d)/\sqrt{2} > f(n, 0)$, a contradiction. This proved Claim 7.
The final step: By Claim 7, take a triangle \( C = uvw \) in \( G \) where \( d(u) = 3 \) and \( d(v) = d(w) = 2 \). Let \( N(u) = \{x, v, w\} \). Then either \( d(x) = 2 \) and both neighbors of \( x \) are of degree at least three by Claim 4 or \( d(x) \geq 3 \). If \( d(x) = 2 \) and both neighbors of \( x \) are of degree at least three, we consider the graph \( G - \{u, v, w, x\} \) which is in \( \mathcal{L}(n-4, 0) \). If \( d(x) \geq 3 \), we consider the graph \( G - \{u, v, w\} \) which is in \( \mathcal{L}(n-3, 0) \). In the following we only consider the case that \( d(x) \geq 3 \).

Let \( N(x) = \{u, x, \ldots, x_d\} \) where \( d = d(x) \). Since \( x \) is not adjacent to \( v, w \), we have \( d \leq n-2 \). Consider the graph \( G' = G - \{u, v, w\} \in \mathcal{L}'(n-3, 0) \). Then

\[
R(G) = R(G') + \frac{1}{2} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3d}} + \left( \sqrt{d} - \sqrt{d-1} \right) \sum_{i=2}^{d} \frac{1}{\sqrt{d(d-1) + 1}}
\geq f(n-3, 0) + \frac{1}{2} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3d}} - \frac{d-1}{\sqrt{d}} \left( \frac{1}{\sqrt{d(d-1) + 1}} \right)
= f(n-3, 0) + \frac{1}{2} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3d}} - \frac{d-1}{\sqrt{d}} \left( \frac{1}{\sqrt{d(d-1) + 1}} \right)
\geq f(n-3, 0) + \frac{1}{2} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3d}} - \frac{1}{\sqrt{d}} \left( \frac{1}{\sqrt{d(d-1) + 1}} \right)
> f(n-3, 0) + \frac{1}{2} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3d}} - \frac{1}{\sqrt{d}} \left( \frac{1}{\sqrt{d(2)}} \right)
= f(n-3, 0) + \frac{1}{2} + \frac{2}{\sqrt{6}} + \left( \frac{1}{\sqrt{3}} - \frac{1}{2\sqrt{2}} \right) \frac{1}{\sqrt{d}}
\geq f(n-3, 0) + \frac{1}{2} + \frac{2}{\sqrt{6}} + \left( \frac{1}{\sqrt{3}} - \frac{1}{2\sqrt{2}} \right) \frac{1}{\sqrt{n-2}}
\text{ (since } d \leq n-2 \).

Thus,

\[
R(G) > \begin{cases} 
\frac{n-4}{4} + \frac{\sqrt{n-4}}{\sqrt{2}} + \frac{1}{2} + \frac{2}{\sqrt{6}} \\
\quad + \left( \frac{1}{\sqrt{3}} - \frac{1}{2\sqrt{2}} \right) \frac{1}{\sqrt{n-2}} & \text{if } n-3 \text{ is odd,} \\
\frac{n-3}{4} + \frac{\sqrt{n-5}}{\sqrt{2}} + \frac{1}{2} + \frac{2}{\sqrt{6}} \\
\quad + \left( \frac{1}{\sqrt{3}} - \frac{1}{2\sqrt{2}} \right) \frac{1}{\sqrt{n-2}} & \text{if } n-3 \text{ is even.}
\end{cases}
\]

Therefore

\[
R(G) > \begin{cases} 
\frac{n-3}{4} + \frac{\sqrt{n-5}}{\sqrt{2}} + \frac{1}{2} + \frac{2}{\sqrt{6}} + \left( \frac{1}{\sqrt{3}} - \frac{1}{2\sqrt{2}} \right) \frac{1}{\sqrt{n-2}} & \text{if } n \text{ is odd,} \\
\frac{n-4}{4} + \frac{\sqrt{n-4}}{\sqrt{2}} + \frac{1}{2} + \frac{2}{\sqrt{6}} + \left( \frac{1}{\sqrt{3}} - \frac{1}{2\sqrt{2}} \right) \frac{1}{\sqrt{n-2}} & \text{if } n \text{ is even.}
\end{cases}
\]
If \( n \) is odd, then \( n \geq 7 \) and

\[
R(G) > n - \frac{1}{4} + \frac{\sqrt{n-1}}{\sqrt{2}} + \frac{\sqrt{n-5}}{\sqrt{2}} - \frac{\sqrt{n-1}}{\sqrt{2}} + \frac{2}{\sqrt{6}} + \left( \frac{1}{\sqrt{3}} - \frac{1}{2\sqrt{2}} \right) \frac{1}{\sqrt{n-2}}
\]

\[
= f(n, 0) + \frac{2}{\sqrt{6}} - \frac{2\sqrt{2}}{\sqrt{n-5} + \sqrt{n-1}} + \left( \frac{1}{\sqrt{3}} - \frac{1}{2\sqrt{2}} \right) \frac{1}{\sqrt{n-2}}.
\]

For \( n \geq 7 \), it is easy to check that

\[
\frac{2}{\sqrt{6}} - \frac{2\sqrt{2}}{\sqrt{n-5} + \sqrt{n-1}} + \left( \frac{1}{\sqrt{3}} - \frac{1}{2\sqrt{2}} \right) \frac{1}{\sqrt{n-2}} > 0.
\]

Therefore \( R(G) > f(n, 0) \) if \( n \) is odd, a contradiction. Hence \( n \) must be even. We then have

\[
R(G) > n - \frac{3}{4} + \frac{\sqrt{n-2}}{\sqrt{2}} + \frac{\sqrt{n-4}}{\sqrt{2}} - \frac{\sqrt{n-2}}{\sqrt{2}} - \frac{1}{2} + \frac{2}{\sqrt{6}} + \left( \frac{1}{\sqrt{3}} - \frac{1}{2\sqrt{2}} \right) \frac{1}{\sqrt{n-2}}
\]

\[
= f(n, 0) + \frac{2}{\sqrt{6}} - \frac{1}{2} - \frac{\sqrt{2}}{\sqrt{n-4} + \sqrt{n-2}} + \left( \frac{1}{\sqrt{3}} - \frac{1}{2\sqrt{2}} \right) \frac{1}{\sqrt{n-2}}.
\]

Again with simple calculations, one can easily check that for \( n \geq 6 \),

\[
\frac{2}{\sqrt{6}} - \frac{1}{2} - \frac{\sqrt{2}}{\sqrt{n-4} + \sqrt{n-2}} + \left( \frac{1}{\sqrt{3}} - \frac{1}{2\sqrt{2}} \right) \frac{1}{\sqrt{n-2}} > 0.
\]

Hence \( R(G) > f(n, 0) \), a contradiction. This completes the proof of the theorem. \( \square \)

References