On the Randić Index of Unicyclic Graphs with Fixed Diameter

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Abstract

The Randić index $R(G)$ of a graph $G$ is the sum of the weights $\frac{1}{\sqrt{d(u)d(v)}}$ of all edges $uv$ of $G$, where $d(u)$ denotes the degree of the vertex $u$. In this paper, we give sharp lower bounds of Randić index of unicyclic graphs with $n$ vertices and diameter $d$, which partly confirms a conjecture in \cite{1}(MATCH Commun. Math. Comput. Chem. 58(2007) 83-102) by Aouchiche, Hansen and Zheng.

1. Introduction

The Randić index of an organic molecule whose molecular graph is $G$ is defined in \cite{27} as

$$R(G) = \sum_{u,v} \frac{1}{\sqrt{d(u)d(v)}}.$$
where \( d(u) \) denotes the degree of the vertex \( u \) of \( G \) and the summation goes over all pairs of adjacent vertices of \( G \). The research background of Randić index together with its generalization appears in chemistry or mathematical chemistry and can be found in the literature (see [11]-[13]).

First we introduce some graph notations used in this paper. We only consider finite, undirected and simple graphs. Other undefined terminologies and notations may refer to [3]. For a vertex \( x \) of a graph \( G \), we denote the neighborhood and the degree of \( x \) by \( N(x) \) and \( d(x) \), respectively. Let \( S \subseteq V(G) \), we will use \( G - S \) to denote the graph that arises from \( G \) by deleting the vertices in \( S \) together with their incident edges. If \( S = \{ v \} \), we write \( G - v \) for \( G - \{ v \} \). We will use \( G - uv \) to denote the graph that arises from \( G \) by deleting the edge \( uv \in E(G) \). Similarly, \( G + uv \) is a graph that arises from \( G \) by adding an edge \( uv \notin E(G) \), where \( u, v \in V(G) \). A pendent vertex is a vertex of degree 1. For two vertices \( u, v \in V(G) \) (\( u \neq v \)), the distance between \( u \) and \( v \), denoted by \( d_G(u, v) \), is the number of edges in a shortest path joining \( u \) and \( v \) in \( G \). The diameter of a graph \( G \), denoted by \( \text{diam}(G) \), is the maximum distance between any two vertices of \( G \).

Unicyclic graphs are connected graphs with \( n \) vertices and \( n \) edges. Let \( V_0 = \{ v : v \) is a pendent vertex of \( G \} \) and \( V_1 = \bigcup_{v \in V_0} N(v) \).

Recently, there are many results concerning (general) Randić index of graphs (see [1], [2], [4]-[10], [14]-[26], [28]-[29]). In [1], Aouchiche, Hansen and Zheng proposed the following conjecture.

**Conjecture A.** For any connected graph on \( n \geq 3 \) vertices with Randić index \( R \) and diameter \( d \),

\[
R - d \geq \sqrt{2} - \frac{n+1}{2} \quad \text{and} \quad \frac{R}{d} \geq \frac{n-3+2\sqrt{2}}{2n-2},
\]

with equality if and only if \( G \) is the path \( P_n \).

Li and Zhao [17] considered the relation between the Randić index and the diameter of trees and given the following result.

**Theorem B ([17]).** Let \( T \) be a tree of order \( n \) with diameter \( d \geq 3 \), then

\[
R(T) \geq \frac{n - d + \frac{1}{\sqrt{2}}}{\sqrt{n - d} + 1} + \frac{d - 3 + \sqrt{2}}{2}
\]

(1)

and equality in (1) if and only if \( T \cong S_{n,d}^* \), where \( S_{n,d}^* \) be a tree of order \( n \) obtained from a star \( S_{n-d+1} \) by attaching a path of order \( d - 1 \) to the center of \( S_{n-d+1} \).
If \( \text{diam}(T) = 2 \) for a tree \( T \) of order \( n \geq 3 \), then \( T \cong S_n \), and then
\[
R(T) - 2 = \sqrt{n-2} - 2 \geq \sqrt{2} - \frac{n+1}{2}, \quad \frac{R(T)}{2} = \frac{\sqrt{n-1}}{2} \geq \frac{n-3+2\sqrt{2}}{2n-2}
\]
and equality holds if and only if \( n = 3 \), i.e., \( T \cong P_3 \). Let \( F(d) = \frac{n-d+1}{\sqrt{n-d+1}} + \frac{d-3+\sqrt{2}}{2} \), \( d \geq 3 \). Then
\[
\frac{F(d)}{d} - \frac{1}{2} = \frac{n-d+1}{d\sqrt{n-d+1}} - \frac{3-\sqrt{2}}{2d} \geq \frac{1+\frac{1}{\sqrt{2}}}{d\sqrt{2}} - \frac{3-\sqrt{2}}{2d} = \frac{\sqrt{2} - 1}{d} > 0.
\]
Note that
\[
\frac{\partial(F(d) - d)}{\partial d} = -\frac{1}{2}(n-d+1)^{-\frac{3}{2}} \left( n-d+2 - \frac{1}{\sqrt{2}} \right) - \frac{1}{2} < 0,
\]
\[
\frac{\partial F(d)}{\partial d} = \frac{1}{d} \left[ -\frac{1}{2} (n-d+1)^{-\frac{3}{2}} \left( n-d+2 - \frac{1}{\sqrt{2}} \right) + \frac{1} {2} - \frac{F(d)}{d} \right] < 0.
\]
Hence by (1), we have
\[
R(T) - d \geq F(d) - d \geq F(n-1) - (n-1) = \sqrt{2} - \frac{n+1}{2},
\]
\[
\frac{R(T)}{d} \geq \frac{F(d)}{d} \geq \frac{F(n-1)}{n-1} = \frac{n-3+2\sqrt{2}}{2n-2}.
\]
Moreover, the equalities hold if and only if \( d = n-1 \), that is, \( G \) is the path \( P_n \).

**Note C.** *The Conjecture A is true for trees.*

In the following, we will show that the Conjecture A is true for unicyclic graphs. Let \( \mathcal{U}_{n,d} = \{ G : G \) is a unicyclic graph with \( n \) vertices and diameter \( d \} \), where \( 1 \leq d \leq n-2 \). Then \( \mathcal{U}_{n,1} = \{ C_3 \} \) and \( \mathcal{U}_{n,2} = \{ U_n^*, C_4, C_5 \} \), where \( n \geq 4 \) and \( U_n^* \) is the graph obtained from star \( S_n \) by adding a new edge between its two pendant vertices. It is easy to check \( R(C_n) \geq R(U_n^*) \).

Denote
\[
\varphi(n, d) = \begin{cases} 
\frac{n-4+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{6}}}{\sqrt{n-2}}, & d = 3, \\
\frac{n-5+\sqrt{2}}{\sqrt{n-3}}, & d = 4, \\
\frac{n-d-1+\sqrt{2}}{\sqrt{n-d+1}} + \frac{d-5}{2} + \frac{1+\sqrt{3}}{\sqrt{2}}, & d \geq 5.
\end{cases}
\]

In this paper, we mainly show the the following theorem in Section 2, which partly confirms Conjecture A.
Theorem D. Let $G \in \mathcal{U}_{n,d}$, $3 \leq d \leq n - 2$. Then
\[ R(G) \geq \varphi(n, d) \]  
(2) 
and equality in (2) holds if and only if $G \cong U_{n}^{d}$, where $U_{n}^{d}$ are shown in Fig. 1.

Denote $\varphi(n) = \sqrt{2} - \frac{n + 1}{2}$ and $\psi(n) = \frac{n - 3 + 2\sqrt{2}}{2(n - 2)}$, where $n \geq 3$. Then
\[
\begin{align*}
(R(C_3) - 1) - \varphi(3) &= \frac{5}{2} - \sqrt{2} > 0, \\
\frac{R(C_3)}{1} - \psi(3) &= \frac{3 - \sqrt{2}}{2} > 0, \\
R(U_{n}^{*}) - 2 - \varphi(n) &= \frac{n - 3 + \sqrt{2}}{\sqrt{n - 1}} + \frac{1}{2} - 2 - \sqrt{2} + \frac{n + 1}{2} > 0 \text{ for } n \geq 4, \\
\frac{R(U_{n}^{*})}{2} - \psi(n) &= \frac{n - 3 + \sqrt{2}}{2\sqrt{n - 1}} + \frac{1}{4} - \frac{n - 3 + 2\sqrt{2}}{2n - 2} > 0 \text{ for } n \geq 4, \\
\varphi(n, 3) - 3 - \varphi(n) &= \frac{n - 4 + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}}}{\sqrt{n - 2}} + \frac{n - 5 + \frac{1 + \sqrt{2} - 2\sqrt{3}}{\sqrt{6}}}{\sqrt{2}} > 0 \text{ for } n \geq 5, \\
\frac{\varphi(n, 3)}{3} - \psi(n) &= \frac{n - 4 + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}}}{3n - 2} - \frac{n - 3 + 2\sqrt{2}}{2n - 2} + \frac{1 + \sqrt{2}}{3\sqrt{6}} > 0 \text{ for } n \geq 5, \\
\varphi(n, 4) - 4 - \varphi(n) &= \frac{n - 4 + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}}}{\sqrt{n - 3}} + \frac{n - 7}{2} + \frac{2 + \sqrt{2} - \frac{\sqrt{12}}{\sqrt{6}}}{\sqrt{3}} > 0 \text{ for } n \geq 6, \\
\frac{\varphi(n, 4)}{4} - \psi(n) &= \frac{n - 4 + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}}}{4\sqrt{n - 3}} - \frac{n - 3 + 2\sqrt{2}}{2n - 2} + \frac{2 + \sqrt{2}}{4\sqrt{6}} > 0 \text{ for } n \geq 6.
\end{align*}
\]

Note that, for $d \geq 5$, $\frac{\varphi(n,d)}{d} - \frac{1}{2} = \frac{n - d - 1 + \sqrt{2}}{d\sqrt{n - d + 1}} + \frac{\sqrt{6} + \sqrt{2} - 5}{2d} \geq \frac{2 + \sqrt{2}}{2d} - \frac{\sqrt{6} + \sqrt{2}}{2d} > 0$. Hence
\[
\frac{\partial(\varphi(n,d) - d)}{\partial d} = -\frac{1}{2} (n - d + 1)^{-\frac{1}{2}} - \frac{1}{2} (2 - \sqrt{2}) (n - d + 1)^{-\frac{3}{2}} - \frac{1}{2} < 0,
\]
\[
\frac{\partial(\varphi(n,d) - d)}{\partial d} = \frac{1}{d} \left[ -\frac{1}{2} (n - d + 1)^{-\frac{3}{2}} (n - d + 3 - \sqrt{2}) + \frac{1}{2} - \frac{\varphi(n,d)}{d} \right] < 0.
\]

Thus by (2),
\[
R(G) - d \geq \varphi(n, d) - d \geq \varphi(n, n - 2) - (n - 2) = \frac{5 + \sqrt{3} + \sqrt{2}}{\sqrt{6}} - \frac{n + 3}{2} > \varphi(n),
\]
where \( \zeta \) both \( f \) \( x \) monotone increasing in \( k \) only if \( n \)

\[
\frac{R(G)}{d} \geq \frac{\varphi(n,d)}{d} \geq \frac{\varphi(n,n-2)}{n-2} = \frac{5+\sqrt{7}+\sqrt{3}}{\sqrt{6}} + \frac{n-7}{2} > \frac{n-3+2\sqrt{2}}{2n-2} = \psi(n).
\]

**Note E.** The Conjecture A is true for unicyclic graphs.

### 2. Proof of Theorem D

We first give some lemmas that will be used in the proof of our result.

**Lemma 1.** (i) Let \( f(x) = \frac{x+\sqrt{2}-2}{\sqrt{x}} \) and \( g(x) = \frac{x^2+1/\sqrt{x}+1/\sqrt{3}}{} \), where \( x \geq 3 \). Then both \( f(x) - f(x+1) \) and \( g(x) - g(x) \) are strictly monotone increasing in \( x \geq 3 \);

(ii) Let \( h_1(x) = \frac{x}{2} - \frac{x^2+n}{2\sqrt{x}} \) and \( h_2(x) = \frac{x^2+k_0}{\sqrt{x-4}} - \frac{x^2}{2\sqrt{x}} \), where \( k_0 > 3(\sqrt{3}-1) \), \( k_0 \leq \frac{1}{\sqrt{q}} \) and \( l_0 \geq \sqrt{2} \) are three constant numbers. Then \( h_1(x) \) and \( h_2(x) \) are strictly monotone increasing in \( x \geq 3 \);

**Proof.** (i) Follows from, for \( x \geq 3 \),

\[
\frac{d^2 f(x)}{dx^2} = -x^{-\frac{3}{2}}(x + 6 - 3\sqrt{2}) < 0, \quad \frac{d^2 g(x)}{dx^2} = -x^{-\frac{3}{2}}(x + 6 - \frac{3}{\sqrt{2}} - \frac{3}{\sqrt{3}}) < 0.
\]

(ii) Note that, for \( x \geq 3 \),

\[
\frac{dh_1(x)}{dx} = \frac{1}{2}x^{-\frac{3}{2}} (x\sqrt{x} - x + x_0) > 0;
\]

\[
\frac{dh_2(x)}{dx} = \frac{1}{2} \left[ (x-1)^{-\frac{3}{2}} - x^{-\frac{3}{2}} \right] + \frac{1}{2}k_0(x-1)^{-\frac{3}{2}} - \frac{2l_0}{2}x^{-\frac{3}{2}}
\]

\[
> \frac{1}{4}x^{-\frac{3}{2}} + \frac{1}{2}k_0(x-1)^{-\frac{3}{2}} - \frac{2l_0}{2}x^{-\frac{3}{2}}
\]

where \( \zeta \in (x-1,x) \). Hence (ii) follows.

**Lemma 2.** (i) For \( d = 4 \) and \( n \geq d + 2 \geq 6 \), and \( d \geq 5 \) and \( n \geq d + 3 \geq 7 \),

\[
\frac{n-6}{2} + \frac{2\sqrt{2}+2}{\sqrt{3}} \geq \varphi(n,d) \quad \text{and equality holds if and only if} \quad d = 4 \quad \text{and} \quad n = 6;
\]

(ii) For \( d \geq 5 \) and \( n \geq d + 2 \), \( \frac{n-7}{2} + \frac{5+\sqrt{3}+\sqrt{2}}{\sqrt{6}} \geq \varphi(n,d) \) and equality holds if and only if \( n = d + 2 \geq 7 \);

**Proof.** (i) Let \( h_1(x) = \frac{x}{2} - \frac{x^2+n}{2\sqrt{x}} \). Then by Lemma 1(ii),

\[
\frac{n-6}{2} + \frac{2\sqrt{2}+2}{\sqrt{3}} - \varphi(n,4) = h_1(n-3) + \frac{1+\sqrt{2}}{\sqrt{3}} - \frac{3}{2} \geq h_1(3) + \frac{1+\sqrt{2}}{\sqrt{3}} - \frac{3}{2} = 0;
\]
and for \( d \geq 5, \)
\[
\frac{n - 6}{2} + \frac{2\sqrt{2} + 2}{\sqrt{3}} - \varphi(n, d) = h_1(n - d + 1) + \frac{2}{\sqrt{3}} + \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{2}} - 1 \\
\geq h_1(4)\frac{2}{\sqrt{3}} + \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{2}} - 1 > 0.
\]

From the above arguments, the equality holds if and only if \( d = 4 \) and \( n - 3 = 3. \)

(ii) Let \( h_1(x) \) defined in (i). Then
\[
\frac{n - 7}{2} + \frac{5 + \sqrt{3} + \sqrt{2}}{\sqrt{6}} - \varphi(n, d) \\
= h_1(n - d + 1) + \frac{5 + \sqrt{3} + \sqrt{2}}{\sqrt{6}} - \frac{3}{2} - \frac{3}{\sqrt{6}} - \frac{1}{\sqrt{2}} \\
\geq h_1(3) + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{3}{2} = 0.
\]

From the above arguments, the equality holds if and only if \( n - d + 1 = 3. \)

Let \( H_1, H_2 \) be two connected graphs with \( V(H_1) \cap V(H_2) = \{ v \} \). Let \( H_1vH_2 \) be a graph defined by \( V(G) = V(H_1) \cup V(H_2), V(H_1) \cap V(H_2) = \{ v \} \) and \( E(G) = E(H_1) \cup E(H_2). \)

**Lemma 3** [28]. Let \( H \) be a connected graph and \( T_l \) be a tree of order \( l \) with \( V(H) \cap V(T_l) = \{ v \} \). Then
\[
R(HvT_l) \geq R(HvK_{1,l-1})
\]
and equality holds if and only if \( HvT_l \cong HvK_{1,l-1} \), where \( v \) is identified with the center of the star \( K_{1,l-1} \) in \( HvK_{1,l-1} \).

**Fig. 2**

**Lemma 4** [17]. Let \( G_{s,t} \) be a graph shown in Fig. 2, where \( H \) is a connected graph. If \( s \geq t \geq 2 \) and \( d_G(u) \geq d_G(v) \), then
\[
R(G_{s,t}) > R(G_{s+1,t-1}).
\]

**Lemma 5** [7]. Let \( G \) be a unicyclic graph of order \( n \). Then \( R(G) \leq R(C_n) \) and equality holds if and only if \( G \cong C_n. \)
Let $P_{n,l}$ (see Fig. 3) be unicyclic graphs of order $n$ obtained from a cycle $C_{n-l}$ by attaching a path of length $l$ ($l \geq 1$) at one vertex of $C_{n-l}$, and the only pendent vertex of $P_{n,l}$ is called the tail of $P_{n,l}$. Let $Q_{n,i,j}$ (see Fig. 3) be those unicyclic graphs of order $n$ and diameter $d$ obtained from a cycle $C_{n-i-j}$ by attaching a path $v_1v_2\ldots v_iv_{i+1}$ of length $i$ and a path $v_{d+1-i}v_{d+2-j}\ldots v_dv_{d+1}$ of length $j$ ($i, j \geq 1$) at two vertices of the cycle, respectively. Let $R_{n,i,l}$ (see Fig. 3) be a unicyclic graph of order $n$ and diameter $d$ obtained from a graph $P_{n-d,l}$ by attaching a path $v_1v_2\ldots v_i$ of length $i-1$ and a path $v_iv_{i+1}\ldots v_{d+1}$ of length $d+1-i$ at the tail of $P_{n-d,l}$, respectively.

![Diagram of graphs](image)

**Fig. 3**

**Lemma 6.** Suppose that $G \in \mathcal{U}_{n,d}$ ($3 \leq d \leq n-2$) with $V_0 \neq \emptyset$. If $G - v \in \mathcal{U}_{n-1,d-1}$ for any $v \in V_0$, then

$$R(G) \geq \varphi(n, d).$$

Moreover, the equality in (3) holds if and only if $d = n - 2$ and $G \cong U_{d+2}^d$.

**Proof.** Since $G$ is unicyclic graph and for any $v \in V_0$, $G - v \in \mathcal{U}_{n-1,d-1}$, we have $G \cong P_{n,l}$, or $G \cong Q_{n,i,j}$, or $G \cong R_{n,i,l}$.

**Case 1.** $G \cong P_{n,l}$.

In this case, if $d = 4$, then $n \geq 6$, and thus by Lemma 1(ii), we have

$$R(G) = \begin{cases}
\frac{n-4+\sqrt{2}+\sqrt{6}}{2} = \varphi(n, 4) + \frac{n-4}{2} - \frac{n-5+\sqrt{2}+\sqrt{6}}{\sqrt{n-3}} \geq \varphi(n, 4), & l > 1, \\
n\frac{\sqrt{2}}{\sqrt{3}} + \frac{n-3}{2} = \varphi(n, 4) + \frac{n-3}{2} - \frac{n-5+\sqrt{2}}{\sqrt{n-3}} > \varphi(n, 4), & l = 1.
\end{cases}$$

If $d \geq 5$, then $n - d \geq 2$, and thus by Lemma 1(ii), we have

$$R(G) = \begin{cases}
\frac{n-4+\sqrt{2}+\sqrt{6}}{2} = \varphi(n, d) + \frac{n-d+1}{2} - \frac{n-d+1+\sqrt{2}}{\sqrt{n-d+1}} > \varphi(n, d), & l > 1, \\
n\frac{\sqrt{2}}{\sqrt{3}} + \frac{n-3}{2} = \varphi(n, d) + \frac{n-d+2}{2} - \frac{n-d+1+\sqrt{2}}{\sqrt{n-d+1}} + \frac{\sqrt{2}+\sqrt{6}}{\sqrt{n-d+1}} \geq \varphi(n, d), & l = 1.
\end{cases}$$

**Case 2.** $G \cong Q_{n,i,j}$. 


Subcase 2.1. \( i + j = d \).

In this subcase, \( i, j \geq 2 \) by the assumption. Thus by Lemma 2,
\[
R(G) = \frac{n - 6 + 4\sqrt{2}}{2} = \left(\frac{n - 6}{2} + \frac{2\sqrt{2} + 2}{\sqrt{3}}\right) + 2\sqrt{2} - \frac{2\sqrt{2} + 2}{\sqrt{3}} > \varphi(n, d).
\]

Subcase 2.2. \( i + j = d - 1 \).

In this subcase, if \( d = 3 \), then \( G \cong U_3^3 \) by the assumption, and thus the result holds. If \( d \geq 4 \), then by Lemma 2, we have
\[
R(G) = \begin{cases} 
\frac{n - 6 + \sqrt{2} + \sqrt{6}}{2} + \frac{\sqrt{3} + 1}{3} > \frac{n - 6}{2} + \frac{2\sqrt{2} + 2}{\sqrt{3}} \geq \varphi(n, d), & i = 1; \\
\frac{n - 7 + 2\sqrt{2}}{2} + \frac{\sqrt{6} + 1}{3} > \frac{n - 7}{2} + \frac{5 + \sqrt{3} + \sqrt{2}}{\sqrt{6}} \geq \varphi(n, d), & i > 1.
\end{cases}
\]

Subcase 2.3. \( i + j \leq d - 2 \).

In this subcase, we have \( d \geq 4 \), and \( n - d \geq 3 \) when \( d \geq 5 \). By Lemma 2, we have
\[
R(G) = \begin{cases} 
\frac{n - 6 + \sqrt{2} + \sqrt{6}}{2} + \frac{\sqrt{3} + 1}{3} > \frac{n - 6}{2} + \frac{2\sqrt{2} + 2}{\sqrt{3}} \geq \varphi(n, d), & i = 1; \\
\frac{n - 7 + 2\sqrt{2}}{2} + \frac{\sqrt{6} + 1}{3} > \frac{n - 7}{2} + \frac{5 + \sqrt{3} + \sqrt{2}}{\sqrt{6}} \geq \varphi(n, d), & i > 1.
\end{cases}
\]

The equalities in (4) and (5) hold only if \( G \cong U_4^4 \) and \( G \cong U_d^d \), respectively.

Case 3. \( G \cong R_{n,p,i} \).

In this case, \( i, d - i + 1 \geq 2 \). Thus from the above calculations, we have
\[
R(G) = \begin{cases} 
\frac{n - 7 + \sqrt{2}}{2} + \frac{1 + \sqrt{6}}{3} > \varphi(n, d), & l = 1; \\
\frac{n - 8 + 2\sqrt{2} + \sqrt{6}}{2} > \varphi(n, d), & l > 1.
\end{cases}
\]

Therefore the proof of the theorem is complete.

\[\square\]

Theorem 7. Suppose that \( G \in \mathcal{U}_{n,3}, n \geq 5 \). Then
\[
R(G) \geq \frac{n - 4 + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}}}{\sqrt{n - 2}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}}
\]
and equality in (6) holds if and only if \( G \cong U_n^3 \).

\textbf{Proof.} We apply induction on \( n \). If \( n = 5 \), then the theorem holds by Lemma 6. So in the following proof, we assume that \( n \geq 6 \).

By Lemmas 5 and 6, we may assume that \( V_0 \neq \emptyset \) and there exists a vertex \( u_0 \in V_0 \) such that \( G - u_0 \) containing a path of length 3. Let \( u \) be the neighbor vertex of \( u_0 \) in \( G \). We consider two cases.
Case 1. $|N(u) \setminus V_0| \geq 2$.

Let $d(u) = t$. Then $3 \leq t \leq n - 2$. Denote $N(u) \cap V_0 = \{v_1, \ldots, v_r\}$ and $N(u) \setminus V_0 = \{x_1, \ldots, x_{t-r}\}$. Then $r \geq 1$, $t-r = |N(u) \setminus V_0| \geq 2$ and all $d(x_i) = d_i \geq 2$. Let $G' = G - v_1$. Then $G' \in \mathcal{U}_{n-1,3}$. Note that

$$R(G) = R(G') + \frac{r}{\sqrt{t}} - \frac{r - 1}{\sqrt{t-1}} + \sum_{i=1}^{t-r} \frac{1}{\sqrt{d_i}} \left( \frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}} \right).$$

(7)

Subcase 1.1 $d_i \geq 3$ for some $i$, $1 \leq i \leq t-r$.

Assume, without loss of generality, that $d_1 \geq 3$. By (7), we have

$$R(G) \geq R(G') + \frac{r}{\sqrt{t}} - \frac{r - 1}{\sqrt{t-1}} + \left( \frac{1}{\sqrt{3}} + \frac{t-r-1}{\sqrt{2}} \right) \left( \frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}} \right)
= \varphi(n-1,3) + \frac{t-2 + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}}}{\sqrt{t}} - \frac{t-3 + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}}}{\sqrt{t-1}}
+ (t-r-2) \left( \frac{1}{\sqrt{2}} - 1 \right) \left( \frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}} \right)
\geq \varphi(n,3) + \frac{n-5 + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}}}{\sqrt{n-3}} - \frac{n-4 + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}}}{\sqrt{n-2}}
+ \frac{t-2 + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}}}{\sqrt{t}} - \frac{t-3 + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}}}{\sqrt{t-1}}.
\tag{8}
$$

where $g(x) = \frac{x-2 + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}}}{\sqrt{x}}$. The last inequality follows by Lemma 1(i) as $t \leq n - 2$.

In order for the equality to hold, all inequalities in the above argument should be equalities. Thus we have

$$R(G') = \varphi(n-1,3), \quad t = n-2, \quad t-r = 2 \quad \text{and} \quad d_1 = 3, \ d_2 = 2.$$

By the induction hypothesis, $G' \cong U_{n-1}^3$. Hence $G \cong U_n^3$ and it is easy to check $R(U_n^3) = \varphi(n,3)$.

Subcase 1.2 $d_i = 2$ for all $i$.

In this subcase, $G' \not\cong U_{n-1}^3$. Then $R(G') > \varphi(n-1,3)$ by the induction hypothesis. By (7), we have

$$R(G) \geq R(G') + \frac{r}{\sqrt{t}} - \frac{r - 1}{\sqrt{t-1}} + \frac{t-r}{\sqrt{2}} \left( \frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}} \right).$$
\[ > \varphi(n-1,3) + \sqrt{t} - \sqrt{t-1} + (t-r) \left( \frac{1}{\sqrt{2}} - 1 \right) \left( \frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}} \right) \]

\[ \geq \varphi(n,3) + \frac{n-5+\sqrt{2}}{\sqrt{n-3}} - \frac{n-4+\sqrt{2}}{\sqrt{n-2}} + \frac{t+\sqrt{2}-2}{\sqrt{t}} - \frac{t+\sqrt{2}-3}{\sqrt{t-1}} \]

\[ > \varphi(n,3) + [f(n-3) - f(n-2)] - [f(t-1) - f(t)] \geq \varphi(n,3), \]

where \( f(x) = \frac{x+\sqrt{2}}{\sqrt{2}} \) and the last inequality follows by Lemma 1(i) as \( t \leq n-2 \).

**Case 2.** \( |N(u) \setminus V_0| = 1 \).

In this case, \( G - u \cong K_3 \cup (n-4)P_1 \) as \( d = 3 \). Thus we have

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

\[
= \varphi(n,3) + \frac{n-4 + \frac{1}{\sqrt{3}}}{\sqrt{n-3}} - \frac{n-4 + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}}}{\sqrt{n-2}} + \frac{1}{\sqrt{6}} + \frac{1}{2} - \frac{1}{\sqrt{3}} > \varphi(n,3).
\]

Therefore the proof of the theorem is complete. \( \blacksquare \)

**Theorem 8.** Suppose that \( G \in \mathcal{U}_{n,d}, 4 \leq d \leq n-2 \). Then

\[ R(G) \geq \varphi(n,d) \tag{9} \]

and equality in (9) holds if and only if \( G \cong U_n^d \).

**Proof.** First we note if \( G \cong U_n^d \) for \( d \geq 4 \), then (9) holds.

Now, we choose \( G \in \mathcal{U}_{n,d}, 4 \leq d \leq n-2 \) such that \( R(G) \) is as small as possible. Since \( G \) has a path of length \( d \), \( n \geq d+2 \). For \( d \) fixed, we apply induction on \( n \).

If \( n = d+2 \), then the theorem holds by Lemma 6. So in the following proof, we assume \( n \geq d+3 \). Let \( P = v_1v_2 \cdots v_dw_{d+1} \) be a path of length \( d \) in \( G \) and \( C \) be the only cycle of \( G \).

By Lemmas 5 and 6, we may assume that \( V_0 \neq \emptyset \) and there exists a vertex \( u_0 \in V_0 \) such that \( G - u_0 \) containing a path of length \( d \). Let \( V_0' \) denote the set of all such vertices \( u_0 \) just mentioned.

Let \( u \in V_1 \cap N_G(V_0') \) with \( d(u) = t+1 \). Then \( 1 \leq t \leq n-d \). Denote \( N(u) \cap V_0 = \{w_1, \ldots, w_r\} \) and \( N(u) \setminus V_0 = \{x_1, \ldots, x_{t-r+1}\} \). Then all \( d(x_i) = d_i \geq 2 \).

**Case 1.** There exists some \( u \in V_1 \cap N_G(V_0') \) such that \( |N(u) \setminus V_0| \geq 2 \).

In this case, \( t-r \geq 1 \) and \( r \geq 1 \). Let \( G' = G - w_1 \). Then \( G' \in \mathcal{U}_{n-1,d} \). Thus

\[
R(G) \geq R(G') + \frac{r}{\sqrt{t+1}} - \frac{r-1}{\sqrt{t}} + \frac{t-r+1}{\sqrt{2}} - \frac{1}{\sqrt{t+1}} - \frac{1}{\sqrt{t}}
\]
\[ \varphi(n - 1, d) + \sqrt{t + 1} - \sqrt{t} + (t - r + 1) \left( \frac{1}{\sqrt{2}} - 1 \right) \left( \frac{1}{\sqrt{t + 1}} - \frac{1}{\sqrt{t}} \right) \]

\[ \geq \varphi(n, d) + \frac{n - d + \sqrt{2} - 2}{\sqrt{n - d}} - \frac{n - d + \sqrt{2} - 1}{\sqrt{n - d + 1}} + \frac{t + \sqrt{2} - 1}{\sqrt{t + 1}} - \frac{t + \sqrt{2} - 2}{\sqrt{t}} \]

\[ \geq \varphi(n, d) + [f(n - d) - f(n - d + 1)] - [f(t) - f(t + 1)] \geq \varphi(n, d), \]

where \( f(x) = \frac{x + \sqrt{2} - 2}{\sqrt{x}} \) and the last inequality follows by Lemma 1(i) as \( t \leq n - d \).

In order for the equality to hold, all inequalities in the above argument should be equalities. Thus we have

\[ R(G') = \varphi(n - 1, d), \quad t = n - d, \quad t - r = 1 \quad \text{and} \quad d_1 = d_2 = 2. \]

By the induction hypothesis, \( G' \cong U_{n-1}^d \). Hence \( G \cong U_n^d \).

**Case 2.** For every \( u \in V_1 \cap N_G(V_0') \), \( |N(u) \setminus V_0| = 1 \).

In this case, \( t \leq n - d - 1 \). Now we will show that \( u \in \{v_2, v_d\} \). Otherwise, \( u \notin V(P) \cup V(C) \). Let \( G^+ = G - uw_1 - \cdots - uw_r + x_1w_1 + \cdots + x_1w_r \). Then \( G^+ \in \mathcal{W}_{n,d} \) and \( R(G^+) < R(G) \) by Lemma 3, a contradiction to the choice of \( G \). Moreover, we may assume that \( u = v_2 \) and \( w_1 = v_1 \) by Lemma 4. Hence \( G - \{w_2, \ldots, w_r\} \cong P_{n-t+1,t} \), or \( G - \{w_2, \ldots, w_r\} \cong Q_{n-t+1,i,j} \), or \( G - \{w_2, \ldots, w_r\} \cong R_{n-t+1,i,t} \).

**Subcase 2.1.** \( G - \{w_2, \ldots, w_r\} \cong P_{n-t+1,t} \).

In this subcase, if \( l \geq 3 \), then, by Lemma 1(ii), for \( d = 4 \),

\[ R(G) = \frac{n - 5 + \frac{1}{\sqrt{2}}}{\sqrt{n - 4}} + \frac{1 + \sqrt{6}}{2} \]

\[ = \varphi(n, 4) + \frac{n - 5 + \frac{1}{\sqrt{2}}}{\sqrt{n - 4}} - \frac{n - 5 + \sqrt{2}}{\sqrt{n - 3}} + \frac{1 + \sqrt{6}}{2} - \frac{1}{\sqrt{3}} - \frac{\sqrt{2}}{\sqrt{3}} \]

\[ \geq \varphi(n, 4) + \frac{2 + \frac{1}{\sqrt{2}}}{\sqrt{3}} - \frac{2 + \sqrt{2}}{\sqrt{4}} + \frac{1 + \sqrt{6}}{2} - \frac{1}{\sqrt{3}} - \frac{\sqrt{2}}{\sqrt{3}} > \varphi(n, 4); \]

and for \( d \geq 5 \),

\[ R(G) = \frac{t + \frac{1}{\sqrt{2}}}{\sqrt{t + 1}} + \frac{3}{\sqrt{6}} + \frac{n - t - 4}{2} \geq \frac{n - d - 1 + \frac{1}{\sqrt{2}}}{\sqrt{n - d}} + \frac{3}{\sqrt{6}} + \frac{d - 3}{2} \]

\[ = \varphi(n, d) + \frac{n - d - 1 + \frac{1}{\sqrt{2}}}{\sqrt{n - d}} - \frac{n - d - 1 + \sqrt{2}}{\sqrt{n - d + 1}} + 1 - \frac{1}{\sqrt{2}} \]

\[ \geq \varphi(n, d) + \frac{2 + \frac{1}{\sqrt{2}}}{\sqrt{3}} - \frac{2 + \sqrt{2}}{\sqrt{4}} + 1 - \frac{1}{\sqrt{2}} > \varphi(n, d). \]
If $l = 2$, then by an argument similar to the above, we have

$$R(G) = \begin{cases} \frac{t+\frac{1}{\sqrt{2}}}{\sqrt{t+1}} + \frac{5}{\sqrt{8}} + \frac{n-t-5}{2} \geq \frac{n-d-1+\frac{1}{\sqrt{d}}}{\sqrt{n-d}} + \frac{5}{\sqrt{8}} + \frac{d-5}{2} > \varphi(n,d), & d = 4; \\
\frac{t+\frac{1}{\sqrt{3}}}{\sqrt{t+1}} + \frac{2}{\sqrt{6}} + \frac{n-t-3}{2} \geq \frac{n-d-1+\frac{1}{\sqrt{d}}}{\sqrt{n-d}} + \frac{2}{\sqrt{6}} + \frac{d-2}{2} > \varphi(n,d), & d \geq 5. \end{cases}$$

**Subcase 2.2.** $G - \{w_2, \ldots, w_r\} \cong Q_{n-t+1, i, j}$.

**Subcase 2.2.1.** $i + j = d$.

In this subcase, $i, j \geq 2$ by the assumption. Thus by Lemma 1(ii), for $i = 2$,

$$R(G) = \frac{t+\frac{1}{\sqrt{4}}}{\sqrt{t+1}} + \frac{5}{\sqrt{8}} + \frac{n-t-5}{2} \geq \frac{n-d-1+\frac{1}{\sqrt{d}}}{\sqrt{n-d}} + \frac{5}{\sqrt{8}} + \frac{d-4}{2} > \varphi(n,d);$$

and for $i \geq 3$,

$$R(G) = \frac{t+\frac{1}{\sqrt{3}}}{\sqrt{t+1}} + \frac{3}{\sqrt{2}} + \frac{n-t-6}{2} \geq \frac{n-d-1+\frac{1}{\sqrt{d}}}{\sqrt{n-d}} + \frac{3}{\sqrt{2}} + \frac{d-5}{2} \geq \varphi(n,d) + \frac{2+\frac{1}{\sqrt{2}}}{\sqrt{3}} - \frac{2+\sqrt{2}}{\sqrt{4}} + \sqrt{2} - \frac{\sqrt{6}}{2} = \varphi(n,d).$$

**Subcase 2.2.2.** $i + j = d - 1$.

In this subcase, if $d = 4$, then $i = 2, j = 1$ and $t + 1 = n - 4$ or $n - 5$, thus for $t + 1 = n - 4$, we have

$$R(G) = \frac{n-5+\frac{1}{\sqrt{3}}}{\sqrt{n-4}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{1}{3} > \frac{n-5+\sqrt{2}}{\sqrt{n-3}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} = \varphi(n,4).$$

and for $t + 1 = n - 5$, we have

$$R(G) = \frac{n-6+\frac{1}{\sqrt{3}}}{\sqrt{n-5}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{1}{3} + \frac{1}{2} > \frac{n-5+\sqrt{2}}{\sqrt{n-3}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} = \varphi(n,4).$$

If $d \geq 5$, then by Lemma 1(ii), for $i \geq 3, j \geq 2$, we have

$$R(G) = \frac{t+\frac{1}{\sqrt{2}}}{\sqrt{t+1}} + \frac{4+\sqrt{3}}{\sqrt{6}} - \frac{19}{6} + \frac{n-t}{2} \geq \frac{n-d-1+\frac{1}{\sqrt{d}}}{\sqrt{n-d}} + \frac{4+\sqrt{3}}{\sqrt{3}} - \frac{8+d}{3} \geq \varphi(n,d).$$
\[ \varphi(n, d) + \frac{n - d - 1 + \frac{1}{\sqrt{2}}}{\sqrt{n - d}} + \frac{n - d - 1 + \sqrt{2}}{\sqrt{n - d + 1}} + \frac{\sqrt{6} - 1}{6} \]

\[ \geq \varphi(n, d) + \frac{2 + \frac{1}{\sqrt{2}}}{\sqrt{3}} - \frac{2 + \sqrt{2}}{\sqrt{4}} + \frac{\sqrt{6} - 1}{6} > \varphi(n, d); \]

and for \( i = 2, j \geq 2, \)

\[ R(G) = \frac{t + \frac{1}{\sqrt{3}}}{\sqrt{t + 1}} + \frac{1 + \sqrt{3}}{\sqrt{2}} - \frac{8 + n - t - 2}{3} \geq \frac{n - d - 1 + \frac{1}{\sqrt{3}}}{\sqrt{n - d}} + \frac{1 + \sqrt{3}}{\sqrt{2}} - \frac{13 + d - 2}{6} \]

\[ = \varphi(n, d) + \frac{n - d - 1 + \frac{1}{\sqrt{3}}}{\sqrt{n - d}} - \frac{n - d - 1 + \sqrt{2}}{\sqrt{n - d + 1}} + \frac{1}{3} \]

\[ \geq \varphi(n, d) + \frac{2 + \frac{1}{\sqrt{3}}}{\sqrt{3}} - \frac{2 + \sqrt{2}}{\sqrt{4}} + \frac{1}{3} > \varphi(n, d); \]

and for \( i \geq 3, j = 1, \)

\[ R(G) = \frac{t + \frac{1}{\sqrt{2}}}{\sqrt{t + 1}} + \frac{3 + \sqrt{2}}{\sqrt{6}} - \frac{8 + n - t - 2}{3} \geq \frac{n - d - 1 + \frac{1}{\sqrt{2}}}{\sqrt{n - d}} + \frac{3 + \sqrt{2}}{\sqrt{6}} - \frac{13 + d - 2}{6} \]

\[ = \varphi(n, d) + \frac{n - d - 1 + \frac{1}{\sqrt{2}}}{\sqrt{n - d}} - \frac{n - d - 1 + \sqrt{2}}{\sqrt{n - d + 1}} + \frac{1}{3} \]

\[ \geq \varphi(n, d) + \frac{2 + \frac{1}{\sqrt{2}}}{\sqrt{3}} - \frac{2 + \sqrt{2}}{\sqrt{4}} + \frac{1}{3} > \varphi(n, d). \]

**Subcase 2.2.3.** \( i + j \leq d - 2. \)

In this subcase, \( d \geq 5. \) Thus by Lemma 1(ii), for \( i \geq 3, j \geq 2, \)

\[ R(G) = \frac{t + \frac{1}{\sqrt{2}}}{\sqrt{t + 1}} + \frac{6 + \sqrt{3}}{\sqrt{6}} + \frac{n - t - 8}{2} \geq \frac{n - d - 1 + \frac{1}{\sqrt{2}}}{\sqrt{n - d}} + \frac{6 + \sqrt{3}}{\sqrt{6}} + \frac{d - 7 - 2}{2} \]

\[ = \varphi(n, d) + \frac{n - d - 1 + \frac{1}{\sqrt{2}}}{\sqrt{n - d}} - \frac{n - d - 1 + \sqrt{2}}{\sqrt{n - d + 1}} + \frac{3}{\sqrt{6}} - \frac{2}{2} \]

\[ \geq \varphi(n, d) + \frac{2 + \frac{1}{\sqrt{2}}}{\sqrt{3}} - \frac{2 + \sqrt{2}}{\sqrt{4}} + \frac{3}{\sqrt{6}} - \frac{2}{2} > \varphi(n, d); \]

and for \( i = 2, j \geq 2, \)

\[ R(G) = \frac{t + \frac{1}{\sqrt{3}}}{\sqrt{t + 1}} + \frac{5 + \sqrt{3}}{\sqrt{6}} + \frac{n - t - 7}{2} \geq \frac{n - d - 1 + \frac{1}{\sqrt{3}}}{\sqrt{n - d}} + \frac{5 + \sqrt{3}}{\sqrt{6}} + \frac{d - 6 - 2}{2} \]

\[ = \varphi(n, d) + \frac{n - d - 1 + \frac{1}{\sqrt{3}}}{\sqrt{n - d}} - \frac{n - d - 1 + \sqrt{2}}{\sqrt{n - d + 1}} + \frac{2}{\sqrt{6}} - \frac{1}{2} \]

\[ \geq \varphi(n, d) + \frac{2 + \frac{1}{\sqrt{3}}}{\sqrt{3}} - \frac{2 + \sqrt{2}}{\sqrt{4}} + \frac{2}{\sqrt{6}} - \frac{1}{2} > \varphi(n, d); \]
and for $i \geq 3$, $j = 1$,

\[
R(G) = \frac{t + \frac{1}{\sqrt{2}}}{\sqrt{t+1}} + \frac{5 + \sqrt{2}}{\sqrt{6}} + \frac{n-t-7}{2} \geq \frac{n-d-1 + \frac{1}{\sqrt{2}}}{\sqrt{n-d}} + \frac{5 + \sqrt{2}}{\sqrt{6}} + \frac{d-6}{2} \\
= \varphi(n,d) + \frac{n-d-1 + \frac{1}{\sqrt{2}}}{\sqrt{n-d}} - \frac{n-d-1 + \sqrt{2}}{\sqrt{n-d+1}} + \frac{\sqrt{2} + 1}{\sqrt{3}} - \frac{\sqrt{2} + 1}{2} \\
\geq \varphi(n,d) + \frac{2 + \frac{1}{\sqrt{2}}}{\sqrt{3}} - \frac{2 + \sqrt{2}}{\sqrt{4}} + \frac{\sqrt{2} + 1}{\sqrt{3}} - \frac{\sqrt{2} + 1}{2} > \varphi(n,d);
\]

and for $i = 2$, $j = 1$,

\[
R(G) = \frac{t + \frac{1}{\sqrt{2}}}{\sqrt{t+1}} + \frac{4 + \sqrt{2}}{\sqrt{6}} + \frac{n-t-6}{2} \geq \frac{n-d-1 + \frac{1}{\sqrt{3}}}{\sqrt{n-d}} + \frac{4 + \sqrt{2}}{\sqrt{6}} + \frac{d-5}{2} \\
= \varphi(n,d) + \frac{n-d-1 + \frac{1}{\sqrt{3}}}{\sqrt{n-d}} - \frac{n-d-1 + \sqrt{2}}{\sqrt{n-d+1}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \\
\geq \varphi(n,d) + \frac{2 + \frac{1}{\sqrt{3}}}{\sqrt{3}} - \frac{2 + \sqrt{2}}{\sqrt{4}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} > \varphi(n,d).
\]

**Subcase 2.3.** $G - \{w_2, \ldots, w_r\} \cong R_{n-t+1,i,l}$.

In this subcase, $d \geq 5$. Then by the similar calculations as above, we have

\[
R(G) = \begin{cases} 
\frac{i+\frac{1}{\sqrt{2}}}{\sqrt{i+1}} + \frac{4}{\sqrt{6}} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{n-t-7}{2} > \varphi(n,d), & i \geq 3, \ l = 1; \\
\frac{i+\frac{1}{\sqrt{2}}}{\sqrt{i+1}} + \frac{6}{\sqrt{6}} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{n-t-8}{2} > \varphi(n,d), & i \geq 3, \ l \geq 2; \\
\frac{i+\frac{1}{\sqrt{2}}}{\sqrt{i+1}} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{n-t-6}{2} > \varphi(n,d), & i = 2, \ l = 1; \\
\frac{i+\frac{1}{\sqrt{2}}}{\sqrt{i+1}} + \frac{5}{\sqrt{6}} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \frac{n-t-7}{2} > \varphi(n,d), & i = 2, \ l \geq 2.
\end{cases}
\]

Therefore the proof of the theorem is complete.

**References**


