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Research Paper

MAXIMUM RANDIĆ ENERGY OF UNICYCLIC GRAPHS

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Abstract. Given a graph $G = (V, E)$, the randić matrix of G is $R(G) = (r_{ij})$, where $r_{ij} = \frac{1}{\sqrt{d_{v_i} d_{v_j}}}$ if $v_iv_j \in E(G)$ and 0 otherwise, and d_{v_i} is the degree of the vertex v_i in G. The randić energy is the sum of absolute values of the eigenvalues of randić matrix. The R-polynomial of G is defined by $\phi_R(G, x) = det(xI_n - R(G))$. In this paper, we obtain the R-polynomial as well as the randić energy of a unicyclic graph. In particular, we determine all unicyclic graphs with maximum randić energy.

1. Introduction

Let $G = (V, E)$ be a *simple connected* graph of order n and $A(G)$ its *adjacency* matrix. For a vertex v in G, the *degree* of v, denoted by $d_v = d_G(v)$, is the number of vertices adjacent to v. A vertex of degree one is referred as a *leaf* and its unique neighbor is referred as a *support*

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vertex. Let the *characteristic polynomial* $\phi(G,x)$ (or just $\phi(G)$) of G be

$$\phi(G,x) = det(xI_n - A(G)) = \sum_{k=0}^{n} a_k x^{n-k},$$

where $a_0(G), a_1(G), \ldots, a_n(G)$ are the *coefficients* of the characteristic polynomial of the graph G. Since the adjacency matrix $A(G)$ is a real symmetric matrix, its characteristic roots (eigenvalues) are all real, and can be sorted as $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$.
The *randić matrix* of a graph G is defined as $r_{ij} = \frac{1}{\sqrt{d_{v_i} d_{v_j}}}$ if $v_i v_j \in E(G)$ and 0 otherwise. Since the randić matrix $R(G)$ is real symmetric, we can order its eigenvalues so that $\rho_1 \geqslant \rho_2 \geqslant \cdots \geqslant \rho_n$. In addition, the *R-polynomial* of G defined by $\phi_R(G,x) = det(xI_n - R(G))$ is the R-characteristic polynomial of G. For references on chemical graph theory variants, see for example, [1, 2, 3, 4, 5, 6, 7, 8, 10, 11, 12, 13].

A connected graph of order n is a *tree* (*unicyclic*) if it has $n-1$ (n, respectively) edges. It is clear that a unicyclic graph contains precisely one cycle as an induced subgraph. In this paper we use the following representation of a unicyclic graph. Let G be a unicyclic graph of order n with the induced cycle $C : v_1 v_2 \ldots v_m$ of order m. Then removing all edges of C results m trees $T_1, \ldots, T_m$, where $v_i \in V(T_i)$, for $i = 1, 2, \ldots, m$. We denote G by $U(n, m; T_1, T_2, \ldots, T_m)$. Thus for any unicyclic graph G of order n, there is an integer $3 \leq m \leq n$ and m trees $T_1, \ldots, T_m$ such that $G = U(n, m; T_1, T_2, \ldots, T_m)$.

In this paper, we obtain the *R-polynomial* as well as the randić energy of a unicyclic graph. In particular, we determine all unicyclic graphs with maximum randić energy.

For an integer $k \geq 1$, we denote by $m(G,k)$ the number of k-matchings of a graph G, that is, the number of ways in which k independent edges can be selected in G. By definition, $m(G,0) = 1$ for all graphs, and $m(G,1)$ is equal to the number of edges of G. We also denote by K_n, P_n and C_m to refer the complete graph, the path and the cycle on n vertices, respectively.

The organization of the paper is as follows. In Section 2, we state the main result of this paper. In Section 3, we state some known results including the Sachs theorem and known results on R-polynomials of trees. In Section 4, we prove necessary lemmas and theorems by introducing three operations and proving three lemmas on them. In Section 5, we prove the main result of this paper.

2. Main result

The *subdivision* of an edge uv is the deletion of uv and the addition of two edges uw and wv along with a new vertex w. A tree T is 2-*spider* if $T = P_3$, $T = P_5$ or T is obtained from a star of order at least four by subdivision of all edges of the star. The *center* of a 2-spider T

is a leaf of T if $T = P_3$, the central vertex of T if $T = P_5$ and the vertex of maximum degree, otherwise. We will prove the following result.

Theorem 2.1. *Let $G = U(n, m; T_1, T_2, \ldots, T_m)$ be a unicyclic graph with maximum randić energy. then:*

1. Assume that $n - m$ is odd. If $n - m = 1$, then there is precisely one integer $j \in \{1, \ldots, m\}$ such that $T_j = K_2$ and $T_i = K_1$ for all $i \in \{1, 2, \ldots, m\} - \{j\}$, and if $n - m \geq 3$ then there are integers $j_1, \ldots, j_k \in \{1, \ldots, m\}$, where $1 \leq k \leq m$, such that T_{j_l} is obtained by joining the vertex v_{j_l} to the center of a 2-spider for $l = 1, 2, .., k$, and $T_i = K_1$ for all $i \in \{1, 2, \ldots, m\} - \{j_1, \ldots, j_k\}$.

2. Assume that $n - m$ is even. If $n - m = 0$, then $G = C_m$, and if $n - m > 0$ then G is obtained from $U(n - 1, m; T_1, T_2, \ldots, T_m)$ by adding a leaf to a leaf of $U(n - 1, m; T_1, T_2, \ldots, T_m)$.

3. Known results

A *weighted graph G_w* is a graph whose edges are assigned values (weight of the edge $w(e_{ij})$). The matrix where entry (i, j) is the value of edge between vertices i and j is called the *adjacency matrix of the weighted graph A_w*. A subgraph of G called a *Sachs subgraph*, if it K_2 or a cycle C_m for some $m \geq 3$. The following Sachs theorem determines the coefficients of characteristic polynomial of a graph depending on the structure of the graph G.

Theorem 3.1. *(Sachs theorem) Let $\phi(G, x) = | xI - A | = \sum_{k=0}^{n} a_k x^{n-k}$ be the characteristic polynomial of an arbitrary G. Then*

$$a_k = \sum_{L \in L_k} (-1)^{P(L)} 2^{C(L)} \ (k = 1, \ldots, n),$$

where L_k denotes the set of all the Sachs subgraphs in G with exactly i vertices, which each of its components is either a K_2 or a cycle; and $P(L)$ and $C(L)$ are the number of components and cycles of L respectively, where the summation is taken over all Sachs subgraphs in G. In addition, $a_0 = 1$.

Now Sach's theorem can be reformulated for weighted graphs as follows. Let G_w be an arbitrary weighted graph with characteristic polynomial $\phi(G_w, x) = | xI - A_w | = \sum_{k=0}^{n} a_k x^{n-k}$. Then

$$a_k = \sum_{L \in L_k} (-1)^{P(L)} 2^{C(L)} \prod_{e \in E(L)} w(e)^{t(e,L)},$$

where L_k denotes the set of all the Sachs subgraphs in G_w with exactly k vertices, such that each of its components is either a K_2 or a cycle; and $P(L)$ and $C(L)$ are the number of components and cycles of L, respectively, $t(e, L)$ is 1 if $e \in E(C_i)$ and 2 otherwise, and $\prod_{e \in E(L)} w(e)^{t(e,L)}$ is the product of the weights of the edges that are contained in subgraphs to the power of $t(e, L)$, where $E(L)$ is the set of edges of L.

Since the Randić matrix is the adjacency matrix of the weighted graph, where the weight of each edge is $w(e_{ij}) = \frac{1}{\sqrt{d_G(v_i)d_G(v_j)}}$, we have a new formula when applied to Randić matrix R immediately (for more details see [4]).

Corollary 3.2. *Let G be a arbitrary graph with R-polynomial*

$$\phi_R(G, x) = \sum_{k=0}^{n} q_k x^{n-k}.$$

For $e_i = v_i v_i$ we have $\prod_{e_i \in E(L)} w(e_i) = \prod_{e_i \in E(L)}(\frac{1}{\sqrt{d_G(v_i)d_G(u_i)}}) = \frac{1}{\prod_{v_i \in V(L)} d_G(v_i)}$. Let $V(L) = \{v_1, v_2, \ldots, e_k\}$ denotes the set of vertices of L. Then the coefficients of R-polynomial as follows

$$q_k = \sum_{L \in L_k} (-1)^{P(L)} . \frac{2^{C(L)}}{\prod_{v_i \in V(L)} d_G(v_i)},$$

where $i = 1, 2, \ldots, k$.

We next state some results on the *R-polynomial* of trees which was presented in [5]. Since in a tree T the set all Sachs subgraphs with k vertex are k-matchings $L_k(G) = M_k(G) \in \Gamma(G)$, and $C(L) = 0$ for $L \in L_k$ (acyclic) and $P(L) = k$, we find that for $V(L) = \{v_1, v_2, \ldots, v_k\}$ the *R-polynomial* graph G is

$$\phi_R(G, x) = \sum_{k=0}^{n} q_k x^{n-k} = \sum_{k=0}^{n} (-1)^k (\sum_{L \in L_k} \frac{1}{\prod_{v_i \in V(L)} d_G(v_i)}) x^{n-k},$$

since all the odd coefficients k of R-polynomial are equal to zero, and its even coefficients are related to $k = 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor$, and in addition $a_0(G) = 1$. The *R-polynomial* of trees has been calculated in [5], as follows: Let T be a tree of order n and $L_k(T) = M_k(T)$ be the set of all k-matchings of T, for $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$. For $e_i = u_i v_i \in E(T)$ and $L = \{e_1, e_2, \ldots, e_k\} \in M_k(T)$, the *R-polynomial* of T can be written as

$$\phi_R(T, x) =\mid xI - R(T) \mid= \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T), k) x^{n-2k},$$

where $b(R(T), 0) = 1$ and $b(R(T), k) = \sum\limits_{L \in M_k(T)} (R_T(L))$ for $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$ with

$$R_T(L) = \frac{1}{\prod_{e_i \in L} d_T(u_i) d_T(v_i)}.$$

4. Operations and lemmas

In this section we introduce three operations, namely, Operation 1, Operation 2 and Operation 3 on a unicyclic graph $U(n, m; T_1, T_2, \ldots, T_m)$.

Operation 4.1. *Assume that there is a tree T_i with two leaves u_s, w_q at distance at least two from v_i, where u_s has a support vertex u_{s-1} with $d_T(u_{s-1}) = 2$. Then remove the edge $u_s u_{s-1}$ and add the edge $w_q u_s$, (see Figure 1).*

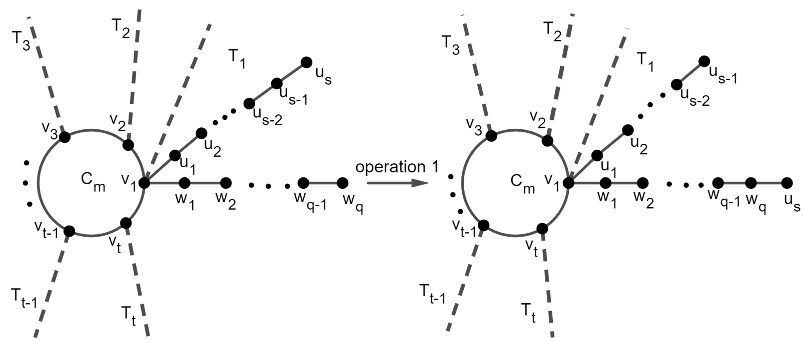

Figure 1. Unicyclic graphs U and U'.

Operation 4.2. *Assume that there is a tree T_i with at least two leaves $u \neq v_i$ and $w_q \neq v_i$ such that $d(w_q, v_i) \geq d(w_s, v_i)$ for every leaf w_s of T_i. Then remove u and add a new vertex and join it to w_q, (see Figure 2).*

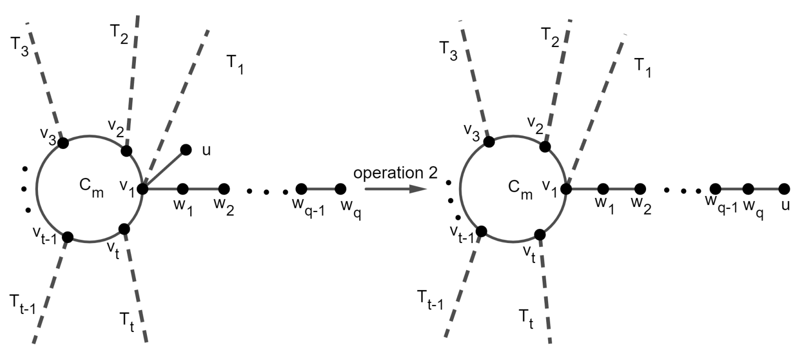

Figure 2. Unicyclic graphs U and U'.

Operation 4.3. *Assume that there is a T_i of order $n_i > 4$ such that $T_i - \{v_i, u_i\}$ has precisely one component P_k, where $k \geq 4$) and all other components are P_2, where u_i is adjacent to v_i.*

Assume that $u_s \neq u_i$ *is the leaf of the* P_k*-component of* $T_i - \{v_i, u_i\}$ *and* u_{s-1} *is adjacent to* u_s $(s \geq 5)$*. Then remove the non-pendant edge of* u_{s-1} *and join* u_i *to* u_{s-1}*, (see Figure 3).*

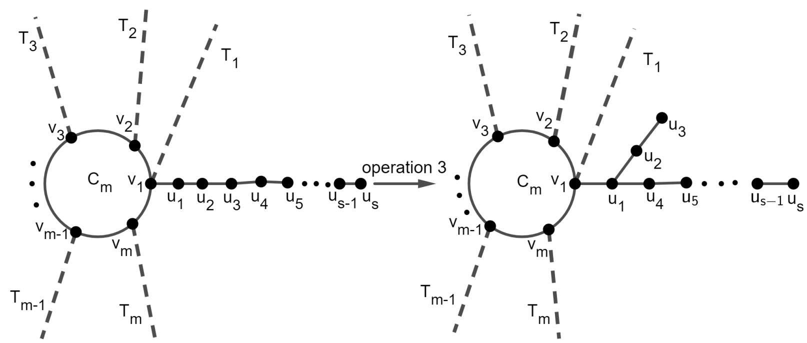

FIGURE 3. Unicyclic graphs U and U'.

To use the above operations in proving our main result we need to prove the following two theorems.

Theorem 4.4. *For an arbitrary unicyclic graph* U*,*

$$\begin{aligned}\phi_R(U,x) &= \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor}(-1)^k b(R(U)),k)x^{n-2k} \\ &\quad + \frac{2}{d_{v_1}\dots d_{v_m}} \sum_{k=0}^{\lfloor \frac{n-m}{2} \rfloor}(-1)^{k+1} b(R(U-C_m),k)x^{n-|V(C_m)|-2k},\end{aligned}$$

where $b(R(T),0) = 1$ *and for* $e_i = v_i u_i$*,* $b(R(U),k) = \sum_{L \in L_k(U)} (R_T(L))$ *for* $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$ *with* $R_T(L) = \dfrac{1}{\prod_{e_i \in L} d_T(u_i) d_T(v_i)}$.

Proof. Suppose that $U = U(n, m; T_1, T_2, \dots, T_m)$ is a unicyclic graph with n vertices and C_m is its cycle. Since the R-polynomial $\phi_R(U,x)$ is determined by its coefficients, $\phi_R(U,x)$ can be calculated by $\Gamma(U)$, the set of all Sachs subgraphs U and $L_k(U) \in \Gamma(U)$ are either matchings or a cycle with k vertices. By corollary 3.2 we have

$$\phi_R(U,x) = \sum_{k=0}^{n} q_k x^{n-k} = \sum_{k=0}^{n}(\sum_{L \in L_k}(-1)^{P(L)}.\frac{2^{C(L)}}{\prod_{v_i \in V(L)} d_U(v_i)})x^{n-k},$$

where $b(R(U),0) = 1$,$b(R(U),k) = \sum_{L \in L_i(U)} (R_U(L))$, $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$ with $R_U(L) = \dfrac{1}{\prod_{v_i \in V(L)} d_U(v_i)}$ and $V(L) = \{v_1, v_2, \dots, e_k\}, i = 1, 2, \dots, k$. Firstly, note that there is no Sachs graphs with one vertex and so $b(R(U)),1) = 0$. Furthermore, the Sachs graphs with two vertices have one component which is a K_2-graph and the Sachs graphs with three vertices have one component which is a triangle (C_3) and the Sachs graphs with four vertices are those that are corresponding to either a cycle C_4 or two K_2-graphs, and Sachs graphs with five vertices are either a cycle C_5 or have two-component consisting of a triangle C_3 and a K_2-graph. The other Sachs graph can be also described. So, all Sachs subgraphs are in the form $\Gamma(U) = \Gamma_1(U) \cup \Gamma_2(U)$, where Γ_1 contains only k-matchings, and $\Gamma_2(U)$ contains the rest Sachs subgraphs. Now, we write the R-polynomial of a graph in terms of R-polynomial of sachs subgraphs according to the classes $\Gamma_1(U)$ and $\Gamma_2(U)$.

Case 1: $\Gamma_1(U)$.

The coefficients of the R-polynomial is determined only by number k-matchings. Then by means of corollary 3.2, the *R-polynomial* of this class of sachs subgraphs of U can be written as:

$$\sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(U), k) x^{n-2k},$$

where for $e_i = u_i v_i$, $b(R(U), k) = \sum_{L \in L_k(U)} (\frac{1}{\prod_{e_i \in L} d_U(u_i) d_U(v_j)})$ and $\lfloor \frac{n}{2} \rfloor$ is the integer part of the real $\frac{n}{2}$ value.

Case 2: $\Gamma_2(U)$.

If $k = m$, then since there are only one cycle C_m contained in unicyclic graphs, there is only one sachs subgraph that is C_k. Thus, $L_k = \{C_k\} \in \Gamma_2(U)$. Also we have $C(L) = 1$ and $p(L) = 1$, and so by corollary 3.2 we have $\dfrac{2}{d_{v_1} \dots d_{v_m}}$ and $b(R(U), 0) = 1$. Then the *R-polynomial* of U can be written as $\dfrac{2}{d_{v_1} \dots d_{v_m}} x^{n-m}$. Thus assume that $k > m$. We know that the subgraphs $U - C_m$ have no cycles, thus the graph $U - C_m$ is acyclic, and so we consider Sachs subgraphs of U that are cycle C_m together with $\frac{k-m}{2}$-matchings of $U - C_m$, that is, $\Gamma_2(U)$ is the set of all $\frac{k-m}{2}$-matchings of U together with the cycle C_m. Thus, the Sachs subgraphs are of two types, either disjoint copies of K_2 (arising only when $k - m$ is even) or one copy of C_m. In particular, we have $C(L) = 1$, for $1 \leq k \leq \frac{k-m}{2}$. Hence $L_k(U) = \{C_m, e_1, e_2, \dots, e_{\frac{k-m}{2}}\} \in \Gamma_2(U)$, where $\{e_1, e_2, \dots, e_{\frac{k-m}{2}}\}$ is the set of all k-matchings of $U - C_m$. By Corollary 3.2, the *R-polynomial* of U can be written as:

$$\frac{2}{d_{v_1} \dots d_{v_m}} \sum_{k=1}^{\lfloor \frac{n-m}{2} \rfloor} (-1)^{k+1} b(R(U - C_m), k) x^{n-2k},$$

where for $e_i = u_i v_i$, $b(R(U), k) = \sum_{L \in L_k(U)} (\frac{1}{\prod_{e_i \in L} d_U(u_i) d_U(v_j)})$. □

We now compare the Randić energies of two unicyclic graphs. In [5], the Randić energies of two bipartite graphs were compared by means of their coulson integral formula. This method can be used to compare the Randic energies of two unicyclic graphs. As a result, for a unicyclic graph U, the coulson integral formula can be rewritten as

$$(1)\ \ \mathcal{E}_R(U) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{1}{x^2}\ln[(\sum_{k=0}^{\lfloor\frac{n}{2}\rfloor} b(R(U),k)x^{2k}) + \frac{2}{d_{v_1}\dots d_{v_m}}(\sum_{k=0}^{\lfloor\frac{n-m}{2}\rfloor} b(R(U-C_m),k)x^{2k})]dx,$$

where $b(R(T),0) = 1$ and for $e_i = v_iu_i$, $b(R(U),k) = \sum_{L\in L_k(U)}(R_T(L))$ for $1 \leq k \leq \lfloor\frac{n}{2}\rfloor$ with $R_T(L) = \frac{1}{\prod_{e_i\in L} d_T(u_i)d_T(v_i)}$.

Theorem 4.5. *Let $U(n,m;T_1,T_2,\dots,T_m)$ and $U'(n,m;T_1',T_2',\dots,T_m')$ be two unicyclic graphs and their R-polynomials be*

$$\phi_R(U,x) = \sum_{k=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^k b(R(U,k)x^{n-2k} + \frac{2}{d_{v_1}\dots d_{v_m}}\sum_{k=0}^{\lfloor\frac{n-m}{2}\rfloor}(-1)^{k+1}b(R(U-C_m),k)x^{n-|V(C_m)|-2k},$$

$$\phi_R(U',x) = \sum_{k=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^k b(R(U',k)x^{n-2k} + \frac{2}{d_{v_1'}\dots d_{v_m'}}\sum_{k=0}^{\lfloor\frac{n-m}{2}\rfloor}(-1)^{k+1}b(R(U'-C_m),k)x^{n-|V(C_m)|-2k},$$

respectively. Assume that $b(R(U'),k) \geq b(R(U),k)$ holds for all $k \geq 1$, and there is an integer k such that $b(R(U),k) > b(R(U'),k)$. Furthermore, assume that $\frac{2}{d_{v_1'}\dots d_{v_m'}}b(R(U'-C_m),k) \geq \frac{2}{d_{v_1}\dots d_{v_m}}b(R(U-C_m),k)$ for all $k \geq 1$, and there is an integer k such that $\frac{2}{d_{v_1'}\dots d_{v_m'}}b(R(U'-C_m),k) > \frac{2}{d_{v_1}\dots d_{v_m}}b(R(U-C_m),k)$. Then $\mathcal{E}_R(U') > \mathcal{E}_R(U)$.

Proof. Let $U = U(n,m;T_1,T_2,\dots,T_m)$ and $U' = U'(n,m;T_1',T_2',\dots,T_m')$ be two unicyclic graphs with the same number of vertices and cycle length m, and let $\phi_R(U,x)$ and $\phi_R(U',x)$ be their R-polynomials of degree n, respectively, where $b(R(U,k))$, $b(R(U-C_m,k))$ and $b(R(U',k))$, $b(R(U'-C_m,k))$ are the coefficients of the R-polynomials. We know the R-polynomials $\phi_R(U,x)$ and $\phi_R(U',x)$ are determined by their coefficients that are the number of k-matchings and cycle C_m in the graphs U, $U-C_m$ and U', $U'-C_m$, respectively. Clearly, for U, we have $k = 0,1,\dots,\lfloor\frac{n}{2}\rfloor$. As a result, to compare the randić energies of U and U', we compare the coefficients of two R-polynomials with the parameter k. Thus, by applying eq. (1), from the coulson integral formula (see eq. (1)), $\mathcal{E}_R(U)$ is a monotonically increasing function of $b(R(U),k)$ for $k=0,1,...,\lfloor\frac{n}{2}\rfloor$ and $b(R(U-C_m),k)$ for $k=0,1,...,\lfloor\frac{n-m}{2}\rfloor$. Consequently, if U and U' are unicyclic graphs for which $b(R(U'),k)\geq b(R(U),k)$ holds for all $k\geq 0$ and $b(R(U'-C_m),k)\geq b(R(U-C_m),k)$ holds for all $k\geq 0$, then $\mathcal{E}_R(U')\geq\mathcal{E}_R(U)$. □

We now are ready to prove three lemmas related to the three operations.

4.1. **Lemmas associated to operations.** We first prove the following lemma associated to Operation 1.

Lemma 4.6. *Let $U(n,m;T_1,T_2,\dots,T_m)$ be a unicyclic graph and $U'(n,m;T'_1,T'_2,\dots,T'_m)$ be the graph obtained from $U(n,m;T_1,T_2,\dots,T_m)$ by Operation 4.1. Then*

$$\mathcal{E}_R(U'(n,m;T'_1,T'_2,\dots,T'_m))=\mathcal{E}_R(U(n,m;T_1,T_2,\dots,T_m)).$$

Proof. Let $U'=U'(n,m;T'_1,T'_2,\dots,T'_m)$ and $U=U(n,m;T_1,T_2,\dots,T_m)$ be unicyclic graphs of order n with cycle C_m and by Theorem 4.4 let the R-polynomials of U and U' be

$$\phi_R(U,x)=\sum_{k=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^k b(R(U,k)x^{n-2k}+\frac{2}{d_{v_1}\dots d_{v_m}}\sum_{k=0}^{\lfloor\frac{n-m}{2}\rfloor}(-1)^{k+1}b(R(U-C_m),k)x^{n-|V(C_m)|-2k},$$

$$\phi_R(U',x)=\sum_{k=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^k b(R(U',k)x^{n-2k}+\frac{2}{d_{v_1}\dots d_{v_m}}\sum_{k=0}^{\lfloor\frac{n-m}{2}\rfloor}(-1)^{k+1}b(R(U'-C_m),k)x^{n-|V(C_m)|-2k}.$$

respectively, where $b(R(U),0)=b(R(U'),0)=b(R(U-C_m),0)=b(R(U'-C_m),0)=1$ and for $e_i=v_iu_i$, $b(R(U),k)=\sum_{L\in L_k(U)}(R_U(L))$ for $1\leq k\leq\lfloor\frac{n}{2}\rfloor$ with $R_U(L)=\frac{1}{\prod_{e_i\in L}d_U(u_i)d_U(v_i)}$ and for $e_i=v_iu_i$, $b(R(U-C_m),k)=\sum_{L\in L_k(U-C_m)}(R_U(L))$ for $1\leq k\leq\lfloor\frac{n-m}{2}\rfloor$ with $R_U(L)=\frac{1}{\prod_{e_i\in L}d_U(u_i)d_U(v_i)}$. Then for $k=1$ we have

$$\begin{aligned}
b(R(U'),1)-b(R(U),1)=&\sum_{L\in L_k(U')}(R_{U'}(L))-\sum_{L\in L_k(U)}(R_U(L))\\
=&R_{U'}(u_{s-2}u_{s-1})+R_{U'}(w_{q-1}w_q)+R_{U'}(w_qu_s)-R_U(u_{s-2}u_{s-1})\\
&-R_U(u_{s-1}u_s)-R_U(w_{q-1}w_q)\\
=&\frac{1}{d_{U'}(u_{s-2})d_{U'}(u_{s-1})}+\frac{1}{d_{U'}(w_{q-1})d_{U'}(w_q)}+\frac{1}{d_{U'}(w_q)d_{U'}(u_s)}\\
&-\frac{1}{d_T(u_{s-2})d_T(u_{s-1})}-\frac{1}{d_T(u_{s-1})d_T(u_s)}-\frac{1}{d_T(w_{q-1})d_T(w_q)}=0.
\end{aligned}$$

That is, $b(R(U'),1)=b(R(U),1)$. Now similar to the case $k=0$ in the second summation

$$b(R(U'-C_m),0)=b(R(U-C_m),0)=1,$$
$$\frac{1}{d_{U'}(v_1)\dots d_{U'}(v_m)}=\frac{1}{d_U(v_1)\dots d_U(v_m)}.$$

Similar to the case $k=1$ in $U-C_m$ we have $b(R(U'-C_m),1)-b(R(U),1)=0$. That is,

$$b(R(U'-C_m),1)=b(R(U-C_m),1).$$

For $k=2,\dots,\lfloor\frac{n}{2}\rfloor$, let $U_1=U-\{u_{s-1}u_s\}-\{w_q\}$ and $U_1'=U'-\{u_{s-1}\}-\{w_qu_s\}$ be subgraphs of U and U', respectively. Then

$$\begin{aligned}
b(R(U'),k)=&\sum_{L\in L_k(U_1')}R_{U'}(L)+\left(\frac{1}{d_{U'}(u_{s-2})d_{U'}(u_{s-1})}+\frac{1}{d_{U'}(w_q)d_{U'}(u_s)}\right)\\
&\times\sum_{L\in L_{k-1}(U_1'-\{u_{s-2}\})}R_{U_1'-\{u_{s-2}\}}(L)\\
&+\left(\frac{1}{d_{U'}(w_{q-1})d_{U'}(w_q)}+\frac{1}{d_{U'}(w_q)d_{U'}(u_s)}\right)\sum_{L\in L_{k-1}(U_1'-\{w_{q-1}\})}R_{U_1'-\{w_{q-1}\}}(L)\\
&+\left(\frac{1}{d_{U'}(u_{s-2})d_{U'}(u_{s-1})}+\frac{1}{d_{U'}(w_{q-1})d_{U'}(w_q)}+\frac{1}{d_{U'}(w_q)d_{U'}(u_s)}\right)\\
&\times\sum_{L\in L_{k-1}(U_1'-\{u_{s-2}\}-\{w_{q-1}\})}R_{U_1'-\{u_{s-2}\}-\{w_{q-1}\}}\\
&+\left(\frac{1}{d_{U'}(u_{s-2})d_{U'}(u_{s-1})}\times\frac{1}{d_{U'}(w_{q-1})d_{U'}(w_q)}+\frac{1}{d_{U'}(u_{s-2})d_{U'}(u_{s-1})}\right.\\
&\left.\times\frac{1}{d_{U'}(w_q)d_{U'}(u_s)}\right)\sum_{L\in L_{k-2}(U_1'-\{u_{s-2}\}-\{w_{q-1}\})}R_{U_1'-\{u_{s-2}\}-\{w_{q-1}\}}(L).
\end{aligned}$$

Similarly,

$$\begin{aligned}
b(R(U),k)=&\sum_{L\in L_k(U_1)}R_U(L)+\left(\frac{1}{d_U(u_{s-2})d_U(u_{s-1})}+\frac{1}{d_U(u_{s-1})d_U(u_s}\right)\\
&\times\sum_{L\in L_{k-1}(U_1-\{u_{s-2}\})}R_{U_1-\{u_{s-2}\}}(L)\\
&+\left(\frac{1}{d_U(w_{q-1})d_U(w_q}+\frac{1}{d_U(u_{s-1})d_U(u_s)}\right)\sum_{L\in L_{k-1}(U_1-\{w_{q-1}\})}R_{U_1-\{w_{q-1}\}}(L)\\
&+\left(\frac{1}{d_U(u_{s-2})d_U(u_{s-1}}+\frac{1}{d_U(u_{s-1})d_U(u_s)}+\frac{1}{d_U(w_{q-1})d_U(w_q)}\right)\\
&\times\sum_{L\in L_{k-1}(U_1-\{u_{s-2}\}-\{w_{q-1}\})}R_{U_1-\{u_{s-2}\}-\{w_{q-1}\}}
\end{aligned}$$

$$+\left(\frac{1}{d_U(u_{s-2})d_U(u_{s-1}} \times \frac{1}{d_U(w_{q-1})d_U(w_q)} + \frac{1}{d_U(u_{s-1})d_U(u_s} \times \frac{1}{d_U(w_{q-1})d_U(w_q)}\right)$$
$$\times \sum_{L\in L_{k-2}(U_1-\{u_{s-2}\}-\{w_{q-1}\})} R_{U_1-\{u_{s-2}\}-\{w_{q-1}\}}(L).$$

Note that in U' and U we have

$$\sum_{L\in L_k(U_1')} R_{U'}(L) = \sum_{L\in L_k(U_1)} R_U(L),$$
$$\sum_{L\in L_k(U_1'-\{u_{s-2}\})} R_{U_1'-\{u_{s-2}\}}(L) = \sum_{L\in L_k(U_1-\{w_{q-1}\})} R_{U_1-\{w_{q-1}\}}(L),$$
$$\sum_{L\in L_k(U_1'-\{w_{q-1}\})} R_{U_1'-\{w_{q-1}\}}(L) = \sum_{L\in L_k(U_1-\{u_{s-2}\})} R_{U_1-\{u_{s-2}\}}(L),$$
$$\sum_{L\in L_{k-2}(U_1'-\{u_{s-2}\}-\{w_{q-1}\})} R_{U_1'-\{u_{s-2}\}-\{w_{q-1}\}}(L) = \sum_{L\in L_{k-2}(U_1-\{u_{s-2}\}-\{w_{q-1}\})} R_{U_1-\{u_{s-2}\}-\{w_{q-1}\}}(L).$$

Since the corresponding coefficients are equal, so

$$b(R(U'),k) = b(R(U),k).$$

Similarly, $b(R(U'-C_m)),k) - b(R(U-C_m),k) = 0$, which implies that

$$b(R(U'-C_m),k) = b(R(U-C_m),k).$$

By Theorem 4.5, the lemma holds. □

We next prove the following lemma associated to Operation 2.

Lemma 4.7. *Let $U(n,m;T_1,T_2,\dots,T_m)$ be a unicyclic graph and $U'(n,m;T_1',T_2',\dots,T_m')$ be the graph obtained from $U(n,m;T_1,T_2,\dots,T_m)$ by Operation 4.2. Then*

$$\mathcal{E}_R(U(n,m;T_1,T_2,\dots,T_m)) \le \mathcal{E}_R(U'(n,m;T_1',T_2',\dots,T_m')).$$

Proof. Let $U' = U'(n,m;T_1',T_2',\dots,T_m')$ and $U = U(n,m;T_1,T_2,\dots,T_m)$ be unicyclic graphs of order n with cycle C_m and by Theorem 4.4 let the R-polynomials of U and U' be

$$\phi_R(U,x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(U,k)x^{n-2k}$$
$$+ \frac{2}{d_{v_1}\dots d_{v_m}} \sum_{k=0}^{\lfloor \frac{n-m}{2} \rfloor} (-1)^{k+1} b(R(U-C_m),k)x^{n-|V(C_m)|-2k},$$

$$\phi_R(U',x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(U',k)x^{n-2k} + \frac{2}{d_{v_1}\dots d_{v_m}} \sum_{k=0}^{\lfloor \frac{n-m}{2} \rfloor} (-1)^{k+1} b(R(U'-C_m),k)x^{n-|V(C_m)|-2k},$$

respectively, where $b(R(U),0) = b(R(U'),0) = b(R(U-C_m),0) = b(R(U'-C_m),0) = 1$ for $e_i = v_iu_i$, $b(R(U),k) = \sum_{L\in L_k(U)} (R_U(L))$ for $1 \le k \le \lfloor \frac{n}{2} \rfloor$ with $R_U(L) = \frac{1}{\prod_{e_i\in L} d_U(u_i)d_U(v_i)}$ and for $e_i = v_iu_i$, $b(R(U-C_m),k) = \sum_{L\in L_k(U-C_m)} (R_U(L))$, where $1 \le k \le \lfloor \frac{n-m}{2} \rfloor$ and $R_U(L) = \frac{1}{\prod_{e_i\in L} d_U(u_i)d_U(v_i)}$.

Since $d_{U'}(v_2) = d_U(v_2)$ and $d_{U'}(v_t) = d_{U'}(v_t)$, for $k = 1$ we have

$$\begin{aligned}
b(R(U'),1) - b(R(U),1) = &\sum_{L\in L_k(U')} (R_{U'}(L)) - \sum_{L\in L_k(U)} (R_U(L)) \\
=&R_{U'}(v_1v_2) + R_{U'}(v_1v_t) + R_{U'}(v_1w_1) + R_{U'}(w_{q-1}w_q) + R_{U'}(w_qu) \\
&- R_U(v_1v_2) - R_U(v_1v_t) - R_U(v_1u) - R_U(v_1w_1) - R_U(w_{q-1}w_q) \\
=&\frac{1}{d_{U'}(v_1)d_{U'}(v_2)} + \frac{1}{d_{U'}(v_1)d_{U'}(v_t)} + \frac{1}{d_{U'}(v_1)d_{T'}(w_1)} \\
&+ \frac{1}{d_{U'}(w_{q-1})d_{U'}(w_q)} + \frac{1}{d_{U'}(w_q)d_{U'}(u)} - \frac{1}{d_U(v_1)d_U(u)} \\
&- \frac{1}{d_U(v_1)d_U(v_2)} - \frac{1}{d_U(v_1)d_U(v_t)} - \frac{1}{d_U(v_1)d_U(w_1)} \\
&- \frac{1}{d_U(w_{q-1})d_U(w_q)} \\
=&\frac{1}{d_{U'}(v_1)d_{U'}(v_2)} + \frac{1}{d_{U'}(v_1)d_{U'}(v_t)} + \frac{3}{4} + \frac{1}{2d_{U'}(v_1)} \\
&- \frac{1}{(d_{U'}(v_1)+1)d_{U'}(v_2)} - \frac{1}{d_{U'}(((v_1)+1))d_{U'}(v_t)} - \frac{3}{4} \\
&- \frac{1}{2(d_{U'}(v_1)+1))} > 0.
\end{aligned}$$

Then $b(R(U'),1) > b(R(U),1)$.

For $k = 2,\dots,\lfloor \frac{n}{2} \rfloor$, we denote $P = w_1w_2\dots w_{q-1}$. Then

$$\begin{aligned}
b(R(U'),k) =&\frac{1}{d_{U'}(w_q)d_{U'}(u)} \sum_{L\in L_{k-1}(C_m\cup P)} R_{U'}(\alpha_{k-1}) + \frac{1}{d_{U'}(w_q)d_{U'}(u)} \sum_{L\in L_{k-1}(C_m-v_1\cup P)} R_{U'}(\alpha_{k-1}) \\
&+ (\frac{1}{d_{U'}(w_{q-1})d_{U'}(w_q)} + \frac{1}{d_{U'}(w_q)d_{U'}(u)}) \sum_{L\in L_{k-1}(C_m\cup(P-w_{q-1}))} R_{U'}(L) \\
&+ (\frac{1}{d_{U'}(w_q)d_{U'}(u)}) \sum_{L\in L_{k-1}(C_m\cup(P-w_1))} R_{U'}(L)
\end{aligned}$$

$$+\Big(\frac{1}{d_{U'}(v_1)d_{U'}(w_1)}+\frac{1}{d_{U'}(w_q)d_{U'}(u)}\Big)\sum_{L\in L_{k-1}((C_m-v_1)\cup(P-w_1)}R_{U'}(L)$$
$$+\frac{1}{d_{U'}(v_1)d_{U'}(w_1)}\times\frac{1}{d_{U'}(w_q)d_{U'}(u)}\Big)\sum_{L\in L_{k-1}((C_m-v_1)\cup(P-w_1)}R_{U'}(L)$$
$$+\Big(\frac{1}{d_{U'}(w_{q-1})d_{U'}(w_q)}+\frac{1}{d_{U'}(w_q)d_{U'}(u)}\Big)\sum_{L\in L_{k-1}((C_m-v_1)\cup(P-w_{q-1})}R_{U'}(L)$$
$$+\Big(\frac{1}{d_{U'}(w_{q-1})d_{U'}(w_q)}+\frac{1}{d_{U'}(w_q)d_{U'}(u)}\Big)\sum_{L\in L_{k-1}((C_m)\cup(P-w_1-w_{q-1})}R_{U'}(L).$$

Similarly, we have $d_U(u)=1$ and

$$b(R(U),k)=\frac{1}{d_U(w_{q-1})d_U(w_q)}\sum_{L\in L_{k-1}(C_m\cup P-w_{q-1})}R_U(L)$$
$$+\frac{1}{d_U(v_1)d_U(u)}\sum_{L\in L_{k-1}(C_m-v_1\cup P)}R_U(L)+\sum_{L\in L_{k-1}(C_m\cup P-w_1)}R_U(L)$$
$$+(\frac{1}{d_U(w_{q-1})d_U(w_q)}+\frac{1}{d_U(v_1)d_U(u)})\sum_{L\in L_{k-1}(C_m-v_1\cup(P-w_{q-1})}R_U(L)$$
$$+(\frac{1}{d_U(w_{q-1})d_U(w_q)}\times\frac{1}{d_U(v_1)d_U(u)})\sum_{L\in L_{k-1}(C_m-v_1\cup(P-w_{q-1})}R_U(L)$$
$$+(\frac{1}{d_U(v_1)d_U(u)}+\frac{1}{d_U(v_1)d_U(w_1)})\sum_{L\in L_{k-1}(C_m-v_1\cup(p-w_1)}R_U(\alpha_{k-1})$$
$$+(\frac{1}{d_U(w_{q-1})d_U(w_q)})\sum_{L\in L_{k-1}(C_m\cup(P-w_1-w_{q-1})}R_U(L).$$

Note that

$$\sum_{L\in L_k(C_m-v_1\cup P)}R_{U'}(L)=\sum_{L\in L_k(C_m-v_1\cup P)}R_U(L),$$
$$\sum_{L\in L_{k-1}(C_m\cup(P-w_{q-1})}R_{U'}(L)=\sum_{L\in L_{k-1}(C_m\cup(P-w_{q-1})}R_U(L),$$
$$\sum_{L\in L_{k-1}(C_m\cup(P-w_1)}R_{U'}(L)=\sum_{L\in L_{k-1}(C_m\cup(P-w_1)}R_U(L),$$
$$\sum_{L\in L_{k-1}(C_m-v_1\cup(P-w_1)}R_{U'}(L)=\sum_{L\in L_{k-1}(C_m-v_1\cup(P-w_1)}R_U(L),$$
$$\sum_{L\in L_{k-1}(C_m-v_1\cup(P-w_{q-1})}R_{U'}(L)=\sum_{L\in L_{k-1}(C_m-v_1\cup(P-w_{q-1})}R_U(L),$$
$$\sum_{L\in L_{k-1}(C_m\cup(P-w_1-w_{q-1})}R_{U'}(L)=\sum_{L\in L_{k-1}(C_m\cup(P-w_1-w_{q-1})}R_U(L).$$

So, we obtain

$$\begin{aligned}
b(R(U'),k)-b(R(U),k)=&\sum_{L\in L_{k-1}(C_m\cup P)} R_{U'}(L)+(\frac{1}{2}-\frac{1}{d_U(v_1)})\sum_{L\in L_{k-1}(C_m-v_1\cup(P)} R_U(L)\\
&+(\frac{3}{4}-\frac{1}{2})\sum_{L\in L_{k-1}(C_m\cup(P-w_{q-1})} R_{U'}(L)\\
&+(\frac{1}{2}-1)\sum_{L\in L_{k-1}(C_m\cup P-w_1)} R_U(L)\\
&+(\frac{1}{2}-\frac{3}{4d_U(v_1)}+\frac{1}{2d_{U'}(v_1)})\sum_{L\in L_{k-1}(C_m-v_1\cup(P-w_1)} R_U(L)\\
&+(\frac{3}{4}-\frac{1}{2d_U(v_1)})\sum_{L\in L_{k-2}(C_m-v_1\cup(P-w_{q-1})} R_U(L)\\
&+(\frac{3}{4}-\frac{1}{2})\sum_{L\in L_{k-2}(C_m\cup(P-w_1-w_{q-1})} R_U(L).
\end{aligned}$$

On the other hand $d_U(v_1)=(d_{U'}(v_1))+1$ and $d_{U'}(v_1)\geq 3$, $d_U(v_1)\geq 4$, also since

$$\begin{aligned}
\sum_{L\in L_{k-1}(C_m\cup P)} R_U(L) &\geq \sum_{L\in L_{k-2}(C_m-v_1\cup(P)} R_U(L),\\
\sum_{L\in L_{k-1}(C_m\cup(P-w_{q-1})} R_U(L) &\geq \sum_{L\in L_{k-2}(C_m-v_1\cup P(-w_{q-1})} R_U(L),\\
\sum_{L\in L_{k-1}(C_m\cup P-w_1)} R_U(L) &\geq \sum_{L\in L_{k-2}(C_m-v_1\cup(P-w_1)} R_U(L),\\
\sum_{L\in L_{k-1}(C_m\cup P-w_1)} R_U(L) &\geq \sum_{L\in L_{k-2}(C_m\cup(P-w_1-w_{q-1})} R_U(L),\\
\sum_{L\in L_{k-1}(C_m-v_1\cup P)} R_U(L) &\geq \sum_{L\in L_{k-2}(C_m-v_1\cup(P-w_1)} R_U(L),
\end{aligned}$$

we obtain that

$$\begin{aligned}
b(R(U'),k)-b(R(U),k)\geq&(\frac{1}{2}-\frac{3}{4d_U(v_1)}+\frac{3}{2d_{U'}(v_1)})\sum_{L\in L_{k-2}(C_m-v_1\cup(P-w_1)} R_U(L))\\
&+(1-\frac{1}{2d_U(v_1)})\sum_{L\in L_{k-2}(C_m-v_1\cup(P-w_{q-1})} R_U(L))\\
&+\sum_{L\in L_{k-2}(C_m\cup(P-w_1-w_{q-1})} R_U(L))\\
&>0.
\end{aligned}$$

That is, $b(R(U'),k)>b(R(U),k)$. Now, for $k=0$ in the second summation we have

$$\frac{1}{d_{U'}(v_1)\ldots d_{U'}(v_m)}>\frac{1}{d_{U'}(((v_1)+1))\ldots d_{U'}(v_m)}=\frac{1}{d_U(v_1)\ldots d_U(v_m)}.$$

Next, let $U_1 = U - C_m$ and $U_1' = U' - C_m$. For $k = 1$ in the second summation we have

$$b(R(U_1'),1) - b(R(U_1),1) = (\frac{1}{d_{U'}(w_{q-1})d_{U_1'}(w_q)} + \frac{1}{d_{U_1'}(w_q)d_{U_1'}(u)}) - (\frac{1}{d_{U_1}(w_{q-1})d_{U_1}(w_q)})$$
$$> 0.$$

For $k = 2, \ldots, \lfloor \frac{n}{2} \rfloor$ let $P = w_1 w_2 \ldots w_{q-1}$ and note that the edges outside the cycle in the second summation are in $U_1' = U' - C_m$, $U_1' = U' - C_m$. Then

$$\begin{aligned} b(R(U_1',k) - b(R(U_1,k) &= (\frac{1}{d_{U'}(w_{q-1})d_{U_1'}(w_q)} + \frac{1}{w_q u})(\frac{2}{d_{U_1'}(v_1)\ldots d_{U'}(v_m)}) \sum_{\alpha_{k-1}\in M_{k-1}(U_1')} R_{U_1'}(L) \\ &- (\frac{1}{d_U(w_{q-1})d_U(w_q)})(\frac{2}{d_U((v_1))\ldots d_U(v_m)}) \sum_{L\in L_{k-1}(U_1)} R_U(L) \\ &= (\frac{3}{4})(\frac{2}{d_{U'}(v_1)\ldots d_{U'}(v_m)}) \sum_{L\in L_{k-1}(U_1')} R_{U'}(L) \\ &- (\frac{1}{2})(\frac{2}{d_{U'}(((v_1)+1))\ldots d_{U'}(v_m)}) \sum_{L\in L_{k-1}(U_1)} R_U(L). \end{aligned}$$

Since $d_U((v_1)+1) > d_U(v_1)$, and

$$\sum_{L\in L_{k-1}(U_1')} R_{U'}(L) \geq \sum_{L\in L_{k-1}(U_1)} R_U(L),$$

we have

$$b(R(U'),k) - b(R(U),k) > 0.$$

By Theorem 4.5, the lemma holds. □

Next we prove the following lemma associated to Operation 3.

Lemma 4.8. *Let $U(n,m;T_1,T_2,\ldots,T_m)$ be a unicyclic graph and $U'(n,m;T_1',T_2',\ldots,T_m')$ be the graph obtained from $U(n,m;T_1,T_2,\ldots,T_m)$ by Operation 4.3. Then*

$$\mathcal{E}_R(U(n,m;T_1,T_2,\ldots,T_m)) \leq \mathcal{E}_R(U'(n,m;T_1',T_2',\ldots,T_m')).$$

Proof. Let $U' = U'(n,m;T_1',T_2',\ldots,T_m')$ and $U = U(n,m;T_1,T_2,\ldots,T_m)$ and let the R-polynomials of U and U' be

$$\begin{aligned} \phi_R(U,x) = &\sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(U,k) x^{n-2k} - \frac{2}{d_{v_1}\ldots d_{v_m}} x^{n-m} \\ &+ \frac{2}{d_{v_1}\ldots d_{v_m}} \sum_{k=1}^{\lfloor \frac{n-m}{2} \rfloor} (-1)^{k+1} b(R(U - C_m - \{v_i v_j | v_i \in V(C_m)\}), k) x^{n-2k}, \end{aligned}$$

$$\phi_R(U',x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(U',k)x^{n-2k} - \frac{2}{d_{v_1}\dots d_{v_m}} x^{n-m}$$
$$+ \frac{2}{d_{v_1}\dots d_{v_m}} \sum_{k=1}^{\lfloor \frac{n-m}{2} \rfloor} (-1)^{k+1} b(R(U' - C_m - \{v_iv_j | v_i \in V(C_m)\}), k)x^{n-2k},$$

respectively, where $b(R(U),0) = b(R(U'),0) = b(R(U - C_m - \{v_iv_j|v_i \in V(C_m)\}),0) = b(R(U' - C_m - \{v_iv_j|v_i \in V(C_m)\}),0) = 1$. Since $d_{U'}(u_i) = (d_U(u_i)+1)$, $d_{U'}(v_i) = d_U(v_i)$, $d_{U'}(u_i) = j+3$, $d_U(u_i) = j+2$, $d_U(v_i) \geq 3$, for $k = 1$ we have

$$\begin{aligned}
b(R(U'),1) - b(R(U),1) =& \frac{1}{d_{U'}(u_{s-3})d_{U'}(u_{s-2})} + \frac{j+2}{2(d_U(u_i)+1)} + \frac{1}{(d_U(u_i)+1)d_U(u_{i_1})} \\
&- \frac{1}{d_T(u_{s-3})d_T(u_{s-2})} - \frac{1}{d_T(u_{s-2})d_T(u_{s-1})} - \frac{j+1}{2d_T(u_i)} - \frac{1}{d_T(v_i)(d_T(u_i))} \\
=& \frac{j+2}{2(j+3)} + \frac{1}{2} + \frac{1}{(d_U(v_i))(j+3)} - \frac{1}{2} - \frac{j+1}{2(j+2)} - \frac{1}{d_U(v_i)(j+2)} \\
=& \frac{(j+2)^2 d_U(v_i)) + 2(j+2) - (j+1)(j+3)d_U(v_i) - 2(j+3)}{2(j+2)(j+3)d_U(v_i))} \\
=& \frac{d_U(v_i) - 2}{2(j+2)(j+3)d_U(v_i))} \\
&> 0.
\end{aligned}$$

That is, $b(R(U'),1) > b(R(U),1)$.
Now, for $k = 0$ in the second summation we have

$$\frac{1}{d_{U'}(v_1)\dots d_{U'}(v_m)} = \frac{1}{d_U(v_1)\dots d_U(v_m)}.$$

Next, for $k = 2, \dots, \lfloor \frac{n}{2} \rfloor$, in the second summation let $P = u_{i_1}u_{i_2}\dots u_{s-3}$. Then

$$\begin{aligned}
b(R(U',k) =& (\sum_{k=1}^{j} \frac{1}{d_{U'}(u'_k)d_{C_m \cup P}(u_i)}) \sum_{L \in L_{k-1}(C_m \cup (p)} R_{U'}(L)) \\
&+ (\frac{1}{d_{U'}(v_i)d_{U'_1}(u_i)} \times \frac{1}{d_{U'}(u_{s-1})d_{U'_1}(u_s)}) \sum_{L \in L_{k-2}(C_m - v_i \cup (P)} R_{U'}(L)) \\
&+ (\frac{1}{d_{U'}(u_i)d_{U'_1}(u_{i_1})} (\sum_{k=1}^{j} \frac{1}{d_{U'}(u'_k)d_{C_m \cup P}(u_k)})) \sum_{L \in L_{k-2}(C_m \cup (P - u_{i_1})} R_{U'}(L)) \\
&+ (\frac{1}{d_{U'}(u_i)d_{U'_1}(u_{i_1})} \times \frac{1}{d_{U'}(u_{s-1})d_{U'_1}(u_s)}) \sum_{L \in L_{k-2}(C_m \cup (P - u_{i_1})} R_{U'}(L)) \\
&+ (\frac{1}{d_{U'}(u_{s-3})d_{U'_1}(u_{s-2})} (\sum_{k=1}^{j} \frac{1}{d_{U'}(u'_k)d_{C_m \cup P}(u_k)})) \sum_{L \in L_{k-2}(C_m \cup (P - u_{s-3})} R_{U'}(L))
\end{aligned}$$

$$
\begin{aligned}
&+(\frac{1}{d_{U'}(u_{s-3})d_{U'_1}(u_{s-2})}(\sum_{k=1}^{j}\frac{1}{d_{U'}(u'_k)d_{C_m\cup P}(u_i)}))\sum_{L\in L_{k-2}(C_m\cup(P-u_{s-3})}R_{U'}(L))\\
&+(\frac{1}{d_{U'}(u_{s-1})d_{U'_1}(u_s)}\times\frac{1}{d_{U'}(u_{s-3})d_{U'_1}(u_{s-2})}\\
&+\frac{1}{d_{U'}(u_{s-1})d_{U'_1}(u_i)}\times\frac{1}{d_{U'}(u_{s-3})d_{U'_1}(u_{s-2})})\sum_{L\in L_{k-2}(C_m\cup(P-u_{s-3})}R_{U'}(L))\\
=&(\frac{j}{2})\sum_{L\in L_{k-1}(C_m\cup(P)}R_{U'}(L)+(\frac{j}{4(j+3)}\sum_{L\in L_{k-2}(C_m\cup(P-u_{i_1})}R_{U'}(L))\\
&+\frac{1}{4(j+3)}\sum_{L\in L_{k-2}(C_m\cup(P-u_{i_1})}R_{U'}(L))+((\frac{j}{4})\sum_{L\in L_{k-2}(C_m\cup(P-u_{s-3})}R_{U'}(L))\\
&+((\frac{1}{4(j+3)})\sum_{L\in L_{k-2}(C_m\cup(P-u_{s-3})}R_{U'}(L))+(\frac{1}{4}\\
&+\frac{1}{4(j+3)})\sum_{L\in L_{k-2}(C_m\cup(P-u_{s-3})}R_{U'}(L)),
\end{aligned}
$$

and

$$
\begin{aligned}
b(R(U,k)=&((\sum_{k=1}^{j}\frac{1}{d_{U'}(u'_k)d_{C_m\cup P}(u_i)}))\sum_{L\in L_{k-1}(C_m\cup(P)}R_U(L))\\
&+(\frac{1}{d_U(u_i)d_U(u_{i_1})}\sum_{k=1}^{j}\frac{1}{d_{U'}(u'_k)d_{C_m\cup P}(u_k)}+\frac{1}{d_U(u_i)d_U(u_{i_1})}(\frac{1}{d_U(u_{s-2})d_U(u_{s-1})}\\
&+\frac{1}{d_U(u_{s-1})d_U(u_s)}))\sum_{L\in L_{k-2}(C_m\cup(P-u_{i_1})}R_U(L))\\
&+(\frac{1}{d_U(u_{s-3})d_U(u_{s-2})}+\frac{1}{d_U(u_{s-2})d_U(u_{s-1})}+\frac{1}{d_U(u_{s-1})d_U(u_s)}\\
&\times(\sum_{k=1}^{j}\frac{1}{d_{U'}(u'_k)d_{C_m\cup P}(u_i)}+(\sum_{k=1}^{j}\frac{1}{d_{U'}(u'_k)d_{C_m\cup P}(u_k)}))\sum_{L\in L_{k-2}(C_m\cup(P-u_{s-3})}R_U(L))\\
&+(\frac{1}{d_{U'}(u'_k)d_{C_m\cup P}(u_{s-3})}\times\frac{1}{d_{U'}(u'_{s-1})d_{C_m\cup P}(u_s)})\sum_{L\in L_{k-2}(C_m\cup(P-u_{s-3})}R_U(L))\\
=&(\frac{j}{2})\sum_{L\in L_{k-1}(C_m\cup(P)}R_U(L))+(\frac{1}{(j+2)}(\frac{j}{4})+\frac{1}{2(j+2)}(\frac{3}{4}))\sum_{L\in L_{k-2}(C_m\cup(P-u_{i_1})}R_U(L))\\
&+((\frac{j}{2(j+2)})+(\frac{j}{2})\sum_{L\in L_{k-2}(C_m\cup(P-u_{s-3})}R_U(L))\\
&+(\frac{1}{4}\times\frac{1}{2})\sum_{L\in L_{k-2}(C_m\cup(P-u_{s-3})}R_U(L)).
\end{aligned}
$$

Since in graphs U' and U we have

$$\sum_{L\in L_{k-1}(C_m\cup P)} R_{U'}(L) = \sum_{L\in L_{k-1}(C_m\cup(P)} R_U(L),$$
$$\sum_{L\in L_{k-2}(C_m\cup(P-u_{i_1})} R_{U'}(L) = \sum_{L\in L_{k-2}(C_m\cup P-u_{i_1})} R_U(L),$$
$$\sum_{L\in L_{k-2}(C_m\cup(P-u_{s-3}})R_{U'}(L) = \sum_{L\in L_{k-2}(C_m\cup P-u_{s-3})} R_U(L),$$
$$\sum_{L\in L_{k-2}(C_m\cup(P-u_{i_1})} R_{U'}(L) = \sum_{L\in L_{k-2}(C_m\cup P-u_{s-3})} R_U(L),$$

and also

$$\sum_{L\in L_{k-2}(C_m\cup(P} R_{U'}(L) \geq \sum_{L\in L_{k-2}(C_m\cup P-u_{s-3})} R_U(L),$$
$$\sum_{L\in L_{k-2}(C_m\cup(P} R_{U'}(L) \geq \sum_{L\in L_{k-2}(C_m\cup P-u_{i_1}} R_U(L),$$

we obtain that

$$b(R(U',k) - b(R(U,k) > 0.$$

By Theorem 4.5, the lemma holds. □

5. Proof of Theorem 2.1

We are now ready to present the proof of the main result of this paper.

Proof. Let $G = U(n, m; T_1, T_2, \ldots, T_m)$ be a unicyclic graph with maximum randić energy and $C_m = v_1v_2\cdots v_mv_1$ be the unique cycle of G and T_i, $1 \leq i \leq m$, be the trees attaching to the vertices of C_m. We know that the number of vertices outside the cycle is $n - m$. We proceed with the following cases.

Case 1: $n-m$ is odd. If $n-m = 1$, then clearly G is cycle C_m with a leaf attached to one of its vertices and the result follows.

Now assume that $n - m \geq 3$. Assume that there is a T_i with at least two leaves u_s, w_q at distance at least two from v_i. Let u_i be a leaf of T_i such that $d_{T_i}(v_i, u_i)$ is as maximum as possible, and let P be the shortest path from v_i to u_i. We apply Operation 4.1, repeatedly, to enlarge the path P (by adding vertices at the end of P), to obtain a tree T_i'. Assume that U' is the resulted unicyclic graph, and let P' be the path from v_i to the farthest leaf of T' of v_i. By Lemma 4.6, $\mathcal{E}_R(U) \leq \mathcal{E}_R(U')$. We apply Operation 4.2, repeatedly, to change T_i' to a path. Assume that U'' is the resulted unicyclic graph that shown in Figure 4. By Lemma 4.7, $\mathcal{E}_R(U') \leq \mathcal{E}_R(U'')$.

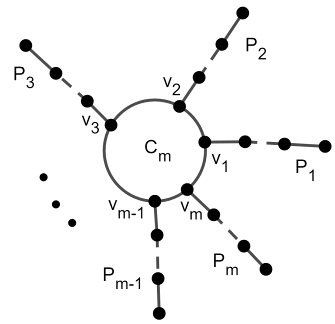

FIGURE 4. Unicyclic graphs U''.

Now we apply Operation 4.3, repeatedly. Assume that U''' is the resulted unicyclic graph that shown in Figure 5. By Lemma 4.8, $\mathcal{E}_R(U') \le \mathcal{E}_R(U''')$.

Case 2: $n-m$ is even. If $n-m=0$, then clearly $G = C_m$. Thus assume that $n-m>0$. Then similar to the first case, we apply Operations 4.1, 4.2 and 4.3 on the graph G. Then a leaf remains, which we join it to the graph obtained in the first case, that is G is obtained from first case graph by adding a leaf to it. □

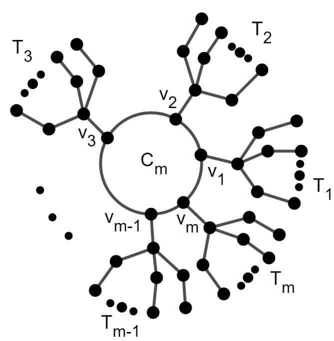

FIGURE 5. Unicyclic graphs U'''.

REFERENCES

[1] A. Ali, I. Gutman and I. Redzepović, *Atom-bond sum-connectivity index of unicyclic graphs and some applications*, El. J. Math., **5** (2023) 1-17.

[2] S. Alikhani and N. Ghanbari, *Randć energy of specific graphs*, Applied Math. Comput., **269** (2015) 722-730.

[3] S. B. Bozkurt and A. D. Gungor, I. Gutman, A. S. Cevik, *Randić Matrix and randi ́c energy*, MATCH Commun. Math. Comput. Chem., **64** (2010) 239-250.

[4] D. M. Cvetković, M. Doob and H. Sachs, *Spectra of Graphs, Theory and Applications*, Barth Verlag, Heidelberg, 1980.

[5] Y. Gao, W. Gao and Y. Shao, *The minimal randić energy of trees with given diameter*, Appl. Math. Comput., **411** (2021) 126489.

[6] S. He, Q. Geng and R.-X. Hao, *The extremal unicyclic graphs with given diameter and minimum edge revised Szeged index*, AIMS Math., **8** (2023) 26301-26327.

[7] R. Horn and C. Johnson, *Matrix Analysis*, Cambridge University Press, Cambridge, 2013.

[8] X. Li, Y. Shi and I. Gutman, *Graph Energy*, Springer, New York, 2012.

[9] B. Liu, Y. Huang and J. Feng, *A note on the randić spectral radius*, MATCH Commun. Math. Comput. Chem., **68** (2012) 913-916.

[10] J. A. Rodrıguez and J. M. Sigarreta, *On the randić index and conditional parameters of a graph*, MATCH Commun. Math. Comput. Chem., **54** (2005) 403-416.

[11] S. Sepidbon, N. Jafari Rad and A. Jahanbani, *On the maximal randć energy of trees with given diameter*, Alg. Struct. Appl., **11** (2024) 217-228.

[12] H. Song and L. Tian, *On the maximal-adjacency-spectrum unicyclic graphs with given maximum degree*, Math. Prob. Eng., (2020) ID9861834.

[13] W. -F. Xia and Y. -M. Chu, *Schur-convexity for a class of symmetric functions and its applications*, J. Ineq. Appl., (2009) 493759.

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