Extremal degree resistance distances in fully loaded unicyclic graphs

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Abstract

Let G be a connected graph, the degree resistance distance of G is defined as $D_R(G) = \sum_{\{u,v\} \subseteq V(G)} [d(u) + d(v)]r(u,v)$, where d(u) (and

d(v) is the degree of the vertex u (and v), r(u,v) is the resistance distance between vertices u and v. A fully loaded unicyclic graph is a unicyclic graph with the property that there is no vertex with degree less than 3 in its unique cycle. In this paper, we determine the minimum and maximum degree resistance distance among all fully loaded unicyclic graphs with n vertices, and characterize the extremal graphs.

1 Introduction

All graphs considered here are both connected and simple unless otherwise stated. The distance between vertices u and v of the graph G, denoted by d(u,v), is the length of a shortest path between them. The degree of vertex u is d(u); n,m are the number of vertices and edges of G, respectively. The girth of a graph G is the length of the shortest cycle in G.

The famous Wiener index was introduced by Harold Wiener in 1947, defined as[1]

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

A modified version of the Wiener index is the degree distance, was introduce by A. A. Dobrynin and A. A. Kochetova[2], defined as

$$D(G) = \sum_{\{u,v\} \subseteq V(G)} [d(u) + d(v)]d(u,v)$$
 (2)

If G is a tree on n vertices, the Wiener index and the degree distance are related as D(G) = 4W(G) - n(n-1) (for details see [3]).

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In [4], a multiplicative variant of the degree distance, namely modified Schultz index or Gutman index was put forward, defined as

$$S^*(G) = \sum_{\{u,v\} \subseteq V(G)} d(u)d(v)d(u,v)$$
 (3)

If G is a tree on n vertices, the Wiener index and the modified Schultz index are related as $S^*(G) = 4W(G) - (2n-1)(n-1)$ (for details see [4]). The modified Schultz index of graphs attracted attention recently. In [5] an asymptotic upper bound for $S^*(G)$ was reported. In [6], a relation between the edge Wiener index and modified Schultz index was established, and S. Mukwembi in [7] improved on a bound by Dankelmann, Gutman, Mukwembi and Swart established in [6]. The maximal and minimal modified Schultz index of bicyclic graphs are determined in [8] and [9], respectively.

The concept of resistance distance was introduced by Klein and Randić [10] in 1993, on the basis of electrical network theory. They viewed a graph G as an electrical network N such that each edge of G is assumed to be a unit resistor. The resistance distance between the vertices u and v of a graph G, denoted by r(u, v), is defined to be the effective resistance between nodes $u, v \in N$. Analogous to the definition of the Wiener index, the Kirchhoff index Kf(G) of a graph G is defined as [10, 11]

$$Kf(G) = \sum_{\{u,v\} \subseteq V(G)} r(u,v) \tag{2}$$

If G is a tree, then r(u, v) = d(u, v) for any two vertices u and v, the Kirchhoff and Wiener indices of trees coincide.

The Kirchhoff index is an important molecular structure descriptor [12], it has been well studied in both mathematical and chemical literatures. For a general graph G, I. Lukovits et al. [13] showed that $Kf(G) \geq n-1$ with equality if and only if G is complete graph K_n . J. L. Palacios [14] showed that $Kf(G) \leq \frac{n^3-n}{6}$ with equality if and only if G is a path P_n . For a circulant graph G, ref. [15] showed that $n-1 \leq Kf(G) \leq \frac{n^3-n}{12}$, the first equality holds if and only if G is K_n and the second does if and only if G is C_n . The unicyclic graphs with extremal Kirchhoff index were determined in [16, 17]. H. Deng also studied the Kirchhoff index of fully loaded unicyclic graphs [18] and graphs with cut edges [19]. H. Zhang et al. [20] characterized bicyclic graphs with extremal Kirchhoff indices. B. Zhou [21] characterized the extremal graphs with given matching number, connectivity. H. Wang et al. [22] determined the first three minimal Kirchhoff indices among cacti. R. Li in [22] obtained newer lower bounds for the Kirchhoff index of a connected graph.

The degree Kirchhoff index was put forward in [23], and further studied in [24, 25], defined as

$$R^*(G) = \sum_{\{u,v\} \subseteq V(G)} d(u)d(v)r(u,v)$$
 (3)

Comparing Eqs. (2) and (3) we can see that the degree Kirchhoff index may be viewed as the resistance distance analogue of the Schultz index. However, there is a much more subtle reason for the introduction of this novel structure descriptor.

The degree resistance distance was introduced by I. Gutman, L. Feng and G. Yu in [26]:

$$D_R(G) = \sum_{\{u,v\} \subseteq V(G)} [d(u) + d(v)]r(u,v)$$
 (4)

They investigated the degree resistance distance of unicyclic graphs, determined the unicyclic graphs with the minimum and second minimum degree resistance distance. Chen et al. [27] determined unicyclic graphs with the maximum and second maximum degree resistance distance. J. L. Palacios in [28] renamed the degree resistance distance as additive degree Kirchhoff index, gave tight upper and lower bounds for the degree resistance distance of a connected undirected graph.

If G is a tree, the degree distance and the degree resistance distance coincide as well, i.e., $D_R(G) = 4W(G) - n(n-1)$.

A graph G is called a unicyclic graph if it contains exactly one cycle. For convenience, we represent a unicyclic graph G with the unique cycle $C_l = v_1 v_2 \cdots v_l v_1$ as $G = U(C_l; T_1, T_2, \cdots, T_l)$, where T_i is the component of $G - E(C_l)$ and T_i is a tree rooted at v_i ; T_i is trivial if it is an isolated vertex. A fully loaded unicyclic graph is a unicyclic graph with the property that there is no vertex with degree less than 3 in its unique cycle. If $G = U(C_l; T_1, T_2, \cdots, T_l)$ is a fully loaded unicyclic graph, then T_1, T_2, \cdots, T_l are all nontrivial. Let $\mathcal{U}(n; l)$ be the set of all fully loaded unicyclic graphs with n vertices and the unique cycle C_l , $\mathcal{U}(n)$ be the set of all fully loaded unicyclic graphs with n vertices; S_n and P_n be the star and the path on n vertices, respectively.

The paper is organized as follows. In Section 2, we introduce some lemmas and two transformations which decrease the degree resistance of graphs and a transformation which increases the degree resistance degree of a graph. In Section 3, we obtain a formula for calculating the degree resistance distance of graphs in $\mathscr{U}(n;l)$, and determine graphs in $\mathscr{U}(n)$ with the maximum and the minimum degree resistance distance by analytic methods.

2 Preliminary Results

For a graph G with $v \in V(G)$, G - v denotes the graph obtained from G by deleting v (and its incident edges); and for an edge uv of the graph G (the complement of G, respectively), G - uv(G + uv), respectively) denotes the graph resulting from G by deleting (adding, respectively) the edge uv.

For a vertex $v \in V(G)$, let

$$r(v|G) = \sum_{u \in V(G)} r(u, v), \ S'(v|G) = \sum_{u \in V(G)} d(u)r(u, v)$$

 C_n be the cycle on $n \geq 3$ vertices, for any two vertices $v_i, v_j \in V(C_n)$ with i < j, by Ohm's law, we have $r(v_i, v_j) = {(j-i)(n+i-j) \choose n}$; for any vertex $u \in V(C_n)$, it's suffice to see that $r(u|C_n) = {n^2-1 \over 6}$, $S'(u|C_n) = {n^2-1 \over 3}$.

Lemma 2.1([29]). Let T be any n vertices trees, then $(n-1)^2 \leq W(T) \leq \frac{n^3-n}{6}$, the left equality holds if and only if $G \cong S_n$ and the right holds if and only if $G \cong P_n$.

Lemma 2.2([2]). Let x be a cut vertex of a connected graph and a and b be vertices occurring in different components which arise upon deletion of x, then r(a, b) = r(a, x) + r(x, b).

Lemma 2.3([26]). Let G_1 and G_2 be connected graphs with disjoint vertex sets, with n_1 , n_2 vertices, and m_1 , m_2 edges, respectively; $u_1 \in V(G_1)$, $u_2 \in V(G_2)$. Constructing the graph G by identifying the vertices u_1 with u_2 , and denote the so obtained vertex by u. Then $D_R(G) = D_R(G_1) + D_R(G_2) + 2m_2r(u_1|G_1) + 2m_1r(u_2|G_2) + (n_2 - 1)S'(u_1|G_1) + (n_1 - 1)S'(u_2|G_2)$.

Let X and Y be two nontrivial connected graphs, such that $u \in V(X)$, $v \in V(Y)$; G be the graph obtained from X and Y by adding the edge uv. We form a graph $G' = \alpha(G, u)$ by identifying vertices u and v, and adding one pendant edge at u. We say that G' is a α -transform of G(see Figure 1).

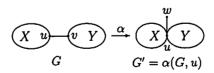


Figure 1. The transformation α

Lemma 2.4. Let $G' = \alpha(G, u)$ be a α -transform of the graph G, then $D_R(G) > D_R(G')$.

Proof. Assume that H is the graph induced by $V(Y) \cup \{u\}$, and $|E(X)| = m_1$, $|E(Y)| = m_2$, $|V(X)| = n_1$, $|V(Y)| = n_2$. By Lemma 2.3, one has $D_R(H) = D_R(Y) + 2r(v|Y) + S'(v|Y) + 2m_2 + n_2 - 1$. Then

$$\begin{split} &D_R(G) \\ &= D_R(X) + D_R(H) + 2(m_2 + 1)r(u|X) + 2m_1r(u|H) + n_2S'(u|X) \\ &+ (n_1 - 1)S'(u|H) \\ &= D_R(X) + D_R(Y) + 2(m_2 + 1)r(u|X) + 2(m_1 + 1)r(v|Y) + n_2S'(u|X) \\ &+ n_1S'(v|Y) + 2m_1n_2 + 2m_2n_1 + n_1 + n_2 \end{split}$$

and analogously,

$$D_R(G') = D_R(X) + D_R(Y) + 2(m_2 + 1)r(u|X) + 2(m_1 + 1)r(v|Y) + n_2S'(u|X) + n_1S'(v|Y) + 2m_1 + 2m_2 + n_1 + n_2$$

So we get $D_R(G) - D_R(G') = 2m_1(n_2 - 1) + 2m_2(n_1 - 1) > 0$. This proves the result.

Let X, Y and Z be three connected graphs with $u' \in V(Y)$ and $v' \in V(Z)$. Suppose that u and v are two vertices of X. Let G be the graph obtained from X, Y, Z by identifying v with v' and u with u', respectively. Let G' be the graph obtained from X, Y, Z by identifying the vertices u, v', u', and G'' be the graph obtained from X, Y, Z by identifying the vertices v, v', u', as shown in Figure 2. Analogously, we say that G' and G'' are β -transformed from G.

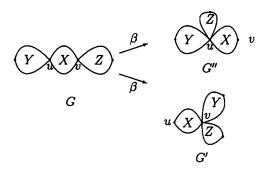


Figure 2. The transformation β

Lemma 2.5. Let G', G'' are graphs β -transformed from G. Then $D_R(G') < D_R(G)$ and $D_R(G'') < D_R(G)$.

Proof. Let $|E(X)| = m_1$, $|E(Y)| = m_2$, $|E(Z)| = m_3$; $|V(X)| = n_1$, $|V(Y)| = n_2$, $|V(Z)| = n_3$. H is the graph induced by $V(X) \cup V(Y)$ in G,

G'. By Lemma 2.3, one has

$$\begin{split} D_R(G) &= D_R(Z) + D_R(H) + 2m_3r(v|H) + 2(m_1 + m_2)r(v|Z) \\ &+ (n_3 - 1)S'(v|H) + (n_1 + n_2 - 2)S'(v|Z) \\ \\ r(v|H) &= \sum_{z \in V(H)} r(v,z) = r(v|X) + r(u|Y) + (n_2 - 1)r(u,v), \\ \\ S'(v|H) &= \sum_{z \in V(H)} d(z)r(v,z) = S'(v|X) + S'(u|Y) + 2m_2r(u,v). \end{split}$$

Thus,

$$D_R(G) = D_R(Z) + D_R(H) + 2m_3[r(v|X) + r(u|Y) + (n_2 - 1)r(u, v)] + 2(m_1 + m_2)r(v|Z) + (n_3 - 1)[S'(v|X) + S'(u|Y) + 2m_2r(u, v)] + (n_1 + n_2 - 2)S'(v|Z)$$

and analogously,

$$D_R(G') = D_R(Z) + D_R(H) + 2m_3[r(v|X) + r(u|Y)] + 2(m_1 + m_2)r(v|Z) + (n_3 - 1)[S'(v|X) + S'(u|Y)] + (n_1 + n_2 - 2)S'(v|Z)$$

Thus, $D_R(G) - D_R(G') = [2m_2(n_3 - 1) + 2m_3(n_2 - 1)]r(u, v) > 0$. By the similar argument, one has

$$D_R(G) - D_R(G'') = [2m_2(n_3 - 1) + 2m_3(n_2 - 1)]r(u, v) > 0.$$

The proof is completed.

Suppose that G be a graph of order $n \geq 7$ obtained from a connected graph $H \neq P_1$ and a cycle $C_r = u_0 u_1 \cdots u_r$, $r \geq 4$ by identifying u_0 with a vertex u of the graph H; $G' = G - u_{r-1} u_{r-2} + u u_{r-2}$ (see Figure 3), We say G' is a graph γ -transformed from G.

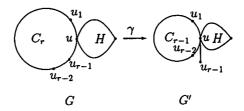


Figure 3. The transformation γ

Lemma 2.6. Let G and G' are two graphs depicted in Figure 3, then $D_R(G) \geq D_R(G')$.

Proof. Assume that $|E(H)| = m_h$, $|V(H)| = n_h$, by Lemma 2.3, one has

$$\begin{split} &D_R(G)\\ &=D_R(C_r)+D_R(H)+2m_hr(v|C_r)+2rr(v|H)+(n_h-1)S'(v|C_r)\\ &+(r-1)S'(v|H)\\ &=\frac{1}{3}(r^3-r)+D_R(H)+2m_h\frac{r^2-1}{6}+2rr(v|H)+(n_h-1)\frac{r^2-1}{3}\\ &+(r-1)S'(v|H)\\ &=D_R(H)+2rr(v|H)+(r-1)S'(v|H)+\frac{r^3-1}{3}+\frac{r^2-1}{3}(m_h+n_h-1)\\ &\text{and analogously,} \end{split}$$

$$D_R(G') = D_R(H) + 2rr(v|H) + (r-1)S'(v|H) + \frac{r^3 - r^2 + 7r - 6}{3} + \frac{r^2 - 2r + 6}{3}m_h + \frac{r^2 - 2r + 3}{3}(n_h - 1)$$

Thus, one has

$$D_R(G) - D_R(G') = \frac{r^2 - 8r + 6}{3} + \frac{2r - 7}{3}m_h + \frac{2r - 4}{3}(n_h - 1)$$

$$= \frac{(r - 4)^2 - 10}{3} + \frac{2r - 7}{3}m_h + \frac{2r - 4}{3}(n_h - 1)$$

$$> \frac{-10}{3} + \frac{1}{3}m_h + \frac{4}{3}(n_h - 1) \ge 0$$

Lemma 2.7[28]. Let G_0 be a connected graphs with $m_0 > 1$ edges, and $u, v \in V(G_0)$ be two distinct vertices with degree at least 3 in G_0 such that r(u, v) = l. Let $P_s = u_1 u_2 \cdots u_s$ and $P_t = v_1 v_2 \cdots v_t$ be two paths of order $s \ge 1$ and $t \ge 1$, respectively; $G_{s,t}$ be the graph obtained from G_0 , P_s and P_t by adding edges uu_1, vv_1 . Suppose that $G_{s-1,t+1} = G_{s,t} - u_r u_{r-1} + v_t u_r$ and $G_{s+1,t-1} = G_{s,t} - v_{t-1} v_t + u_s v_t$. Then either $D_R(G_{s,t}) < D_R(G_{s-1,t+1})$ or $D_R(G_{s,t}) < D_R(G_{s+1,t-1})$.

3 Extremal degree resistance distance in fully loaded unicyclic graphs

3.1 Extremal degree resistance distance of $\mathcal{U}(n;l)$

In this section, we shall determine the graph in $\mathcal{U}(n;l)$ with the maximum and the minimum degree resistance distance.

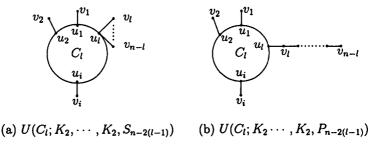


Figure 4.

Theorem 3.1. Let $G \in \mathcal{U}(n;l)$ be an arbitrary fully loaded unicyclic graph with girth l. Then $D_R(U(C_l;K_2,\cdots,K_2,S_{n-2(l-1)})) \leq D_R(G)$ and $D_R(G) \leq D_R(U(C_l;K_2,\cdots,K_2,P_{n-2(l-1)}))$, the first equality holds if and only if $G \cong U(C_l;K_2,\cdots,K_2,S_{n-2(l-1)})$ and the second does if and only if $G \cong U(C_l;K_2,\cdots,K_2,P_{n-2(l-1)})$. $U(C_l;K_2,\cdots,K_2,S_{n-2(l-1)})$ and $U(C_l;K_2,\cdots,K_2,P_{n-2(l-1)})$ are depicted in Figure 4.

Proof. For the left inequality, we suppose that G' be the graph in $\mathscr{U}(n;l)$ has the minimum degree resistance distance. By Lemma 2.4, Lemma 2.5, one has $G' \cong U(C_l; K_2, \dots, K_2, S_{n-2(l-1)})$.

For the right inequality, suppose that G'' has the maximum degree resistance distance, then all trees $T_i (1 \le i \le l)$ attached to the cycle C_l must be paths by Lemma 2.4. Further, from Lemma 2.6, all paths are connected to one vertex of the only cycle C_l , then $G \cong U(C_l; K_2, \dots, K_2, P_{n-2(l-1)})$.

This completes the proof.

3.2 The minimum degree resistance distance of $\mathcal{U}(n)$

In this section, we determine the graph in $\mathscr{U}(n)$ with the minimum degree resistance distance.

Theorem 3.2. Let $G \in \mathcal{U}(n)$ with $n \geq 6$, then $D_R(G) \geq 3n^2 - \frac{n}{3} - 26$, the equality holds if and only if $G \cong U(C_3; K_2, K_2, S_{n-4})$.

Proof. Firstly, we shall compute $D_R(U(C_l; K_2, \dots, K_2, S_{n-2(l-1)}))$. As depicted in Figure 4(a), we let G_1 be the graph induced by u_i and v_i for $i = 1, 2, \dots, l$, G_2 be the graph induced by v_i $(i = l+1, l+2, \dots, n-l)$

and u_l . By the definition of degree resistance distance, one arrives at

$$\begin{split} &D_R(G_1) \\ &= \sum_{1 \leq i < j \leq l} [d(u_i) + d(u_j)] r(u_i, u_j) + \sum_{1 \leq i < j \leq l} [d(v_i) + d(v_j)] r(v_i, v_j) \\ &+ \sum_{i=1}^l \sum_{j=1}^l [d(u_i) + d(v_j)] r(u_i, v_j) \\ &= 6 \sum_{1 \leq i < j \leq l} r(u_i, u_j) + 2 \sum_{1 \leq i < j \leq l} (r(u_i, u_j) + 2) + 4 \sum_{i=1}^l \sum_{j=1}^l (r(u_i, u_j) + 1) \\ &= 6Kf(C_l) + 2Kf(C_l) + 4 \binom{l}{2} + 4(2Kf(C_l) + l^2) \\ &= 16Kf(C_l) + 6l^2 - 2l; \end{split}$$

and

$$D_R(G_2) = D_R(S_{n-2l+1}) = 3(n-2l)^2 - (n-2l);$$

$$r(u_l|G_2) = n-2l, \quad r(u_l|G_1) = l + \frac{l^2-1}{3};$$

$$S'(u_l|G_2) = n-2l, \quad S'(u_l|G_1) = \frac{2}{2}l^2 + l - \frac{2}{3}.$$

By Lemma 2.3, one has

$$D_R(U(C_l; K_2, \dots, K_2, S_{n-2(l-1)}))$$

$$= 16Kf(C_l) + 6l^2 - 2l + 3(n-2l)^2 - (n-2l) + 4l(n-2l)$$

$$+ 2(n-2l)(l + \frac{l^2 - 1}{3}) + (2l-1)(n-2l) + (n-2l)(\frac{2}{3}l^2 + l - \frac{2}{3})$$

$$= \frac{1}{2}(-4l^3 + 4nl^2 - 9nl + 10l + 9n^2 - 10n)$$

Nextly, we determine the graph in $U(C_l; K_2, \dots, K_2, S_{n-2(l-1)})$ with the smallest degree resistance distance.

Let
$$f(l) := D_R(U(C_l; K_2, \dots, K_2, S_{n-2(l-1)})) = \frac{1}{3}(-4l^3 + 4nl^2 - 9nl + 10l + 9n^2 - 10n), 3 \le l \le [\frac{n}{2}].$$

Case 1. If $6 \le n \le 7$, then $[\frac{n}{2}] = 3$ and l = 3. $f(l)_{min} = f(3) = 3n^2 - \frac{n}{3} - 26$.

Case 2. If $8 \le n \le 10$, then $\left[\frac{n}{2}\right] = 4,5$ and l = 3,4,5. Computing directly, one has

(1)
$$f(3) = \frac{490}{3} < f(4) = \frac{504}{3}$$
 for $n = 8$.

(2)
$$f(3) = \frac{642}{3} < f(4) = \frac{675}{3}$$
 for $n = 9$.

(3)
$$f(3) = \frac{812}{3} < f(4) = \frac{864}{3} < f(5) = 300 \text{ for } n = 10.$$

The first derivation of f(l) is $f'(l) = -4l^2 + \frac{8n}{3}l - 3n + \frac{10}{3}$, $3 \le l \le \lfloor \frac{n}{2} \rfloor$.

Let
$$f'(l) = 0$$
, then $l_{1,2} = \frac{2n \mp \sqrt{4n^2 - 27n + 30}}{6}$

Let f'(l) = 0, then $l_{1,2} = \frac{2n \mp \sqrt{4n^2 - 27n + 30}}{\frac{6}{2}}$. It's easy to verify that $l_1 < 3$, $l_2 > [\frac{n}{2}]$. Thus, f'(l) > 0 in the interval $I := \left[3, 4, \cdots, \left[\frac{n}{2}\right]\right]$. Therefore, $f(l)_{min} = f(3) = 3n^2 - \frac{n}{3} - 26$.

Combining above three cases, one proves the theorem.

The maximum degree resistance distance of $\mathcal{U}(n)$ 3.3

In this section, we determine the graph in $\mathcal{U}(n)$ with the maximum degree resistance distance.

Theorem 3.3. Let $G \in \mathcal{U}(n)$ with $n \geq 6$, then $D_R(G) \leq \frac{2}{3}n^3 - 28n +$ 104, the equality holds if and only if $G \cong U(C_3; K_2, K_2, P_{n-4})$

Proof. For the graph $U(C_l; K_2, \dots, K_2, P_{n-2(l-1)})$, as shown in Figure 4(b), we let G_3 be the graph induced by u_i and v_i for $i = 1, 2, \dots, l, G_4$ be the graph induced by v_i $(i = l, l + 1, \dots, n - l)$.

By Theorem 3.2, one has

$$D_R(G_3) = 16Kf(C_l) + 6l^2 - 2l = \frac{4}{3}l^3 + 6l^2 - \frac{10}{3}l$$
, and

$$\begin{split} D_R(G_4) &= D_R(P_{n-2l+1}) \\ &= 4W(P_{n-2l+1}) - (n-2l+1)(n-2l) \\ &= 4 \times \frac{1}{6} \left((n-2l+1)^3 - (n-2l+1) \right) - (n-2l+1)(n-2l) \\ &= -\frac{16}{3} l^3 + (8n+4)l^2 - (4n^2 + 4n + \frac{2}{3})l + \frac{2}{3} n^3 + n^2 + \frac{n}{3}; \\ r(v_l|G_4) &= \frac{1}{2} (n-2l)(n-2l+1), \ r(v_l|G_3) = \frac{l^2}{3} + 3l - \frac{7}{3}; \end{split}$$

$$S'(v_l|G_4) = (n-2l)^2, \quad S'(v_l|G_3) = \frac{2}{3}l^2 + 5l - \frac{8}{3}.$$

By Lemma 2.3, one has

$$\begin{split} &D_R(U(C_l;K_2,\cdots,K_2,P_{n-2(l-1)}))\\ &=\frac{4}{3}l^3+6l^2-\frac{10}{3}l-\frac{16}{3}l^3+(8n+4)l^2-(4n^2+4n+\frac{2}{3})l+\frac{2}{3}n^3+n^2+\frac{n}{3}\\ &+2l(n-2l)(n-2l+1)+\frac{2}{3}(n-2l)(l^2+9l-7)+\frac{n-2l}{3}(2l^2+10l-8)\\ &+(2l-1)(n-2l)^2\\ &=\frac{1}{3}[28l^3-(20n+60)l^2+(39n+32)l+2n^3-21n] \end{split}$$

In the following, we investigate graph in $U(C_l; K_2, \dots, K_2, P_{n-2(l-1)})$ with the largest degree resistance distance.

Let
$$g(l) := D_R(U(C_l; K_2, \dots, K_2, P_{n-2(l-1)})) = \frac{1}{3} [28l^3 - (20n + 60)l^2 + (39n + 32)l + 2n^3 - 21n], 3 \le l \le [\frac{n}{2}].$$

The first derivation of g(l) is $g'(l) = 28l^2 - \frac{2l}{3}(20n + 60) + 13n + \frac{32}{3}$. The roots of g'(l) = 0 are $l_{1,2} = \frac{(10n + 30) \mp \sqrt{100n^2 - 219n + 228}}{42}$.

It's easy to verify that $l_1 < 3$, $l_2 > 3$ for $n \ge 6$.

Case 1. If $l_2 \geq [\frac{n}{2}]$, then g'(l) < 0 for $3 \leq l \leq [\frac{n}{2}]$. $g(l)_{max} = g(3) =$ $\frac{2}{3}n^3 - 28n + 104.$

Case 2. If $l_2 < [\frac{n}{2}]$, then g'(l) < 0 for $3 \le l \le l_2$ and g'(l) > 0 for $l_2 \le l \le \left[\frac{n}{2}\right].$

In this case,

$$\max\{D_R(U(C_l; K_2, \cdots, K_2, P_{n-2(l-1)}))\} = \max\{g(3), g(\lceil \frac{n}{2} \rceil)\}.$$

In the following, we shall compare g(3) with $g([\frac{\pi}{2}])$. Let

$$h(n) = g(3) - g(\left[\frac{n}{2}\right]).$$

If n is even and $n \geq 6$, then

$$h(n) = \left(\frac{2n^3}{3} - 28n + 104\right) - \left(\frac{n^3}{6} + \frac{3n^2}{2} - \frac{5n}{3}\right)$$
$$= \frac{n^3}{2} - \frac{3n^2}{2} - \frac{79n}{3} + 104$$
$$= \frac{1}{6}(n-6)(3n^2 + 9n - 104) \ge 0.$$

Thus,
$$g(3) \ge g(\frac{n}{2})$$
.

$$\max\{D_R(U(C_l;K_2,\cdots,K_2,P_{n-2(l-1)}))\}=D_R(U(C_3;K_2,K_2,P_{n-4})).$$

If n is odd and $n \geq 7$, then

$$h(n) = \left(\frac{2n^3}{3} - 28n + 104\right) - \left(\frac{n^3}{6} + \frac{4n^2}{3} + \frac{11n}{3} - \frac{23}{2}\right)$$
$$= \frac{n^3}{2} - \frac{4n^2}{3} - \frac{95n}{3} + \frac{231}{2}$$
$$= \frac{1}{6}(n-7)(3n^2 + 13n - 99) \ge 0.$$

So,
$$g(3) \ge g(\frac{n-1}{2})$$
.

$$\max\{D_R(U(C_l;K_2,\cdots,K_2,P_{n-2(l-1)}))\}=D_R(U(C_3;K_2,K_2,P_{n-4})).$$

Combining the two cases above, one arrives at the desired result.

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References

- [1] H. Wiener, Structural determination of paraffin boiling points, J. Amer. Chem. Soc. 69 (1947) 17-20.
- [2] A. A. Dobrynin and A. A. Kochetova, Degree distance of a graph: A degree analogue of the Wiener index, J. Chem. Inf. Comput. Sci. 34 (1994) 1082-1086.
- [3] D. J. Klein, Z. Mihalić, D. Plavšić, N. Trinajstić, Molecular topological index: A relation with the Wiener index, J. Chem. Inf. Comput. Sci. 32 (1992) 304-305.
- [4] R. Todeschini, V. Consonni, Molecular Descriptors for Chemoinformatics, Wiley-VCH, Weinheim, 2009.
- [5] P. Dankelmann, I. Gutman, S. Mukwembi, H. C. Swart, The edge-Wiener index of a graph, Discrete Math. 309(2009) 3452-3457.

- [6] S. Mukwembi, On the Upper Bound of Gutman Index of Graphs, MATCH Commun. Math. Comput. Chem. 68(2012) 343-348.
- [7] L. Feng, W. Liu, The Maximal Gutman Index of Bicyclic Graphs, MATCH Commun. Math. Comput. Chem. 66 (2011) 699-708.
- [8] S. Chen, W. Liu, Extremal modified Schultz index of bicyclic graphs, MATCH Commun. Math. Comput. Chem. 64 (2010) 767-782.
- [9] D. J. Klein and M. Randić, Resistance distance, J. Math. Chem. 12 (1993) 81-95.
- [10] D. Bonchev, A. T. Balaban, X. Liu, D. J. Klein, Molecular cyclicity and centricity of polycyclic graphs I. Cyclicity based on resistance distances or reciprocal distances, *Int. J. Quantum Chem.* 50 (1994) 1-20.
- [11] W. Xiao, I. Gutman, Resistance distance and Laplacian spectrum, *Theor. Chem. Acc.* **110** (2003) 284-289.
- [12] I. Lukovits, S. Nikolić, N. Trinajstić, Resistance distance in regular graphs, Int. J. Quantum Chem. 71 (1999) 217-225.
- [13] J. L. Palacios, Foster's Formulas via Probability and the Kirchhoff index, Methodology and Computing in Applied Probability. 6 (2004) 381-387.
- [14] J. L. Palacios, Resistance distance in graphs and random walks, Int. J. Quantum Chem. 81 (2001) 29-33.
- [15] Y. J. Yang, X. Y. Jiang, Unicyclic graphs with extremal Kirchhoff index, MATCH Commun. Math. Comput. Chem. 60 (2008) 107-120.
- [16] W. Zhang, H. Deng, The second maximal and minimal Kirchhoff Indices of Unicyclic Graphs, MATCH Commun. Math. Comput. Chem. 61 (2009) 683-695.
- [17] Q. Guo, H. Deng, D. Chen, The extremal Kirchhoff index of a class of unicyclic graphs, MATCH Commun. Math. Comput. Chem. 61 (2009) 713-722.
- [18] H. Deng, D. Chen, On the minimum Kirchhoff index of graphs with a given number of cut-edges, MATCH Commun. Math. Comput. Chem. 63 (2010) 171-180.
- [19] H. P. Zhang, X. Jiang, Y. J. Yang, Bicyclic graphs with extremal Kirchhoff index, MATCH Commun. Math. Comput. Chem. 61 (2009) 697-712.

- [20] B. Zhou, N. Trinajstić, The Kirchhoff index and matching number, Int. J. Quantum Chem. 109 (2009) 2978-2981.
- [21] H. Wang, H. Hua, D. Wang, Cacti with minimum, second-minimum, and third-minimum Kirchhoff indices, *Math. Commun.* 15 (2010) 347-358.
- [22] R. Li, Lower bounds for the Kirchhoff index, MATCH Commun. Math. Comput. Chem. 70 (2013) 163-174.
- [23] H. Chen, F. Zhang, Resistance distance and the normalized Laplacian spectrum, *Discr. Appl. Math.* 155 (2007) 654-661.
- [24] J. Palacios, J. M. Renom, Another look at the degree Kirchhoff index, Int. J. Quantum Chem. 111 (2011) 3453-3455.
- [25] L. Feng, I. Gutman, G. Yu, Degree Kirchhoff Index of Unicyclic Graphs, MATCH Commun. Math. Comput. Chem. 69 (2013) 629-648.
- [26] I. Gutman, L. Feng, G. Yu, Degree resistance distance of unicyclic graphs, *Transactions on Combinatorics*, 1(2) (2012) 27-40.
- [27] S. Chen, Q. Chen, X. Cai, Z. Guo, Maximal Degree Resistance Distance of Unicyclic Graphs, MATCH Commun. Math. Comput. Chem. In press.
- [28] J. L. Palacios, Upper and lower bounds for the additive degree Kirch-hoff index, MATCH Commun. Math. Comput. Chem. 70 (2013) 651-655.
- [29] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: Theory and applications, Acta Appl. Math. 66 (2001) 211-249.