



Article Further Results on the Resistance-Harary Index of Unicyclic Graphs

Jian Lu¹, Shu-Bo Chen², Jia-Bao Liu^{3,*}, Xiang-Feng Pan¹ and Ying-Jie Ji¹

- ¹ School of Mathematical Sciences, Anhui University, Hefei 230601, China; lujianmath@163.com (J.L.); xfpan@ustc.edu (X.-F.P.); jyjgood66@163.com (Y.-J.J.)
- ² College of Mathematics, Hunan City University, Yiyang 413000, China; shuobo.chen@163.com
- ³ School of Mathematics and Physics, Anhui Jianzhu University, Hefei 230601, China
- * Correspondence: liujiabaoad@163.com

Received: 20 December 2018; Accepted: 14 February 2019; Published: 20 February 2019

Abstract: The Resistance-Harary index of a connected graph *G* is defined as $RH(G) = \sum_{\substack{\{u,v\} \subseteq V(G)}} \frac{1}{r(u,v)}$, where r(u,v) is the resistance distance between vertices *u* and *v* in *G*. A graph *G* is called a unicyclic graph if it contains exactly one cycle and a fully loaded unicyclic graph is a unicyclic graph that no vertex with degree less than three in its unique cycle. Let U(n) and $\mathfrak{U}(n)$ be the set of unicyclic graphs and fully loaded unicyclic graphs of order *n*, respectively. In this paper, we determine the graphs of U(n) with second-largest Resistance-Harary index and determine the graphs of $\mathfrak{U}(n)$ with largest Resistance-Harary index.

Keywords: Resistance-Harary Index; resistance distance; unicyclic graphs; fully loaded unicyclic graphs

1. Introduction

The topological index is the mathematical descriptor of the molecular structure, which can effectively reflect the chemical structure and properties of the material. The famous Wiener index W(G) (also Wiener number) introduced by H. Wiener, is a topological index of a molecule, defined as the sum of the lengths of the shortest paths between all pairs of vertices, i.e., $W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)$

in the chemical graph representing the non-hydrogen atoms in the molecule. In 1993, Klein and Randić [1] defined a new distance function named resistance distance on the basis of electrical network theory replacing each edge of a simple connected graph *G* by a unit resistor. Let *G* be a simple connected graph with vertices set $V = \{v_1, v_2, \dots, v_n\}$. The resistance distance between the vertices v_i and v_j , denoted by $r(v_i, v_j)$ (if more than one graphs are considered, we write $r_G(v_i, v_j)$ to avoid confusion), is defined to be the effective resistance between the vertices v_i and v_j in *G*. If the ordinary distance is replaced by resistance distance in the expression for the Wiener index, one arrives at the Kirchhoff index [1,2]

$$Kf(G) = \sum_{\{u,v\}\subseteq V(G)} r(u,v),$$

which has been widely studied [3–12].

Another distance-based graph invariant index named Harary index was introduced independently by Plavšić et al. [13] and by Ivanciuc et al. [14] in 1993 for the characterization of molecular graphs. The Harary index H(G) is defined as

$$H(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d(u,v)},$$

which is the sum of reciprocals of distances between all pairs of vertices of *G*. For more related results to Harary index, please refer to [15–22]. In 2017, Chen et al. [23,24] introduced a new graph invariant reciprocal to Kirchhoff index, named Resistance-Harary index, as

$$RH(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{r(u,v)}.$$

To understand the results and concepts, we introduce some definitions and notions. All of the graphs considered in this paper are connected and simple. A graph *G* is called a unicyclic graph if it contains exactly one cycle, simply denoted as $G = U(C_l; T_1, T_2, \dots, T_l)$, where C_l is the unique cycle with vertices $v_1v_2 \cdots v_l$, T_i is a tree rooted at v_i , $1 \le i \le l$. A fully loaded unicyclic graph is a unicyclic graph with the property that there is no vertex with degree less than three in its unique cycle. Let S_n^l denote the graph obtained from cycle C_l by adding n - l pendant edges to a vertex of C_l . Let $\mathcal{U}(n;l)$ be the set of unicyclic graphs with n vertices and the unique cycle C_l and $\mathcal{U}(n)$ be the set of unicyclic graphs with n vertices and the unique cycle graphs with n vertices and the unique cycle C_l and $\mathcal{U}(n)$ be the set of unicyclic graphs with n vertices and the unique cycle C_l and $\mathcal{U}(n)$ be the set of unicyclic graphs with n vertices. Let $\mathfrak{U}(n;l)$ be the set of all fully loaded unicyclic graphs with n vertices and the unique cycle C_l , and $\mathfrak{U}(n)$ be the set of unicyclic graphs with n vertices. Let \mathfrak{S}_n and P_n be the star and the path on n vertices, respectively.

In this paper, we improve the results of the recent paper (Chen et al. [23]) and we determine the largest Resistance-Harary index among all unicyclic graphs. Additionally, we determine the second-largest Resistance-Harary index among all unicyclic graphs and determine the largest Resistance-Harary index among all fully loaded unicyclic graphs and characterize the corresponding extremal graphs, respectively.

2. Preliminaries

In this section, we introduce some useful lemmas and two transformations. Let $R_G(u) = \sum_{u \in V(G) \setminus \{u\}} \frac{1}{r_G(u,v)}$, then $RH(G) = \frac{1}{2} \sum_{u \in V(G)} R_G(u)$. Let $C_g = v_1 v_2 \cdots v_g v_1$ be the cycle on g vertices where $g \ge 3$. By Ohm's law, for any two vertices $v_i, v_j \in V(C_g)$ with i < j, one has

$$r_{C_g}(v_i, v_j) = \frac{(j-i)(g+i-j)}{g}$$

By a simple calculation, we can obtain the Resistance-Harary index of C_g , which is

$$RH(C_g) = \sum_{u \in V(C_g)} \frac{1}{2} R_{C_g}(v) = g \sum_{i=1}^{g-1} \frac{1}{i}.$$

Lemma 1 ([1]). *Let x be a cut vertex of a connected graph G and let a and b be vertices occurring in different components which arise upon deletion of x. Then,*

$$r_G(a,b) = r_G(a,x) + r_G(x,b).$$

Definition 1 ([23]). Let v be a vertex of degree p + 1 in a graph G, such that $vv_1, vv_2, ..., vv_p$ are pendent edges incident with v, and u is the neighbor of v distinct from $v_1, v_2, ..., v_p$. We form a graph $G' = \sigma(G, v)$ by deleting the edges $vv_1, vv_2, ..., vv_p$ and adding new edges $uv_1, uv_2, ..., uv_p$. We say that G' is a σ -transform of the graph G (see Figure 1).



Figure 1. The σ -transform at v.

Lemma 2 ([23]). Let $G' = \sigma(G, v)$ be a σ -transform from the graph G, $d(u) \ge 1$ described in Figure 1. Then, $RH(G') \ge RH(G)$, with equality holds if and only if G is a star with v as its center.

Definition 2 ([23]). Let u, v be two vertices in a graph G, such that u_1, u_2, \dots, u_s are pendents incident with u and v_1, v_2, \dots, v_t are pendents incident with v in $G_0 \subseteq G$, respectively. G' and G'' are two graphs β transformed from G, such that $G' = G - \{vv_1, vv_2, \dots, vv_t\} + \{uv_1, uv_2, \dots, uv_t\}, G'' = G - \{vv_1, vv_2, \dots, vv_s\} + \{uv_1, uv_2, \dots, uv_s\}$, (see Figure 2).



Figure 2. The β -transform.

Lemma 3 ([23]). Let G', G'' be the graphs transformed from the graph $G, d(u) \ge 1$ described in Figure 2. Then, RH(G) < RH(G'), or RH(G) < RH(G'').

Corollary 1 ([23]). Let G be a connected graph with $u, v \in V(G)$. Denote by G(s;t) the graph obtained by attaching s > 1 pendent vertices to vertex u and t > 1 pendent vertices to vertex v. Then, we have RH(G(1, s + t - 1)) > RH(G) or RH(G(s + t - 1, 1)) > RH(G).

Lemma 4. The function $f(x) = \frac{2(k-1)}{(x+1)(k-1)-x^2} - \frac{1}{x+1} - \frac{1}{k-x} - \frac{2}{k-2}$ for $k \ge 3$ and $1 \le x \le \frac{k-1}{2}$ is strictly decreasing.

Proof. By simple calculation,

$$\begin{aligned} f'(x) &= \frac{2(1-k)(k-2x-1)}{(k(x+1)-x^2-x-1)^2} - \frac{1}{(k-x)^2} + \frac{1}{(x+1)^2} \\ &= (k-2x-1) \Big(\frac{2(1-k)}{(k(x+1)-x^2-x-1)^2} + \frac{(k+1)}{(x+1)^2(k-x)^2} \Big), \end{aligned}$$

Let $g(x) = \left(\frac{2(1-k)}{(k(x+1)-x^2-x-1)^2} + \frac{(k+1)}{(x+1)^2(k-x)^2}\right)$, then we have $g'(x) = \frac{2(k+1)}{(x+1)^2(k-x)^3} - \frac{2(k+1)}{(x+1)^3(k-2)^2} - \frac{4(k-1)(k-2x-1)}{(-kx+(1-k)+x^2+x)^3} < 0$ since $1 \le x \le \frac{k-1}{2}$ and $g(1) = \frac{2(1-k)}{4k^2-12k+9} - \frac{k+1}{4k^2-8k+4} < 0$ since $k \ge 3$. Thus, g(x) < 0, since $1 \le x \le \frac{k-1}{2}$. It follows that f'(x) < 0, since $1 \le x \le \frac{k-1}{2}$ and $k \ge 3$, thus implying the conclusion of the theorem. \Box

3. Main Results

By Lemmas 2 and 3, we claim that $RH(G) \leq RH(S_n^g)$ if $G \in U(n;g)$. Next, we will determine the graphs in U(n) with the largest Resistance-Harary index and the second-largest Resistance-Harary index.

3.1. The Largest Resistance-Harary Index

Theorem 1. *If* $G \in U(n)$ *, then*

$$\max_{G \in \mathcal{U}(n)} \{ RH(G) \} = \begin{cases} RH(C_n) & \text{if } n \le 7, \\ RH(S_8^5) & \text{if } n = 8, \\ RH(S_n^4) & \text{if } 9 \le n \le 15, \\ RH(S_n^3) & \text{if } n \ge 16. \end{cases}$$

Proof. Let $H = G - C_g$, by the definition of Resistance-Harary index, one has,

$$\begin{split} RH(S_n^g) &= \sum_{\{u,v\} \subseteq V(G)} \frac{1}{r(u,v)} \\ &= \sum_{\{u,v\} \subseteq V(C_g)} \frac{1}{r(u,v)} + \sum_{\{u,v\} \subseteq V(H)} \frac{1}{r(u,v)} + \sum_{u \in V(C_g), v \in V(H)} \frac{1}{r(u,v)} \\ &= g\Big(1 + \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{g-1}\Big) + \frac{1}{4}(n-g)(n+3-g) \\ &+ g(n-g)\Big(\frac{1}{2g-1} + \frac{1}{3g-4} + \dots + \frac{1}{g^2 - (g-1)^2}\Big). \end{split}$$

Similarly,

$$RH(S_n^{g-1}) = (g-1)\left(1 + \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{g-2}\right) + \frac{1}{4}(n+1-g)(n+4-g) + (g-1)(n+1-g)\left(\frac{1}{2g-3} + \frac{1}{3g-7} + \dots + \frac{1}{(g-1)^2 - (g-2)^2}\right).$$

Further, by the symmetry of C_g , one has,

$$\begin{split} \triangle &= RH(S_n^{g-1}) - RH(S_n^g) \\ &= (g-1)(n+1-g) \Big(\frac{1}{2g-3} + \frac{1}{3g-7} + \dots + \frac{1}{(g-1)^2 - (g-2)^2} \Big) \\ &+ \frac{1}{2}(n-g) - g(n-g) \Big(\frac{1}{2g-1} + \frac{1}{3g-4} + \dots + \frac{1}{g^2 - (g-1)^2} \Big) \\ &- \Big(1 + \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{g-1} \Big) \\ &= (n-g) \Big\{ \Big[\underbrace{\Big(\frac{g-1}{2g-3} + \frac{g-1}{3g-7} + \dots + \frac{g-1}{2g-3} \Big)}_{g-2} + \frac{1}{2} \Big] \\ &- \Big(\underbrace{\frac{g}{2g-1} + \frac{g}{3g-4} + \dots + \frac{g}{2g-1}}_{g-1} \Big) \Big\} + (g-1) \Big(\frac{1}{2g-3} + \frac{1}{3g-7} \\ &+ \dots + \frac{1}{(g-1)^2 - (g-2)^2} \Big) - \Big(1 + \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{g-1} \Big). \end{split}$$
(1)

To explore the relationship between \triangle and parameters g, we first discuss the part of the first brace of Equation (1). Let

$$\Theta_1 = \left[\left(\frac{g-1}{2g-3} + \frac{g-1}{3g-7} + \ldots + \frac{g-1}{2g-3} \right) + \frac{1}{2} \right] - \left(\frac{g}{2g-1} + \frac{g}{3g-4} + \ldots + \frac{g}{2g-1} \right),$$

then

$$\Theta_1 = \begin{cases} \left(\frac{g-1}{2g-3} - \frac{g}{2g-1}\right) + \left(\frac{g-1}{3g-7} - \frac{g}{3g-4}\right) + \ldots + \left(\frac{g-1}{2g-3} - \frac{g}{2g-1}\right) \\ + \frac{1}{2} - \frac{4}{g+4} > 0, & \text{if } g \ge 4 \text{ and } g \text{ is even,} \\ \left(\frac{g-1}{2g-3} - \frac{g}{2g-1}\right) + \left(\frac{g-1}{3g-7} - \frac{g}{3g-4}\right) + \ldots + \left(\frac{g-1}{2g-3} - \frac{g}{2g-1}\right) \\ + \frac{1}{2} - \frac{4g}{(g+2)^2-5} > 0, & \text{if } g \ge 5 \text{ and } g \text{ is odd.} \end{cases}$$

Next, we consider the rest of Equation (1). Let

$$\Theta_2 = (g-1)\left(\frac{1}{2g-3} + \frac{1}{3g-7} + \ldots + \frac{1}{(g-1)^2 - (g-2)^2}\right) - \left(1 + \frac{1}{2} + \frac{1}{3} + \ldots + \frac{1}{g-1}\right).$$

(i) If g is even, then

$$\begin{split} \Theta_2 &= (g-1) \sum_{i=1}^{g-2} \frac{1}{(i+1)(g-1) - i^2} - \sum_{i=1}^{g-1} \frac{1}{i} \\ &= \sum_{i=1}^{\frac{g-2}{2}} \frac{2(g-1)}{(i+1)(g-1) - i^2} - \left(\sum_{i=1}^{g-2} \frac{1}{i+1} + 1\right) \\ &= \sum_{i=1}^{\frac{g-2}{2}} \frac{2(g-1)}{(i+1)(g-1) - i^2} - \left[\sum_{i=1}^{\frac{g-2}{2}} \left(\frac{1}{i+1} + \frac{1}{g-i}\right) + \underbrace{\left(\frac{2}{g-2} + \frac{2}{g-2} + \dots + \frac{2}{g-2}\right)}_{\frac{g-2}{2}}\right] \\ &= \sum_{i=1}^{\frac{g-2}{2}} \left[\frac{2(g-1)}{(i+1)(g-1) - i^2} - \frac{1}{i+1} - \frac{1}{g-i} - \frac{2}{g-2}\right]. \end{split}$$

By Lemma 4, the function

$$F(x) = \frac{2(g-1)}{(x+1)(g-1) - x^2} - \frac{1}{x+1} - \frac{1}{g-x} - \frac{2}{g-2}$$

is a monotonically decreasing function on $[1, \frac{g-1}{2}]$. Thus, when $x = \frac{g-2}{2}$, F(x) get the minimum value

$$F(\frac{g-2}{2}) = \frac{8(g-1)}{g^2 + 2g - 4} - \frac{2}{g-2} - \frac{2}{g} - \frac{2}{g+2},$$

since

$$g \to \infty, F(\frac{g-2}{2}) \to \frac{2}{g} > 0.$$

Actually, by simple calculation, we have F(x) > 0 when $g \ge 8$, it follows that $\Theta_2 > 0$ when $g \ge 8$. (ii) Using the same argument as Equation (1), we can check that if g is an odd integer, $\Theta_2 > 0$ for all $g \ge 8$.

Comparing Θ_1 and Θ_2 , it is easy to see that

$$RH(S_n^g) < RH(S_n^{g-1}),$$

since $g \ge 8$. For g = 3, 4, ..., 7, we calculate $RH(S_n^3)$, $RH(S_n^4)$, $RH(S_n^5)$, $RH(S_n^6)$, $RH(S_n^7)$ and compare the values. We have

$$\begin{split} RH(S_n^3) &= RH(C_3) + \sum_{x,y \in V(G \setminus C_3)} \frac{1}{r(x,y)} + \sum_{x \in V(G), y \in V(C_3)} \frac{1}{r(x,y)} \\ &= \frac{1}{20} (5n^2 + 9n + 18), \\ RH(S_n^4) &= RH(C_4) + \sum_{x,y \in V(G \setminus C_4)} \frac{1}{r(x,y)} + \sum_{x \in V(G), y \in V(C_4)} \frac{1}{r(x,y)} \\ &= \frac{1}{84} (21n^2 + 33n + 148). \end{split}$$

Then,

$$RH(S_n^3) - RH(S_n^4) = \frac{2n}{35} - \frac{181}{210}.$$

Thus, we can get

$$\begin{cases} RH(S_n^3) < RH(S_n^4) & \text{if } n \le 15, \\ RH(S_n^3) > RH(S_n^4) & \text{if } n \ge 16. \end{cases}$$

In a similar way, by calculating $RH(S_n^5)$, $RH(S_n^6)$, and $RH(S_n^7)$ and comparing the values, we can get the following set of inequalities,

$$\begin{cases} RH(S_n^3) < RH(S_n^4) < \dots < RH(S_n^{n-1}) < RH(S_n^n) & \text{if } n \le 7, \\ RH(S_n^3) < RH(S_n^7) < RH(S_n^6) < RH(S_n^4) < RH(S_n^5) & \text{if } n = 8, \\ RH(S_n^7) < RH(S_n^3) < RH(S_n^6) < RH(S_n^5) < RH(S_n^4) & \text{if } n = 9, \\ RH(S_n^7) < RH(S_n^6) < RH(S_n^3) < RH(S_n^5) < RH(S_n^4) & \text{if } n = 10, \\ RH(S_n^7) < RH(S_n^6) < RH(S_n^5) < RH(S_n^3) < RH(S_n^3) < RH(S_n^4) & \text{if } 11 \le n \le 15, \\ RH(S_n^7) < RH(S_n^6) < RH(S_n^5) < RH(S_n^4) < RH(S_n^3) & \text{if } n \ge 16. \end{cases}$$

To sum up, we can get $RH(C_n)$ has the largest value $\frac{343}{20}$ if $n \le 7$, $RH(S_n^5)$ has the largest value $\frac{923}{44}$ if n = 8, $RH(S_n^4)$ has the largest value $\frac{1}{84}(21n^2 + 33n + 148)$ if $9 \le n \le 15$ and $RH(S_n^3)$ has the largest value $\frac{1}{20}(5n^2 + 9n + 18)$ if $n \ge 16$. The proof is completed. \Box

In [23], the unique element of U(n) with the largest Resistance-Harary index is determined. Herewith, we point out some minor errors in [23]. These do not affect the validity of the final result of [23] but deserve to be corrected. We list the error as follows and we give a counterexample.

Theorem 2. [23] Let $G \in U(n)$, then we have $RH(G) \leq \frac{1}{20}(n^2 + 9n + 18)$ with equality holding if and only if $G \cong S_n^3$ for $n \geq 9$ and $G \cong C_n$ for $n \leq 8$.

Counterexample

If n = 9, according to Theorem 2 in [23], the largest Resistance-Harary index is $HR(S_9^3) = 25.2000$. However, $HR(S_9^4) = 25.5476$, $HR(S_9^3) < HR(S_9^4)$, is a contradiction. If n = 8, according to the Theorem 2 in [23], the result is $RH(C_8) = 20.7429$ has the largest value. However, $RH(S_8^5) = 20.9773$, $RH(C_8) < RH(S_8^5)$, is a contradiction. Actually, according to our Theorem 1, we have $HR(S_9^4) > HR(S_9^3)$ if n = 9 and $RH(S_8^5) > RH(C_8)$ if n = 8. Obviously, the result is consistent with our theorem.

3.2. The Second-Maximum Resistance-Harary Index

By Lemmas 2 and 3 and Equation (2) of the proof of Theorem 1, we can conclude that for $n \ge 16 G$ which has the second-largest Resistance-Harary index in U(n) and those must be one of the graphs G_1, G_2 , and $G_3(S_n^4)$, as shown in Figure 3.



Theorem 3. If $G \in U(n)$, let $max^* \{RH(G)\}$ denote the second-largest Resistance-Harary index of graph *G*, then

$$\max_{G \in \mathcal{U}(n)}^{*} \{RH(G)\} = \begin{cases} RH(S_n^{n-1}) & \text{if } n \leq 7, \\ RH(S_n^4) & \text{if } n = 8, \\ RH(S_n^5) & \text{if } n = 9, 10, \\ RH(S_n^3) & \text{if } 11 \leq n \leq 15, \\ RH(S_n^4) & \text{if } n \geq 16. \end{cases}$$

Proof. (i) For $n \ge 16$.

Case 1. Let H_1 be the common subgraph of S_n^3 and G_1 . Thus, we can view graphs S_n^3 and G_1 as the graphs depicted in Figure 4.

Then, we have

$$\begin{aligned} RH(S_n^3) &= RH(H_1) + \frac{1}{2} + 2\sum_{x \in H_1} \frac{1}{1 + r(x, v_1)} \\ &= RH(H_1) + \frac{1}{2} + 2\left[1 + \frac{n-5}{2} + \frac{6}{5}\right], \\ RH(G_3) &= RH(H_1) + 1 + \sum_{x \in H_2} \frac{1}{1 + r(x, v_1)} + \sum_{x \in H_2} \frac{1}{2 + r(x, v_1)} \\ &= RH(H_1) + 1 + \left(1 + \frac{6}{5} + \frac{n-5}{2} + \frac{1}{2} + \frac{n-5}{3} + \frac{3}{4}\right). \end{aligned}$$

Therefore, we can get the difference

$$RH(S_n^3) - RH(G_1) = \frac{n}{6} - \frac{23}{60}.$$



Figure 4. The graphs S_n^3 and G_1 .

Case 2. Let H_2 be the common subgraph of S_n^3 and G_2 . Thus, we can view graphs S_n^3 and G_2 as the graphs depicted in Figure 5.

Then, we have

$$RH(S_n^3) = RH(S_n^3) + \sum_{x \in H_2} \frac{1}{1 + r(x, v_1)}$$
$$= RH(H_2) + \left[1 + \frac{n-4}{2} + \frac{6}{5}\right],$$
$$RH(G_2) = RH(H_2) + \sum_{x \in H_2} \frac{1}{1 + r(x, v_2)}$$
$$= RH(H_2) + \left[1 + \frac{3(n-4)}{8} + \frac{6}{5}\right].$$

Therefore, we can get the difference

$$RH(S_n^3) - RH(G_2) = \frac{n}{8} - \frac{1}{2}$$



Figure 5. The graphs S_n^3 and G_2 .

Case 3. Let H_3 be the common subgraph of S_n^3 and G_3 . Thus, we can view graphs S_n^3 and G_3 as the graphs depicted in Figure 6.

Then, we have

$$RH(S_n^3) = RH(H_3) + RH(S_4^3) + \sum_{x \in H_3, y \in S_4^3} \frac{1}{r(x, y)}$$
$$= RH(H_3) + \frac{67}{10} + \frac{27(n-4)}{10},$$
$$RH(G_3) = RH(H_3) + RH(C_4) + \sum_{x \in H_3, y \in C_4} \frac{1}{r(x, y)}$$
$$= RH(H_3) + \frac{22}{3} + \frac{37(n-4)}{14}.$$

Therefore, we can get the difference

$$RH(S_n^3) - RH(G_3) = \frac{2n}{35} - \frac{181}{210}.$$

By the above expressions for the Resistance-Harary index of G_1 , G_2 and G_3 , we immediately have the desired result.



Figure 6. The graphs S_n^3 and G_3 .

(ii) *For* $9 \le n \le 15$.

By the same arguments as used in (i), we conclude that the possible candidates having the second-largest Resistance-Harary index must be one of the graphs G_4 , G_5 , G_6 , $G_7(S_n^5)$ (as shown in Figure 7) and S_n^3 .



Figure 7. The graphs $G_4 - G_7$.

Let H_4 , H_5 , H_6 denote the common subgraphs of S_n^4 and $G_4 - G_7$, respectively. Thus, we can view graphs $G_4 - G_7$ as the graphs depicted in Figure 8.



Figure 8. The graphs $G_4 - G_7$.

Then, in a similar way, we have

$$RH(S_n^4) - RH(G_4) = \frac{n}{6} - \frac{193}{402},$$

$$RH(S_n^4) - RH(G_5) = \frac{3n}{22} - \frac{12}{22},$$

$$RH(S_n^4) - RH(G_6) = \frac{n}{6} - \frac{5}{6},$$

$$RH(S_n^4) - RH(G_7) = \frac{85n}{693} - \frac{2921}{2772}$$

Therefore, we have $HR(G_4) < HR(G_6) < HR(G_5) < HR(G_7)$. In connection with Equation (2), we have $G_7(S_n^5) < S_n^3$ if $11 \le n \le 15$, so for $11 \le n \le 15$, S_n^3 is the second largest. For n = 9, 10, in connection with Equation (2), we have S_n^5 is the second largest.

(iii) For $n \leq 7$ and n = 8.

In connection with Equation (2), we have S_n^{n-1} , S_n^4 is the second largest, respectively. The result follows. \Box

4. Application

Now, we give a specific application of formation mentioned in the Section 3. Fully loaded graphs as a special class of unicyclic graphs also have some special properties about Resistance-Harary index. In this section, we determine the largest Resistance-Harary index among all fully loaded unicyclic graphs.

By a sequence of α and β transformations to a fully loaded graph *G*, we can obtain a new graph, denoted by Q_n^l , which is obtained by attaching a pendent edge to each vertex of the unique cycle C_l and attaching n - 2l + 1 pendent edges to a vertex of C_l . Then, by Lemma 2 and Corollary 1, we arrive at,

Theorem 4. $G \in \mathfrak{U}(n;g)$, then $RH(G) \leq RH(Q_n^g)$.

Next, we determine the graph in $\mathfrak{U}(n)$ with the largest Resistance-Harary index.

Theorem 5. *If* $G \in \mathfrak{U}(n)$ *, then*

$$\max_{G \in \mathfrak{U}(n)} \{ RH(G) \} = \begin{cases} RH(Q_n^3) & \text{if } n \le 7, \\ RH(Q_n^4) & \text{if } n = 8,9, \\ RH(Q_n^3) & \text{if } n \ge 10. \end{cases}$$

Proof. Using a similar way as in Section 3.2, we can conclude that the unicyclic graphs with $n \ge 16$ in Figure 9 have the second largest or third largest Resistance-Harary index.



Figure 9. The graphs with second maximal or third maximal Resistance-Harary index.

Only one graph Q_n^3 is fully loaded (Graph 9 in Figure 9). Thus, Q_n^3 has the largest Resistance-Harary index among all fully loaded graphs with $n \ge 16$. For $n \le 15$, from Lemmas 2 and 3 we can conclude that the fully loaded graph with largest Resistance-Harary index must be one of the five situations $Q_n^3, Q_n^4, Q_n^5, Q_n^6, Q_n^7$.

For completeness of the proof, we list all possible values as follows. For $n \le 7$, there is only one situation Q_7^3 with n = 7 and Q_6^3 with n = 6, so we begin at n = 8.

Case 1. *n* = 8.

$$RH(Q_8^3) = 19.625, RH(Q_8^4) = 20.026.$$

Then, $\max_{G \in \mathfrak{U}(n)} \{RH(G)\} = RH(Q_8^4).$ Case 2. n = 9.

$$RH(Q_9^3) = 24.075, RH(Q_9^4) = 24.229.$$

Then, $\max_{G \in \mathfrak{U}(n)} \{RH(G)\} = RH(Q_9^4)$. **Case 3.** n = 10.

$$RH(Q_{10}^3) = 29.025, RH(Q_{10}^4) = 28.933, RH(Q_{10}^5) = 28.866$$

Then, $\max_{G \in \mathfrak{U}(n)} \{ RH(G) \} = RH(Q_{10}^3).$ Case 4. n = 11.

$$RH(Q_{11}^3) = 34.475, RH(Q_{11}^4) = 34.136, RH(Q_{11}^5) = 33.725.$$

Then, $\max_{G \in \mathfrak{U}(n)} \{ RH(G) \} = RH(Q_{11}^3).$ Case 5. n = 12.

$$RH(Q_{12}^3) = 40.425, RH(Q_{12}^4) = 39.840, RH(Q_{12}^5) = 39.085, RH(Q_{12}^6) = 38.563$$

Then, $\max_{G \in \mathfrak{U}(n)} \{ RH(G) \} = RH(Q_{12}^3).$ Case 6. n = 13.

$$RH(Q_{13}^3) = 46.875, RH(Q_{13}^4) = 46.043, RH(Q_{13}^5) = 44.944, RH(Q_{13}^6) = 44.003.$$

Then, $\max_{G \in \mathfrak{U}(n)} \{RH(G)\} = RH(Q_{13}^3).$ **Case 7.** n = 14. $RH(Q_{14}^3) = 53.825, RH(Q_{14}^4) = 52.747, RH(Q_{14}^5) = 51.303,$ $RH(Q_{14}^6) = 49.942, RH(Q_{14}^7) = 49.987.$ Then, $\max_{G \in \mathfrak{U}(n)} \{RH(G)\} = RH(Q_{14}^3).$ **Case 8.** n = 15. $RH(Q_{15}^3) = 61.275, RH(Q_{15}^4) = 59.950, RH(Q_{15}^5) = 58.163,$ $RH(Q_{15}^6) = 56.382, RH(Q_{15}^7) = 54.946.$ Then $\max \{RH(G)\} = RH(Q_{13}^3)$

Then, $\max_{G \in \mathfrak{U}(n)} \{RH(G)\} = RH(Q_{15}^3)$. The proof is completed. \Box

5. Conclusions

This paper focuses on Resistance-Harary index in unicyclic graphs. Let $\mathcal{U}(n)$ and $\mathfrak{U}(n)$ be the set of unicyclic graphs and fully loaded unicyclic graphs, respectively. Here, we first give a more precise proof about the largest Resistance-Harary index among all unicyclic graphs, then determine the graph of $\mathcal{U}(n)$ with second-largest Resistance-Harary index and apply this way to fully loaded unicyclic graphs determine the graph of $\mathfrak{U}(n)$ with largest Resistance-Harary index.

Author Contributions: Funding Acquisition, J.L. and J.-B.L.; Methodology, J.-B.L. and J.L.; Supervision, X.-F.P.; and Writing—Original Draft, J.L. and S.-B.C. All authors read and approved the final manuscript.

Funding: This work was supported by the National Natural Science Foundation of China (11601006), the China Postdoctoral Science Foundation (2017M621579), the Postdoctoral Science Foundation of Jiangsu Province (1701081B), the Project of Anhui Jianzhu University (2016QD116 and 2017dc03) and the Anhui Province Key Laboratory of Intelligent Building and Building Energy Saving.

Conflicts of Interest: The authors declare no conflict of interest.

References

- 1. Klein, D.J.; Randić, M. Resistance distance. J. Math. Chem. 1993, 12, 81–95. [CrossRef]
- Du, J.; Su, G.; Tu, J.; Gutman, I. The degree resistance distance of cacti. *Discrete Appl. Math.* 2015, 188, 16–24. [CrossRef]
- 3. Bu, C.; Yan, B.; Zhou, X.; Zhou, J. Resistance distance in subdivision-vertex join and subdivision-edge join of graphs. *Linear Algebra Appl.* **2014**, *458*, 454–462. [CrossRef]
- 4. Feng, L.H.; Yu, G.; Liu, W. Futher results regarding the degree Kirchhoff index of a graph. *Miskolc Math. Notes* **2014**, *15*, 97–108. [CrossRef]
- 5. Feng, L.H.; Yu, G.; Xu, K.; Jiang, Z. A note on the Kirchhoff index of bicyclic graphs. *ARS Combin.* **2014**, *114*, 33–40.
- Gao, X.; Luo, Y.; Liu, W. Resistance distance and the Kirchhoff index in Cayley graphs. *Discrete Appl. Math.* 2011, 159, 2050–2057. [CrossRef]
- 7. Gao, X.; Luo, Y.; Liu, W. Kirchhoff index in line, subdivision and total graphs of a regular graph. *Discrete Appl. Math.* **2012**, *160*, 560–565. [CrossRef]
- 8. Gutman, I.; Feng, L.; Yu, G. On the degree resistance distance of unicyclic graphs. Trans. Comb. 2012, 1, 27–40.
- 9. Liu, J.; Pan, X.; Yu, L.; Li, D. Complete characterization of bicyclic graphs with minimal Kirchhoff index. *Discrete Appl. Math.* 2016, 200, 95–107. [CrossRef]
- 10. Liu, J.; Wang, W.; Zhang, Y.; Pan, X. On degree resistance distance of cacti. *Discrete Appl. Math.* **2016**, 203, 217–225. [CrossRef]
- 11. Liu, J.; Pan, X. Minimizing Kirchhoff index among graphs with a given vertex bipartiteness. *Appl. Math. Comput.* **2016**, 291, 84–88. [CrossRef]

- 12. Pirzada, S.; Ganie, H.A.; Gutman, I. On Laplacian-Energy-Like Invariant and Kirchhoff Index. *MATCH Commun. Math. Comput. Chem.* **2015**, *73*, 41–59.
- 13. Plavšić, D.; Nikolić, S.; Mihalić, Z. On the Harary index for the characterization of chemical graphs. *J. Math. Chem.* **1993**, *12*, 235–250.
- 14. Ivanciuc, O.; Balaban, T.S.; Balaban, A.T. Reciprocal distance matrix, related local vertex invariants and topological indices. *J. Math. Chem.* **1993**, *12*, 309–318. [CrossRef]
- 15. Furtula, B.; Gutman, I.; Katanić, V. Three-center Harary index and its applications. *Iranian J. Math. Chem.* **2016**, *7*, 61–68.
- 16. Feng, L.H.; Lan, Y.; Liu, W.; Wang, X. Minimal Harary index of graphs with samll parameters. *MATCH Commun. Math. Comput. Chem.* **2016**, *76*, 23–42.
- 17. Li, X.; Fan, Y. The connectivity and the Harary index of a graph. *Discrete Appl. Math.* **2015**, *181*, 167–173. [CrossRef]
- 18. Xu, K.; Das, K.C. On Harary index of graphs. Discrete Appl. Math. 2011, 159, 1631–1640. [CrossRef]
- 19. Xu, K. Trees with the seven smallest and eight greatest Harary indices. *Discrete Appl. Math.* **2012**, *160*, 321–331. [CrossRef]
- 20. Xu, K.; Das, K.C. Extremal unicyclic and bicyclic graphs with respect to Harary index. *Bull. Malays. Math. Sci. Soc.* **2013**, *36*, 373–383.
- 21. Xu, K.; Wang, J.; Das, K.C.; Klavžar, S. Weighted Harary indices of apex trees and k-apex trees. *Discrete Appl. Math.* 2015, 189, 30–40. [CrossRef]
- 22. Yu, G.; Feng, L. On the maximal Harary index of a class of bicyclic graphs. Util. Math. 2010, 82, 285–292.
- Chen, S.B.; Guo, Z.J.; Zeng, T.; Yang, L. On the Resistance-Harary index of unicyclic graphs. *MATCH Commun. Math. Comput. Chem.* 2017, 78, 189–119.
- 24. Wang, H.; Hua, H.; Zhang, L.; Wen, S. On the Resistance-Harary Index of Graphs Given Cut Edges. *J. Chem.* 2017, 2017, 3531746.



© 2019 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/).