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The Reciprocal Reverse Wiener Index of Unicyclic Graphs

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Abstract. The reciprocal reverse Wiener index $R\Lambda(G)$ of a connected graph G is defined in mathematical chemistry as the sum of weights $\frac{1}{d(G)-d_G(u,v)}$ of all unordered pairs of distinct vertices u and v with $d_G(u,v) < d(G)$, where $d_G(u,v)$ is the distance between vertices u and v in G and $d(G)$ is the diameter of G. We determine the minimum and maximum reciprocal reverse Wiener indices in the class of n-vertex unicyclic graphs and characterize the corresponding extremal graphs.

1. Introduction

A topological index is a numerical structural descriptor of the molecular structure based on certain topological features of the molecular graph [7]. The Wiener index [8] introduced in 1947 is one of the oldest and most widely used topological indices, see [5, 6]. There are also many variants of the Wiener index, for example, the reverse Wiener index [1, 3] and the reciprocal reverse Wiener index [3, 10]. See [9] for a recent survey for such distance based topological indices.

We consider simple graphs. Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For $u, v \in V(G)$, $d_G(u,v)$ denotes the distance between u and v in G. The diameter of G is the maximum distance among all pairs of vertices of G, denoted by $d(G)$. Let G be a graph with $V(G) = \{v_1, v_2, \ldots, v_n\}$. The distance matrix $D(G)$ of G is an $n \times n$ matrix (d_{ij}) such that $d_{ij} = d_G(v_i, v_j)$ for $i, j = 1, 2, \ldots, n$, The reciprocal reverse Wiener (RRW) matrix $RRW(G)$ of G is an $n \times n$ matrix (r_{ij}) such that $r_{ij} = \frac{1}{d(G)-d_{ij}}$ if $i \neq j$ and $d_{ij} < d(G)$, and 0 otherwise [3, 4].

For a connected graph G, its Wiener index is defined as the sum of distances between all unordered pairs of distinct vertices of G [2, 8]. In parallel to this definition, the reciprocal reverse Wiener (RRW) index $R\Lambda(G)$ of a connected graph G is defined as [3]

$$R\Lambda(G) = \sum_{i<j} r_{ij} = \sum_{\substack{i<j \\ d_{ij}<d(G)}} \frac{1}{d(G) - d_{ij}}.$$

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For $u, v \in V(G)$, let $r_G(u,v) = \frac{1}{d(G)-d_G(u,v)}$ if $0 < d_G(u,v) < d(G)$, and $r_G(u,v) = 0$ otherwise. Then

$$R\Lambda(G) = \sum_{\{u,v\}\subseteq V(G)} r_G(u,v).$$

The RRW index and some other topological indices derived from the RRW matrix were used to produce QSPR models for the alkane molar heat capacity in [3]. Some basic properties for the RRW index, especially for trees (connected graphs with no cycle), have been established by Zhou et al. [10].

In this paper, we determine the minimum and maximum RRW indices in the class of n-vertex unicyclic graphs (connected graphs with a unique cycle) and characterize the corresponding extremal graphs.

2. Preliminaries

Let C_n and P_n be a cycle and path on $n \geq 3$ vertices, respectively.

If an n-vertex unicyclic graph G has diameter $n-2$, then $G = G_{n,i}$ with $1 \leq i \leq \lfloor \frac{n-1}{2} \rfloor$ or $G = H_{n,i}$ with $1 \leq i \leq \lfloor \frac{n-2}{2} \rfloor$, where $G_{n,i}$ is the graph formed from the path P_{n-1} whose vertices are labelled consecutively as $v_1, v_2, \cdots, v_{n-1}$ by adding vertex v and edges vv_i, vv_{i+1}, and $H_{n,i}$ is the graph formed from the path P_{n-1} by adding vertex v and edges vv_i, vv_{i+2}. By direct calculation, we have

$$R\Lambda(G_{n,1}) = n-2+\sum_{k=2}^{n-3}\frac{1}{k}+\frac{1}{n-3}+\sum_{k=3}^{n-1}\frac{1}{n-k},$$

$$R\Lambda(G_{n,i}) = n-2+\sum_{k=2}^{n-3}\frac{1}{k}+\sum_{k=3}^{i+2}\frac{1}{n-k}+\sum_{k=3}^{n-i+1}\frac{1}{n-k} \text{ for } i \geq 2$$

and

$$R\Lambda(H_{n,i}) = n-2+\sum_{k=2}^{n-3}\frac{1}{k}+\sum_{k=3}^{i+2}\frac{1}{n-k}+\sum_{k=3}^{n-i}\frac{1}{n-k}+\frac{1}{n-4}.$$

If an n-vertex unicyclic graph G different from C_6 and C_7 has diameter three, then it is one of the following four types: (i) $U_3(a,b,c)$, the unicyclic graph formed by attaching a, b and c pendent edges respectively to the vertices of C_3, where $a \geq b \geq \max\{c, 1\}$ and $a+b+c = n-3$; (ii) $U_4(a,b)$, the unicyclic graph formed by attaching a and b pendent edges respectively to the two adjacent vertices of C_4, where $a \geq \max\{b,1\}$ and $a+b = n-4$; (iii) $U_5(a,b)$, the unicyclic graph formed by attaching a and b pendent edges respectively to the two adjacent vertices of C_5, where $a \geq \max\{b,1\}$ and $a+b = n-5$; (iv) $U_3^*(a,b)$, be the unicyclic graph formed by attaching $b+1$ pendent edges to a vertex of C_3 and then attaching a pendent edges to a pendent vertex, where $a \geq 1$ and $a+b = n-4$.

3. Minimum RRW index and extremal graphs

Lemma 3.1. *For $n \geq 6$, $n < R\Lambda(C_n) < \frac{n^2-4n+8}{2}$.*

Proof. Let $d = d(C_n) = \lfloor \frac{n}{2} \rfloor$. For $v \in V(C_n)$ and $i = 1, 2, \ldots, d-1$, there are two vertices of distance i from v. Then $R\Lambda(C_n) = n\sum_{i=1}^{d-1}\frac{1}{d-i} = n\sum_{i=1}^{d-1}\frac{1}{i}$. Thus $R\Lambda(C_n) > n$, and since $d \geq 3$, $R\Lambda(C_n) \leq \left[1+\frac{1}{2}+\frac{1}{3}(d-3)\right]n \leq \left[\frac{3}{2}+\frac{1}{3}\left(\frac{n}{2}-3\right)\right]n < \frac{n^2-4n+8}{2}$. □

Lemma 3.2. *Let G be an n-vertex unicyclic graph with $d(G) = n-2$. Then $R\Lambda(G) > n$.*

Proof. Since $d(G) = n-2$, $G = G_{n,i}$ with $1 \le i \le \lfloor \frac{n-1}{2} \rfloor$ or $G = H_{n,i}$ with $1 \le i \le \lfloor \frac{n-2}{2} \rfloor$. The expressions for $R\Lambda(G_{n,i})$ and $R\Lambda(H_{n,i})$ are given in Section 2. Note that $R\Lambda(G_{5,1}) = \frac{11}{2}$, $R\Lambda(H_{5,1}) = R\Lambda(G_{5,2}) = \frac{13}{2}$, $R\Lambda(G_{6,1}) = R\Lambda(H_{6,2}) = 7$, and $R\Lambda(G_{6,2}) = R\Lambda(H_{6,1}) = \frac{15}{2}$. Thus the result is true for $n = 5, 6$. Suppose that $n \ge 7$. Then $\sum_{k=2}^{n-3} \frac{1}{k} \ge \frac{1}{2} + \frac{1}{3} + \frac{1}{4} > 1$, $\frac{1}{n-3} + \sum_{k=3}^{n-1} \frac{1}{n-k} > (n-2) \cdot \frac{1}{n-2} = 1$, $\sum_{k=3}^{i+2} \frac{1}{n-k} + \sum_{k=3}^{n-i+1} \frac{1}{n-k} > (n-1) \cdot \frac{1}{n-1} = 1$, and $\sum_{k=3}^{i+2} \frac{1}{n-k} + \sum_{k=3}^{n-i} \frac{1}{n-k} + \frac{1}{n-4} > (n-1) \cdot \frac{1}{n-1} = 1$. Thus $R\Lambda(G_{n,i}) > n$ and $R\Lambda(H_{n,i}) > n$. □

Lemma 3.3. *Let G be an n-vertex unicyclic graph with* $3 \le d(G) \le n-3$. *Then* $R\Lambda(G) > n$.

Proof. We prove the lemma by induction on n. If $n = 6$, then $d(G) = 3$ and $G \cong C_6$, $U_3(1,1,1)$, $U_3(2,1,0)$, $U_4(2,0)$, $U_4(1,1)$, $U_5(1,0)$, $U_3^*(2,0)$ or $U_3^*(1,1)$, and thus by direct calculation, we have

$$R\Lambda(G) = \begin{cases} 10 & \text{if } G \cong U_3(2,1,0), U_5(1,0), \text{or } U_4(2,0) \\ 8 & \text{if } G \cong U_3^*(2,0) \\ 9 & \text{otherwise} \end{cases} > 6,$$

as desired.

Suppose that $n \ge 7$ and the result is true for unicyclic graphs on $n-1$ vertices. Let G be an n-vertex unicyclic graph with $3 \le d(G) \le n-3$. Let $d = d(G)$.

Case 1. There exists a pendent vertex, say u outside some diametrical path. Then $d(G-u) = d$ and

$$R\Lambda(G) = R\Lambda(G-u) + \sum_{v \in V(G)\setminus\{u\}} r_G(u,v).$$

By the induction hypothesis for $3 \le d \le n-4$, and Lemma 3.2 for $d = n-3$, we have $R\Lambda(G-u) > n-1$. If $d(u,w) = d-1$ for some $w \in V(G) \setminus \{u\}$, then $\sum_{v \in V(G)\setminus\{u\}} r_G(u,v) > r_G(u,w) = 1$. If $d(u,v) \ne d-1$ for any $v \in V(G)\setminus\{u\}$, then $1 \le d_G(u,v) \le d-2$ for any $v \in V(G)\setminus\{u\}$, and thus $\sum_{v \in V(G)\setminus\{u\}} r_G(u,v) \ge \sum_{v \in V(G)\setminus\{u\}} \frac{1}{d-1} = \frac{n-1}{d-1} > 1$. Thus $R\Lambda(G) > n$.

Case 2. There exists no pendent vertex outside any diametrical path. If $G \cong C_n$, then the result follows from Lemma 3.1. Suppose that $G \not\cong C_n$. Let $P = v_1 v_2 \ldots v_d v_{d+1}$ be a diametrical path of G. Then a pendent vertex of G must be v_1 or v_{d+1}. Let $V_1 = V(G) \setminus V(P)$. Obviously, $d_G(u,v) < d$ for $u, v \in V_1$, or $u \in V_1$ and $v \in V(P) \setminus \{v_1, v_{d+1}\}$. If $u \in V_1$, then $d_G(u, v_1) < d$. Thus

$$\begin{aligned} \sum_{u \in V_1, v \in V(G)} r_G(u,v) &= \sum_{\{u,v\} \subseteq V_1} r_G(u,v) + \sum_{u \in V_1} \sum_{v \in V(P)} r_G(u,v) \\ &\ge \frac{1}{d-1} \binom{n-d-1}{2} + \sum_{u \in V_1} \sum_{v \in V(P)} \frac{1}{d-1} \\ &\ge \frac{(n-d-1)(n-d-2)}{2(d-1)} + \sum_{u \in V_1} \frac{d}{d-1} \\ &> \frac{(n-d-1)(n-d-2)}{2(d-1)} + n - d - 1. \end{aligned}$$

It is easily seen that

$$\sum_{\{u,v\} \subseteq V(P)} r_G(u,v) = \sum_{i=1}^{d-1} \frac{d+1-i}{d-i} = d + \sum_{i=2}^{d-1} \frac{1}{i}.$$

Then

$$\begin{aligned} R\Lambda(G) &= \sum_{u\in V_1, v\in V(G)} r_G(u,v) + \sum_{\{u,v\}\subseteq V(P)} r_G(u,v) \\ &> n-1+\sum_{i=2}^{d-1}\frac{1}{i}+\frac{(n-d-1)(n-d-2)}{2(d-1)} \\ &\geq n-1+\frac{d-2}{d-1}+\frac{(n-d-1)(n-d-2)}{2(d-1)} \\ &= n-1+\frac{n^2-2nd+d^2-3n+5d-2}{2(d-1)}. \end{aligned}$$

Let $f(d) = n^2-2nd+d^2-3n+5d-2-2(d-1) = n^2-2nd+d^2-3n+3d$. Since $f'(d) = -2n+3+2d < 0$, $f(d)$ is decreasing for $3 \leq d \leq n-3$. Then $f(d) \geq f(n-3) = 0$, and thus $n^2-2nd+d^2-3n+5d-2 \geq 2(d-1)$. It follows that $R\Lambda(G) > n-1+1 = n$. □

Let U_3^{n-3} be the unicyclic graph formed by attaching $n-3$ pendent vertices to a vertex of C_3.

Theorem 3.4. *Let G be a unicyclic graph with n vertices, $n \geq 4$. Then $R\Lambda(G) \geq n$ with equality if and only if $G \cong C_4$, C_5 or U_3^{n-3}.*

Proof. Obviously, $2 \leq d(G) \leq n-2$. If $d(G) \geq 3$, then by Lemmas 3.2 and 3.3, $R\Lambda(G) > n$. If $d(G) = 2$, then $R\Lambda(G) = n$ and $G \cong C_4$, C_5 or U_3^{n-3}. □

4. Maximum RRW index and extremal graphs

Lemma 4.1. *Let G be an n-vertex unicyclic graph with $d(G) = 3$. Then $R\Lambda(G) \leq \frac{n^2-4n+8}{2}$ with equality if and only if $G \cong U_3(n-4,1,0)$, $U_4(n-4,0)$ or $U_5(1,0)$.*

Proof. If G is a cycle, then $G \cong C_6$ or C_7, and the result follows from Lemma 3.1. Suppose that G is not a cycle, then there are four possibilities:

(i) $G \cong U_3(a,b,c)$, $a \geq b \geq \max\{c,1\}$ and $a+b+c = n-3$; Then

$$\begin{aligned} R\Lambda(G) &= \frac{n}{2}+2(n-3)+\frac{a^2+b^2+c^2-(n-3)}{2} \\ &\leq \frac{n}{2}+2(n-3)+\frac{(n-4)^2+1-(n-3)}{2} \\ &= \frac{n^2-4n+8}{2} \end{aligned}$$

with equality if and only if $a = n-4$, $b = 1$ and $c = 0$, i.e., $G \cong U_3(n-4,1,0)$.

(ii) $G \cong U_4(a,b)$, where $a \geq \max\{b,1\}$ and $a+b = n-4$; Then

$$\begin{aligned} R\Lambda(G) &= \frac{n}{2}+2(n-3)+\frac{a^2+b^2-(n-4)}{2} \\ &\leq \frac{n}{2}+2(n-3)+\frac{(n-4)^2-(n-4)}{2} \\ &= \frac{n^2-4n+8}{2} \end{aligned}$$

with equality if and only if $a = n-4$ and $b = 0$, i.e., $G = U_4(n-4,0)$.

(iii) $G \cong U_5(a,b)$, where $a \geq \max\{b,1\}$ and $a+b = n-5$; Then

$$\begin{aligned} R\Lambda(G) &= \frac{n}{2}+2n-5+\frac{a^2+b^2-(n-5)}{2} \\ &\leq \frac{n}{2}+2n-5+\frac{(n-5)^2-(n-5)}{2} \\ &= \frac{n^2-6n+20}{2} \\ &\leq \frac{n^2-4n+8}{2} \end{aligned}$$

with equality if and only if $n = 6$, i.e., $G \cong U_5(1,0)$.

(iv) $G \cong U_3^*(a,b)$, where $a \geq 1$ and $a+b=n-4$; Then

$$\begin{aligned} R\Lambda(G) &= \tfrac{n}{2}+2+n-4+2b+\tfrac{a^2+b^2-(n-4)}{2} \\ &\leq n+\tfrac{a^2+(b+2)^2-4}{2} \\ &\leq n+\tfrac{1^2+(n-3)^2-4}{2} \\ &= \tfrac{n^2-4n+6}{2} < \tfrac{n^2-4n+8}{2}. \end{aligned}$$

The result follows. □

Lemma 4.2. *Let G be an n-vertex unicyclic graph with $d(G)=n-2$. Then $R\Lambda(G) < \frac{n^2-4n+8}{2}$.*

Proof. Since $d(G)=n-2$, $G=G_{n,i}$ with $1 \leq i \leq \lfloor \frac{n-1}{2} \rfloor$ or $G=H_{n,i}$ with $1 \leq i \leq \lfloor \frac{n-2}{2} \rfloor$. The expressions for $R\Lambda(G_{n,i})$ and $R\Lambda(H_{n,i})$ are given in Section 2. Thus

$$\begin{aligned} R\Lambda(G_{n,1}) &= n-2+\sum_{k=2}^{n-3}\tfrac{1}{k}+\tfrac{1}{n-3}+\sum_{k=3}^{n-1}\tfrac{1}{n-k} \\ &\leq n-2+\tfrac{n-4}{2}+\tfrac{1}{2}+\tfrac{n-4}{2}+1 \\ &= 2n-4-\tfrac{1}{2} \\ &< \tfrac{n^2-4n+8}{2}. \end{aligned}$$

Similarly, $R\Lambda(G_{n,i}) < \frac{n^2-4n+8}{2}$ for $i \geq 2$ and $R\Lambda(H_{n,i}) < \frac{n^2-4n+8}{2}$ for $i \geq 1$. □

Lemma 4.3. *Let G be a unicyclic graph with diameter $d(G)$, where $4 \leq d(G) \leq n-3$. If there exists no pendent vertex outside any diametrical path of G, then $R\Lambda(G) < \frac{n^2-4n+8}{2}$.*

Proof. If $G \cong C_n$, then the result follows from Lemma 3.1. Suppose that $G \ncong C_n$.

Let $P=v_1v_2\ldots v_dv_{d+1}$ be a diametrical path of G. Let $V_1=V(G)\setminus V(P)$. By the proof of Lemma 3.3, we have

$$\sum_{\{u,v\}\subseteq V(P)} r_G(u,v) = d+\sum_{i=2}^{d-1}\frac{1}{i}.$$

Let $u \in V_1$. We will show that $\sum\limits_{v\in V(P)} r_G(u,v) \leq d$. Suppose first that G has exactly one pendent vertex, say v_{d+1}. If $d_G(u,v_{d+1})=d$, then $\sum\limits_{v\in V(P)} r_G(u,v) \leq (d+1)-1=d$. Suppose that $d_G(u,v_{d+1}) \leq d-1$. Then $d_G(u,v_d) \leq d-2$. If v_d lies outside the cycle of G, then $d_G(u,v_{d-1}) < d-2$, and otherwise, $\min\{d_G(u,v_1), d_G(u,v_{d-1})\} \leq d-2$. Thus $\sum\limits_{v\in V(P)} r_G(u,v) \leq (d+1)-2+\frac{1}{2}\cdot 2=d$. If G has two pendent vertices v_1 and v_{d+1}, then $d_G(u,v_2)$, $d_G(u,v_d) \leq d-2$, i.e., $r_G(u,v_2), r_G(u,v_d) \leq \frac{1}{2}$, implying that $\sum\limits_{v\in V(P)} r_G(u,v) \leq (d+1)-2+\frac{1}{2}\cdot 2=d$. It follows that

$$\sum_{u\in V_1}\sum_{v\in V(P)} r_G(u,v) \leq \sum_{u\in V_1} d = (n-d-1)d.$$

If $u,v \in V_1$ and $u \neq v$, then $r_G(u,v) \leq 1$ and $r_G(u,v)=\frac{1}{d-1} < \frac{1}{2}$ if u and v are adjacent. Thus

$$\begin{aligned} \sum_{\{u,v\}\subseteq V_1} r_G(u,v) &\leq 1\cdot\binom{n-d-1}{2}-\frac{1}{2}\cdot(n-d-2) \\ &= \frac{(n-d-1)(n-d-2)}{2}-\frac{n-d-2}{2}. \end{aligned}$$

Note that $-d^2+5d \le 4$ since $d \ge 4$. Then

$$\begin{aligned} R\Lambda(G) &= \sum_{\{u,v\}\subseteq V(P)} r_G(u,v) + \sum_{u\in V_1}\sum_{v\in V(P)} r_G(u,v) + \sum_{\{u,v\}\subseteq V_1} r_G(u,v) \\ &\le d + \sum_{i=2}^{d-1}\tfrac{1}{i} + (n-d-1)d + \tfrac{(n-d-1)(n-d-2)}{2} - \tfrac{n-d-2}{2} \\ &\le d + \tfrac{d-2}{2} + \tfrac{n^2-4n+2-d^2+2d+2}{2} \\ &= \tfrac{n^2-4n+2}{2} + \tfrac{-d^2+5d}{2} \\ &\le \tfrac{n^2-4n+2}{2} + 2 \\ &< \tfrac{n^2-4n+8}{2}, \end{aligned}$$

as desired. □

For $u \in V(G)$, d_u denotes the degree of u in G.

Lemma 4.4. *Let G be a unicyclic graph with $4 \le d(G) \le n-3$. Then $R\Lambda(G) < \frac{n^2-4n+8}{2}$.*

Proof. We prove the lemma by induction on n. Suppose first that $n = 7$. Then $d(G) = 4$. Let $P = v_1v_2v_3v_4v_5$ be the diametrical path of G and C the unique cycle of G. Let $D(v_6) = \sum_{u\in V(P)} r_G(u,v_6)$, and $D(v_7) = \sum_{u\in V(P)} r_G(u,v_7) + r_G(v_6,v_7)$. Note that

$$R\Lambda(G) = \sum_{\{u,v\}\subseteq V(P)} r_G(u,v) + D(v_6) + D(v_7) \ \text{ and } \sum_{\{u,v\}\subseteq V(P)} r_G(u,v) = 4 + \frac{1}{2} + \frac{1}{3} = 4 + \frac{5}{6}.$$

Suppose that $v_6, v_7 \in V(C)$. Then v_6 and v_7 are adjacent, v_6 is also adjacent to a vertex $u \in V(P)$. Let v be a neighbor of u in P. Then $d_G(u,v_6) = 1$ and $d_G(v,v_6) \le 2$, implying that $r_G(u,v_6) = \frac{1}{3}$ and $r_G(v,v_6) \le \frac{1}{2}$. Thus

$$D(v_6) \le (5-2) + \frac{1}{3} + \frac{1}{2} = 3 + \frac{5}{6}.$$

Similarly,

$$D(v_7) \le (6-3) + \frac{1}{3}\times 2 + \frac{1}{2} = 4 + \frac{1}{6}.$$

Hence

$$R\Lambda(G) \le 4 + \frac{5}{6} + 3 + \frac{5}{6} + 4 + \frac{1}{6} = 12 + \frac{5}{6} < \frac{29}{2} = \frac{7^2 - 4\times 7 + 8}{2}.$$

If one of v_6 and v_7 belongs to $V(C)$, then by similar arguments as above we also have the result. Thus the result follows for $n = 7$.

Suppose that $n \ge 8$ and the result follows for unicyclic graphs on $n-1$ vertices. Let G be an n-vertex unicyclic graph with $4 \le d(G) \le n-3$. Let $d(G) = d$.

If there exists no pendent vertex outside any diametrical path, the the result follows from Lemma 4.3.

Suppose there exists a pendent vertex, say u outside some diametrical path, say $P = v_1v_2\ldots v_dv_{d+1}$. Obviously, $d(G-u) = d$. Note that

$$R\Lambda(G) = R\Lambda(G-u) + \sum_{v\in V(G)\setminus\{u\}} r_G(u,v).$$

By the induction hypothesis for $4 \le d \le n-4$, and Lemma 4.2 for $d = n-3$, we have

$$R\Lambda(G-u) < \frac{(n-1)^2 - 4(n-1) + 8}{2} = \frac{n^2 - 6n + 13}{2}.$$

Next we will show that $\sum_{v\in V(G)\setminus\{u\}} r_G(u,v) \le n-\frac{5}{2}$. If $d_G(u,w)=d$ for some $w\in V(G)\setminus\{u\}$, then there is a shortest path P' from u to w with length d, $\sum_{v\in V(P')\setminus\{u\}} r_G(u,v) \le \frac{1}{2}\cdot(d-2)+1$, and thus

$$\begin{aligned}\sum_{v\in V(G)\setminus\{u\}} r_G(u,v) &= \sum_{v\in V(P')\setminus\{u\}} r_G(u,v) + \sum_{v\in V(G)\setminus V(P')} r_G(u,v)\\ &\le \frac{d-2}{2}+1+(n-d-1)\\ &= n-\frac{d}{2}-1\\ &< n-\frac{5}{2}.\end{aligned}$$

Now suppose that $1\le d_G(u,v)\le d-1$ for any $v\in V(G)\setminus\{u\}$. Let w be the unique neighbor of u. If $d_w\ge 3$, then for neighbors x and y of w different from u, $d(u,w), d(u,x), d(u,y)\le 2\le d-2$, implying that

$$\sum_{v\in V(G)\setminus\{u\}} r_G(u,v) \le (n-1)-3+\frac{1}{2}\times 3 = n-\frac{5}{2}.$$

Suppose that $d_w=2$ and x is the neighbor of w different from u. If $d(G)=4$, then for any $y\in V(G)\setminus\{u,w,x\}$, $y\in N_x$ or $d_G(x,y)=2$; In the former case, y is a neighbor of x for any $y\in V(G)\setminus\{u,w,x\}$, which implies $d(G)=3$, a contradiction, while in the latter case, $d_G(u,y)=4$, also a contradiction. Thus $d(G)\ge 5$. Let y be a neighbor x. Then $d(u,w), d(u,x), d(u,y)\le 3\le d-2$, implying that

$$\sum_{v\in V(G)\setminus\{u\}} r_G(u,v) \le (n-1)-3+\frac{1}{2}\times 3 = n-\frac{5}{2}.$$

It follows that $R\Lambda(G) < \frac{n^2-6n+13}{2}+n-\frac{5}{2}=\frac{n^2-4n+8}{2}$. This completes the proof. □

Theorem 4.5. *Let G be a unicyclic graph with n vertices. Then $R\Lambda(G)\le \frac{n^2-4n+8}{2}$ with equality if and only if $G\cong U_3(n-4,1,0)$, $U_4(n-4,0)$ or $U_5(1,0)$.*

Proof. Obviously, $2\le d(G)\le n-2$. If $d(G)=2$, then $R\Lambda(G)=n<\frac{n^2-4n+8}{2}$. Thus the result follows from Lemmas 4.1, 4.2 and 4.4. □

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