Applied Mathematics and Computation 331 (2018) 334–340

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

On the permanental sum of graphs[☆]

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ARTICLE INFO

MSC:
05C31
05C75
15A15
92E10

Keywords:
Permanent
Permanental polynomial
Coefficients
Permanental sum

ABSTRACT

Let G be a graph and $A(G)$ the adjacency matrix of G. The polynomial $\pi(G,x) = \text{per}(xI - A(G))$ is called the permanental polynomial of G, and the permanental sum of G is the summation of the absolute values of the coefficients of $\pi(G, x)$. In this paper, we investigate properties of permanental sum of a graph, prove recursive formulas to compute the permanental sum of a graph, and show that the ordering of graphs with respect to permanental sum. Furthermore, we determine the upper and lower bounds of permanental sum of unicyclic graphs, and the corresponding extremal unicyclic graphs are also determined.

1. Introduction

The *permanent* of an $n \times n$ real matrix $X = (x_{ij})$, with $i, j \in \{1, 2, \dots, n\}$, is defined as

$$\text{per}(X) = \sum_{\sigma} \prod_{i=1}^{n} x_{i\sigma(i)},$$

where the sum is taken over all permutations σ of $\{1, 2, \dots, n\}$. Valiant [19] has shown that compute the permanent is #P-complete even when restricted to (0, 1)-matrices.

Let G be a graph with n vertices and let $A(G)$ be its adjacency matrix. The polynomial

$$\pi(G,x) = \text{per}(xI - A(G)) = \sum_{k=0}^{n} b_k x^{n-k} \tag{1}$$

is called the *permanental polynomial* of G, where I is the n by n identity matrix. To emphasize the graph G, the coefficients are often written as $b_k(G)$, $0 \le k \le n$.

The properties of the coefficients $b_k(G)$ has been one problem that has attracted many researchers. A graph G is a *Sachs graph* if each of whose component is a single edge or a cycle. Given an integer $k \ge 0$ and a graph G, let $S_k(G)$ denote the collection of all Sachs subgraphs H of G on k vertices, and let $c(H)$ be the number of cycles in a graph H. Merris et al. [16] presented a Sachs type result concerning the coefficients of the permanental polynomial of G, as follows,

$$b_k(G) = (-1)^k \sum_{H \in S_k(G)} 2^{c(H)}, \quad 0 \le k \le n. \tag{2}$$

☆ Supported by the National Natural Science Foundation of China (No. 11761056); the NSF of Qinghai Province (No. 2016-ZJ-947Q); and the High-level Personnel of Scientific Research Project of QHMU (No. 2016XJG07).

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https://doi.org/10.1016/j.amc.2018.03.026
0096-3003/

The *permanental sum* of graph G, denoted by $PS(G)$, is the sum of the absolute values of all coefficients of $\pi(G, x)$. By (2), we have,

$$PS(G) = \sum_{k=0}^{n} |b_k(G)| = \sum_{k=0}^{n} \sum_{H \in S_k(G)} 2^{c(H)}. \tag{3}$$

Thus $PS(G) = 1$ if G is an empty graph.

In late 1970s, permanental polynomials of graphs was first introduced in mathematics and chemistry [2,11,16]. The studies on the permanental polynomials have receiving a lot of attention from researchers in recent years. Cash [4,5], Gutman [8] and Chen [6] studied the coefficients of the permanental polynomials of some chemical graphs, such as benzenoid hydrocarbons, fullerenes, and so on. For more and additional information, see [1,3,7,13,14,17,22,23] and the references therein.

The permanental sum of a graph was first considered by Tong [18]. In [21], Xie et al. captured a labile fullerene $C_{50}(D_{5h})$. Tong computed all 271 fullerenes in C_{50}. In his study, Tong found that the permanental sum of $C_{50}(D_{5h})$ achieves the minimum among all 271 fullerenes in C_{50}. He pointed that the permanental sum would be closely related to stability of molecular graphs. Recently, Li et al. in [12] determined the extremal hexagonal chains with respect to permanental sum. Furthermore, the permanental sum of a graph is also related to the Hosoya index, an important topological index of a graph. For an integer $k \geq 0$, let $m(G, k)$ denote the number of k-matchings of a graph G. The *Hosoya index* $Z(G)$ of a graph G is defined to be the total number of matchings of G, that is

$$Z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} m(G, k), \tag{4}$$

where n is the number of vertices of graph G. By (2), (3) and (4), it is shown that the Hosoya index is an lower bound of the permanental sum of G. That is,

Proposition 1.1. *Let G be a graph. Then*

$$Z(G) \leq PS(G), \text{ where the equality holds if and only if } G \text{ is a forest}. \tag{5}$$

In this paper, we investigate the properties of the permanental sum of a graph. Preliminaries are presented in Section 2, and a number of recursive formulas of permanental sum are derived in Section 3. In Section 4, we prove the ordering of graphs with respect to their permanental sum. In Section 5, we determine extremal unicyclic molecular graphs with respect to permanental sum.

2. Preliminaries

All graphs considered in this work are undirected, finite and simple graphs. For notation and terminology not defined here, see [15].

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The *order* of G is the number of vertices of G, and G is called an *empty graph* if it is of zero order. The *neighborhood* of vertex $v \in V(G)$, denoted by $N_G(v)$, is the set of vertices adjacent to v. The path, cycle, star and complete graph of order n are denoted by P_n, C_n, S_n and K_n, respectively. Let $G \cup H$ denote the union of two vertex disjoint graphs G and H. For any positive integer l, lG denotes the union of l disjoint copies of G.

A *unicyclic graph* is a connected graph containing exactly one cycle. Denote by $\mathscr{U}_n$ the set of all unicyclic graphs on n vertices. Let S_n^+ be the graph obtained by adding a new edge to the star S_n, and let $D_{r,n-r}$ be the graph obtained from the disjoint union of a cycle C_r and a path P_{n-r} by identifying one end of P_{n-r} with one of the vertices of C_r. By definitions, $S_n^+, D_{n,n-r} \in \mathscr{U}_n$.

The following are known on the Hosoya index $Z(G)$ of graph G and $m(G, k)$ the number of k-matchings of graph G.

Lemma 2.1. *(Wagner and Gutman [20]) Suppose that* $G \in \mathscr{U}_n$. *Then* $Z(G) \geq 2n - 2$, *where equality holds if and only if G is isomorphic to* S_n^+.

Lemma 2.2. *(Wagner and Gutman [20]) Let* P_n *be a path of order n. Then*

$$Z(P_n) = \begin{cases} 0 & \text{if } n = 0\ , \\ 1 & \text{if } n = 1\ , \\ Z(P_{n-1}) + Z(P_{n-2}) & \text{if } n \geq 2. \end{cases}$$

Thus the sequence $Z(P_0), Z(P_1), Z(P_2), \ldots$ *is the sequence of Fibonacci numbers.*

Lemma 2.3. *(Gutman and Polansky [9]) Let G be a forest of order n. Then* $m(G, k) \leq m(P_n, k)$, *where equality holds if and only if* $G \cong P_n$.

It follows from (4) and Lemma 2.3 that $Z(G) \leq Z(P_n)$. This, together with (5), implies Lemma 2.4 below.

Lemma 2.4. *Let G be a forest of order n. Then* $PS(G, k) \leq PS(P_n, k)$, *where equality holds if and only if* $G \cong P_n$.

With the same arguments, we also obtain similar relationships for disjoint paths.

Lemma 2.5 (Gutman and Zhang [10])**.** *Let s and r be integers with $s \geq 0$ and $0 \leq r \leq 3$, and let P_n be a path of order $n = 4s + r$. Then $m(P_n, k) > m(P_2 \cup P_{n-2}, k) > m(P_4 \cup P_{n-4}, k) > \cdots > m(P_{2s} \cup P_{2s+r}, k) > m(P_{2s+1} \cup P_{2s+r-1}, k) > m(P_{2s-1} \cup P_{2s+r+1}, k) > \cdots > m(P_3 \cup P_{n-3}, k) > m(P_1 \cup P_{n-1}, k)$.*

Lemma 2.6. *Let k and r be integers with $k \geq 0$ and $0 \leq r \leq 3$, and let P_n be a path of order $n = 4k + r$. Then $PS(P_n) > PS(P_2 \cup P_{n-2}) > PS(P_4 \cup P_{n-4}) > \cdots > PS(P_{2k} \cup P_{n-2k}) > PS(P_{2k+1} \cup P_{n-2k-1}) > PS(P_{2k-1} \cup P_{2-2k+1}) > \cdots > PS(P_3 \cup P_{n-3}) > PS(P_1 \cup P_{n-1})$.*

Proof. This lemma follows from (2)–(5) and by Lemma 2.4. □

The following property of the Fibonacci numbers is well known.

Lemma 2.7. *$F(n) = F(k)F(n-k+1) + F(k-1)F(n-k)$ for $1 \leq k \leq n$.*

3. The recursive formulas of permanental sum of a graph

The main result of this section is to derive Theorem 3.1 below. For a graph G, if $e \in E(G)$, then $\mathcal{C}_G(e)$ denote the collection of cycles in G that contains e; and if $v \in V(G)$, then $\mathcal{C}_G(v)$ denote the collection of cycles in G that contains v.

Theorem 3.1. *The permanental sum of a graph satisfies the following identities: (i) Let G and H be two vertex disjoint connected graphs. Then*

$$PS(G \cup H) = PS(G)PS(H).$$

(ii) Let $e = uv$ be an edge of graph G. Then

$$PS(G) = PS(G-e) + PS(G-v-u) + 2\sum_{C \in \mathcal{C}_G(e)} PS(G - V(C)).$$

(iii) Let v be a vertex of graph G. Then

$$PS(G) = PS(G-v) + \sum_{u \in N_G(v)} PS(G-v-u) + 2\sum_{C \in \mathcal{C}_G(v)} PS(G - V(C)).$$

Proof. (i) Each Sachs subgraph of order k in $G \cup H$ consists of a Sachs subgraph of order s in G together with a Sachs subgraph of order $k - s$ in H, where $0 \leq s \leq k$. Hence

$$PS(G \cup H) = \sum_{k=0}^{n} |b_k(G)| = \sum_{k=0}^{n}\sum_{s=0}^{k} |b_s(G)||b_{k-s}(H)| = PS(G)PS(H).$$

For each integer i, let $S_i(G)$ denote the collection of all Sachs subgraphs of G on i vertices.

(ii) Let $e = uv \in E(G)$ be a given edge, and define $S'_i(G, e) = \{H \in S_i(G) : e \in E(H)\}$ and $S''_i(G, e) = \{H \in S_i(G) : e \notin E(H)\}$. Hence by definition, $|S''_i(G, e)| = |b_i(G - uv)|$. For each $H \in S'_i(G)$, either e itself is a component of H, or e lies in a cycle of H. It follows that $|\{H \in S'_i(G, e) : e \text{ is a component of } H\}| = |b_{i-2}(G-u-v)|$, and $|\{H \in S'_i(G, e) : e \text{ lies in a cycle of } H\}| = 2\sum_{k=0}^{i}\sum_{C_k \in \mathcal{C}_G(e)} |b_{i-k}(G - V(C_k))|$. Thus

$$|b_i(G)| = |b_i(G-e)| + |b_{i-2}(G-u-v)| + 2\sum_{k=0}^{i}\sum_{C_k \in \mathcal{C}_G(uv)} |b_{i-k}(G - V(C_k))|$$

for all positive integers i. It follows that

$$\begin{aligned} PS(G) &= \sum_{k=0}^{n} |b_k(G)| \\ &= \sum_{k=0}^{n}(|b_i(G-e)| + |b_{i-2}(G-u-v)| + 2\sum_{k=0}^{i}\sum_{C_k \in \mathcal{C}_G(e)} |b_{i-k}(G - V(C_k))|) \\ &= PS(G-e) + PS(G-v-u) + 2\sum_{C \in \mathcal{C}_G(e)} PS(G - V(C)). \end{aligned}$$

(iii) Similar to the proof of (ii). Let $v \in V(G)$ be a given vertex, and define $S'_i(G, v) = \{H \in S_i(G) : v \in V(H)\}$ and $S''_i(G, v) = \{H \in S_i(G) : v \notin V(H)\}$. Hence by definition, $|S''_i(G, v)| = |b_i(G - v)|$. For each $H \in S'_i(G)$, either v is an endpoint of some single edge of H, or v lies in a cycle of H. It follows that $|\{H \in S_i'(G, v) : v$ is an endpoint of some single edge $e(= uv)$ of $H\}| = |b_{i-2}(G - u - v)|$, and $|\{H \in S_i'(G, v) : v$ lies in a cycle C_k of $H\}| = 2\sum_{k=0}^{i}\sum_{C_k \in \mathcal{C}_G(v)} |b_{i-k}(G - V(C_k))|$. Thus

$$|b_i(G)| = |b_i(G - v)| + |b_{i-2}(G - u - v)| + 2\sum_{k=0}^{i}\sum_{C_k \in \mathcal{C}_G(v)} |b_{i-k}(G - V(C_k))|.$$

Substituting this into the definition of $PS(G)$ (as in the previous paragraph) yields the given identity. □

From Theorem 3.1 it immediately follows:

Corollary 3.2. *Among all graphs with n vertices, the graph nK_1 and the complete graph K_n have, respectively, minimum and maximum permanental sum.*

4. Inequality relationship of permanental sums of graphs

In this section, we will present several inequalities on the permanental sum of graphs. If $e \in E(G)$ is an edge of graph G, then $G - e$ is the spanning subgraph of G with edge set $E(G) - \{e\}$.

Theorem 4.1. *Let G be a graph and e an edge of G. Then*

$$PS(G - e) < PS(G).$$

Proof. This theorem is a direct result of (ii) of Theorem 3.1. □

Suppose that $V(P_n) = \{v_1, v_2, \ldots, v_n\}$ with $v_i v_{i+1} \in E(P_n)$ for each i with $1 \le i \le n - 1$. For a fixed vertex $v \in V(G)$ of a graph G, the graph $P_n(v_i, v)G$ is obtained from the disjoint union of G and P_n by identifying the vertex v_i of P_n with the vertex v of G.

Theorem 4.2. *Let G be a graph and v an arbitrary vertex of G. Then for any integers $k \ge 1$, $r \in \{-1, 0, 1, 2\}$, and $n = 4k + r$, we have $PS(P_n(v_1, v)G) > PS(P_n(v_3, v)G) > \cdots > PS(P_n(v_{2k+1}, v)G) > PS(P_n(v_{2k}, v)G) > PS(P_n(v_{2k-2}, v)G) > \cdots > PS(P_n(v_2, v)G)$.*

Proof. Let $\mathcal{C}_G(v)$ be the set of cycle C_j containing v in G, where $3 \le j \le n$. By Theorem 3.1 (iii), we have

$$\begin{aligned} PS(P_n(v_i, v)G) &= PS(P_{i-1})PS(P_{n-i})PS(G - v) + PS(P_{i-2})PS(P_{n-i})PS(G - v) \\ &\quad + PS(P_{i-1})PS(P_{n-i-1})PS(G - v) + \sum_{u \in N_G(v)} PS(G - v - u)PS(P_{i-1})PS(P_{n-i}) \\ &\quad + 2\sum_{C_j \in \mathcal{C}_G(v)} PS(G - V(C_j))PS(P_{i-1})PS(P_{n-i}). \end{aligned} \tag{6}$$

Suppose that $1 \le l \le k$ is an integer. By (5), (6) and Lemma 2.2, it is routine to verify that

$$\begin{aligned} PS(P_n(v_{2l-1}, v)G) - PS(P_n(v_{2l+1}, v)G) &= [PS(P_{2l-2})PS(P_{n-2l+1}) + PS(P_{2l-3})PS(P_{n-2l+1}) + PS(P_{2l-2})PS(P_{n-2l}) \\ &\quad - PS(P_{2l})PS(P_{n-2l-1}) - PS(P_{2l-1})PS(P_{n-2l-1}) - PS(P_{2l})PS(P_{n-2l-2})]PS(G - v) \\ &\quad + [PS(P_{2l-2})PS(P_{n-2l+1}) - PS(P_{2l})PS(P_{n-2l-1})]\sum_{u \in N_G(v)} PS(G - v - u) \\ &\quad + 2[PS(P_{2l-2})PS(P_{n-2l+1}) - PS(P_{2l})PS(P_{n-2l-1})]\sum_{C_j \in \mathcal{C}_G(v)} PS(G - V(C_j)) \\ &= [F(2l-1)F(n-2l+2) + F(2l-2)F(n-2l+2) + F(2l-1)F(n-2l+1) \\ &\quad - F(2l+1)F(n-2l) - F(2l)F(n-2l) - F(2l+1)F(n-2l-1)]PS(G - v) \\ &\quad + [PS(P_{2l-2})PS(P_{n-2l+1}) - PS(P_{2l})PS(P_{n-2l-1})]\sum_{u \in N_G(v)} PS(G - v - u) \\ &\quad + 2[PS(P_{2l-2})PS(P_{n-2l+1}) - PS(P_{2l})PS(P_{n-2l-1})]\sum_{C_j \in \mathcal{C}_G(v)} PS(G - V(C_j)) \\ &= +[PS(P_{2l-2})PS(P_{n-2l+1}) - PS(P_{2l})PS(P_{n-2l-1})]\sum_{u \in N_G(v)} PS(G - v - u) \\ &\quad + 2[PS(P_{2l-2})PS(P_{n-2l+1}) - PS(P_{2l})PS(P_{n-2l-1})]\sum_{C_j \in \mathcal{C}_G(v)} PS(G - V(C_j)). \end{aligned}$$

By Lemma 2.6, it can be known that $PS(P_{2l-2})PS(P_{n-2l+1}) - PS(P_{2l})PS(P_{n-2l-1}) > 0$. Thus, $PS(P_n(v_{2l-1}, v)G) > PS(P_n(v_{2l+1}, v)G)$.

Similarly, by (5), (6) and Lemma 2.2, we have

$$\begin{aligned}
&PS(P_n(v_{2l,v})G) - PS(P_n(v_{2l-2}, v)G)\\
&= [F(2l)F(n-2l+1) + F(2l-1)F(n-2l+1) + F(2l)F(n-2l)\\
&- F(2l-2)F(n-2l+3) - F(2l-3)F(n-2l+3) - F(2l-2)F(n-2l+2)]PS(G-v)\\
&+ [PS(P_{2l-1})PS(P_{n-2l}) - PS(P_{2l-3})PS(P_{n-2l+2})] \sum_{u\in N_G(v)} PS(G-v-u)\\
&+ 2[PS(P_{2l-1})PS(P_{n-2l}) - PS(P_{2l-3})PS(P_{n-2l+2})] \sum_{C_j\in \mathcal{C}_G(v)} PS(G-V(C_j))\\
&= +[PS(P_{2l-1})PS(P_{n-2l}) - PS(P_{2l-3})PS(P_{n-2l+2})] \sum_{u\in N_G(v)} PS(G-v-u)\\
&+ 2[PS(P_{2l-1})PS(P_{n-2l}) - PS(P_{2l-3})PS(P_{n-2l+2})] \sum_{C_j\in \mathcal{C}_G(v)} PS(G-V(C_j)).
\end{aligned}$$

Thus by Lemma 2.6, we derive that $PS(P_{2l-1})PS(P_{n-2l}) - PS(P_{2l-3})PS(P_{n-2l+2}) > 0$, and so $PS(P_n(v_{2l,v})G) > PS(P_n(v_{2l-2}, v)G)$.

Finally, we will prove that $PS(P_n(v_{2l+1,v})G) > PS(P_n(v_{2l}, v)G)$.

$$\begin{aligned}
&PS(P_n(v_{2l+1,v})G) - PS(P_n(v_{2l}, v)G)\\
&= [F(2l+1)F(n-2l) + F(2l)F(n-2l) + F(2l+1)F(n-2l-1)\\
&- F(2l)F(n-2l+1) - F(2l-1)F(n-2l+1) - F(2l)F(n-2l)]PS(G-v)\\
&+ [PS(P_{2l})PS(P_{n-2l-1}) - PS(P_{2l-1})PS(P_{n-2l})] \sum_{u\in N_G(v)} PS(G-v-u)\\
&+ 2[PS(P_{2l})PS(P_{n-2l-1}) - PS(P_{2l-1})PS(P_{n-2l})] \sum_{C_j\in \mathcal{C}_G(v)} PS(G-V(C_j)).
\end{aligned}$$

It then follows by Lemma 2.6 that $PS(P_{2l})PS(P_{n-2l-1}) - PS(P_{2l-1})PS(P_{n-2l}) > 0$, and so $PS(P_n(v_{2l+1}, v)G) > PS(P_n(v_{2l}, v)G)$. The proof is completed. □

Next we shall introduce a graph operation that can be considered as graph transformations, and we shall show that generally, the transformed graph will have bigger permanental sum than that of the original graph.

Definition 4.3. Let $G \neq P_1$ be a graph and v an arbitrary vertex of G. G_1 denotes the graph that results from identifying v with the vertex v_k of a path $P_n = v_1v_2\dots v_n$, $1<k<n$. G_2 is obtained from G_1 by deleting the path $v_1v_2\dots v_{k-1}$ of P_n and attaching the path $v_1v_2\dots v_{k-1}$ to v_n of P_n. We designate the transformation from G_1 to G_2 as of type **I**.

Corollary 4.4. *Let G_1 and G_2 be the graphs defined in definition 4.3. Then $PS(G_1) < PS(G_2)$.*

Proof. This follows immediately from Theorem 4.2. □

Definition 4.5. Let $P = uu_1u_2\dots u_tv$ be a path of C_r in unicyclic graph G, the degrees of $u, u_1, u_2 \dots u_t, v$ in G be 2. G_1 denotes the graph that results from identifying u with the vertex v_k of a path $v_1v_2\dots v_k$ and identifying v with the vertex v_{k+1} of a path $v_{k+1}v_{k+2}\dots v_n$, $1<k<n-1$. G_2 is obtained from G_1 by deleting the path $v_1v_2\dots v_{k-1}$ and attaching simultaneously the path $v_1v_2\dots v_{k-1}$ to v_n. And G_3 is obtained from G_1 by deleting the path $v_{k+2}v_{k+3}\dots v_n$ and attaching simultaneously the path $v_{k+2}v_{k+3}\dots v_n$ to v_1. We designate the transformation from G_1 to G_2 or G_3 as of type **II**.

Theorem 4.6. *Let G_1, G_2 and G_3 be the unicyclic graphs defined in definition 4.5. Then $PS(G_1) < PS(G_2)$ or $PS(G_1) < PS(G_3)$.*

Proof. Suppose that $N_G(u) = \{u_1, x\}$ and $N_G(v) = \{u_t, y\}$. Set

$$A = PS(G - \{u, u_1, \dots, u_t, v\}),\quad B = PS(G - \{u, u_1, \dots, u_t, v, y\}),$$
$$C = PS(G - \{u, u_1, \dots, u_t, v, x\}),\quad D = PS(G - \{u, u_1, \dots, u_t, v, x, y\}).$$

By Theorem 3.1 and (5), we obtain that

$$\begin{aligned}
PS(G_1) &= PS(G_1 - u) + PS(G_1 - \{u, x\}) + PS(G_1 - \{u, u_1\}) + PS(G_1 - \{u, v_{k-1}\})\\
&\quad + 2PS(G_1 - V(C_r))\\
&= PS(G_1 - \{u, v\}) + PS(G_1 - \{u, v, y\}) + PS(G_1 - \{u, v, u_t\}) + PS(G_1 - \{u, v, v_{k+2}\})\\
&\quad + PS(G_1 - \{u, x, v\}) + PS(G_1 - \{u, x, v, y\}) + PS(G_1 - \{u, x, v, u_t\}) + PS(G_1 -\\
&\quad \{u, x, v, v_{k+2}\}) + PS(G_1 - \{u, u_1, v\}) + PS(G_1 - \{u, u_1, v, y\}) + PS(G_1 - \{u, u_1, v, u_t\})\\
&\quad + PS(G_1 - \{u, u_1, v, v_{k+2}\}) + PS(G_1 - \{u, v_{k-1}, v\}) + PS(G_1 - \{u, v_{k-1}, v, y\})\\
&\quad + PS(G_1 - \{u, v_{k-1}, v, u_t\}) + PS(G_1 - \{u, v_{k-1}, v, v_{k+2}\}) + 2PS(G_1 - V(C_r))
\end{aligned}$$

$$
\begin{aligned}
&= A[F(k)F(n-k)F(t+1)+F(k)F(n-k)F(t)+F(k)F(n-k-1)F(t+1)\\
&\quad +F(k)F(n-k)F(t)+F(k)F(n-k)F(t-1)+F(k)F(n-k-1)F(t)\\
&\quad +F(k-1)F(n-k)F(t+1)+F(k-1)F(n-k)F(t)+F(k-1)F(n-k-1)F(t+1)]\\
&\quad +B[F(k)F(n-k)F(t+1)+F(k)F(n-k)F(t)+F(k-1)F(n-k)F(t+1)]\\
&\quad +C[F(k)F(n-k)F(t+1)+F(k)F(n-k)F(t)+F(k)F(n-k)F(t+1)]\\
&\quad +D(F(k)F(n-k)F(t+1))+2PS(P_{k-1})PS(P_{n-k-1})PS(G-V(C_r))\\
&= A[F(k+1)F(n-k+1)F(t+1)+F(k+1)F(n-k)F(t)+F(k)F(n-k+1)F(t)\\
&\quad +F(k)F(n-k)F(t-1)]+B[F(k+1)F(n-k)F(t+1)+F(k)F(n-k)F(t)]\\
&\quad +C[F(k)F(n-k+1)F(t+1)+F(k)F(n-k)F(t)]+D(F(k)F(n-k)F(t+1))\\
&\quad +2PS(P_{k-1})PS(P_{n-k-1})PS(G-V(C_r)),
\end{aligned}
$$

$$
\begin{aligned}
PS(G_2) &= PS(G_2-u)+PS(G_2-\{u,x\})+PS(G_2-\{u,u_1\})+2PS(G_2-V(C_r))\\
&= PS(G_2-\{u,v\})+PS(G_2-\{u,v,y\})+PS(G_2-\{u,v,u_t\})+PS(G_2-\{u,v,v_{k+2}\})\\
&\quad +PS(G_2-\{u,x,v\})+PS(G_2-\{u,x,v,y\})+PS(G_2-\{u,x,v,u_t\})+PS(G_2-\\
&\quad \{u,x,v,v_{k+2}\})+PS(G_2-\{u,u_1,v\})+PS(G_2-\{u,u_1,v,y\})+PS(G_2-\{u,u_1,v,u_t\})\\
&\quad +PS(G_2-\{u,u_1,v,v_{k+2}\})+2PS(G_2-V(C_r))\\
&= A[F(n)F(t+1)+F(n+1)F(t)+F(n-1)F(t-1)]+B[F(n-1)F(t+1)\\
&\quad +F(n-1)F(t)]+C[F(n)F(t+1)+F(n-1)F(t)]+D(F(n-1)F(t+1))\\
&\quad +2PS(P_{n-2})PS(G-V(C_r)),
\end{aligned}
$$

and

$$
\begin{aligned}
PS(G_3) &= PS(G_3-u)+PS(G_3-\{u,x\})+PS(G_3-\{u,u_1\})+PS(G_3-\{u,v_{k-1}\})\\
&\quad +2PS(G_3-V(C_r))\\
&= PS(G_3-\{u,v\})+PS(G_3-\{u,v,y\})+PS(G_3-\{u,v,u_t\})+PS(G_3-\{u,x,v\})\\
&\quad +PS(G_3-\{u,x,v,y\})+PS(G_3-\{u,x,v,u_t\})+PS(G_3-\{u,u_1,v\})+PS(G_3\\
&\quad -\{u,u_1,v,y\})+PS(G_3-\{u,u_1,v,u_t\})+PS(G_3-\{u,v_{k-1},v\})+PS(G_3-\{u,v_{k-1},v,y\})\\
&\quad +PS(G_3-\{u,v_{k-1},v,u_t\})+2PS(G_3-V(C_r))\\
&= A[F(n)F(t+1)+F(n+1)F(t)+F(n-1)F(t-1)]+B[F(n)F(t+1)\\
&\quad +F(n-1)F(t)]+C[F(n-1)F(t+1)+F(n-1)F(t)]+D(F(n-1)F(t+1))\\
&\quad +2PS(P_{n-2})PS(G-V(C_r)).
\end{aligned}
$$

If follows by Lemma 2.4 that $PS(P_{n-2}) > PS(P_{k-1})PS(P_{n-k-1})$. If $B \le C$, then by Lemma 2.7, we have

$$
\begin{aligned}
\Delta &= PS(G_2)-PS(G_1)\\
&= B[-F(k-1)F(n-k-2)F(t+1)+F(k-1)F(n-k-1)F(t)]\\
&\quad +C[F(k-1)F(n-k)F(t+1)+F(k-1)F(n-k-1)F(t)]+D[F(k-1)F(n-k-1)\\
&\quad F(t+1)]+2[PS(P_{n-2})-PS(P_{k-1})PS(P_{n-k-1})]PS(G-V(C_r))\\
&> 0.
\end{aligned}
$$

If $B > C$, then by Lemma 2.5, we have

$$
\begin{aligned}
\Delta' &= PS(G_3)-PS(G_1)\\
&= B[F(k)F(n-k-1)F(t+1)+F(k-1)F(n-k-1)F(t)]\\
&\quad +C[-F(k-2)F(n-k-1)F(t+1)+F(k-1)F(n-k-1)F(t)]+D[F(k-1)\\
&\quad F(n-k-1)F(t+1)]+2[PS(P_{n-2})-PS(P_{k-1})PS(P_{n-k-1})]PS(G-V(C_r))\\
&> 0.
\end{aligned}
$$

This completes the proof. □

5. Permanental sum of unicyclic graphs

In this section, we shall determine the maximum and minimum permanental sums of unicyclic graphs and characterize the corresponding extremal graphs.

Theorem 5.1. *Let G be a unicyclic graph with $n \geq 5$ vertices. Then*

$$2n \leq PS(G) \leq 6F_{n-2} + 2F_{n-3},$$

where the first equality holds if and only if $G \cong S_n^+$, and where the second equality holds if and only if $G \cong D_{3,n-3}$.

Proof. We start with the first inequality stated in Theorem 5.1. Let $G \in \mathscr{U}_n$ be a graph. By the definition of permanental sum of a graph, it can be seen that $PS(G) = Z(G) + 2w(G)$, where $w(G)$ denotes the number of all Sachs graphs containing the unique cycle of G, and $w(G) \geq 1$. By Lemma 2.1, we know that if $G \neq S_n^+$ then $Z(S_n^+) < Z(G)$. Since $w(S_n^+) = 1$, $2n = Z(S_n^+) + 2 = PS(S_n^+) < PS(G) = Z(G) + 2w(G)$.

Let C_r denote the unique cycle of G and assume that $G \neq C_n$. Repeatedly applying Transformation **I** on G to transform G into G' that results from attaching some paths on some vertices of C_r. By Corollary 4.4, we have $PS(G') \geq PS(G)$. Then, by repeatedly applying transformation **II** on G', to convert G' into the graph $D_{r,n-r}$. By Theorem 4.6, we have $PS(G') \leq PS(D_{r,n-r})$, where equality holds if and only if $G' \cong D_{r,n-r}$. By Theorem 3.1, we conclude that

$$\begin{aligned}
&PS(D_{r-1,n-r+1}) - PS(D_{r,n-r}) \\
&\quad = PS(P_{r-2})PS(P_{n-r+1}) + 2PS(P_{r-3})PS(P_{n-r+1}) + PS(P_{r-2})PS(P_{n-r}) + 2PS(P_{n-r+1}) \\
&\quad - PS(P_{r-1})PS(P_{n-r}) - 2PS(P_{r-2})PS(P_{n-r}) - PS(P_{r-1})PS(P_{n-r-1}) + 2PS(P_{n-r}) \\
&\quad = F(r-1)F(n-r+2) + 2F(r-2)F(n-r+2) + F(r-1)F(n-r+1) + 2F(n-r+2) \\
&\quad - F(r)F(n-r+1) - 2F(r-1)F(n-r+1) - F(r)F(n-r) - 2F(n-r+1) \\
&\quad = F(r-2)F(n-r) - F(r-3)F(n-r+1) + 2F(n-r) \\
&> 0.
\end{aligned}$$

This implies that $PS(D_{r,n-r}) \leq PS(D_{3,n-3})$, where equality holds if and only if $r = 3$. By Lemma 2.2 and Theorem 3.1, we obtain that $PS(D_{3,n-3}) = 6F_{n-2} + 2F_{n-3} > F_{n-1} + F_{n+1} + 2 = PS(C_n)$. Consequently, $PS(D_{3,n-3}) > PS(G)$ provided $\mathscr{U}(n) \setminus D_{3,n-3}$. □

Remark 1. With elementary algebraic manipulations, one can derive that $PS(C_4) > PS(D_{3,1})$. This is the unique exception for Theorem 5.1.

Let $\mathscr{U}(n, r)$ denote the set of all unicyclic graphs with order n and girth r. Checking the proof of Theorem 5.1, it can find the following result.

Theorem 5.2. *Let $G \in \mathscr{U}(n, r)$. Then $PS(G) \leq PS(D_{r,n-r})$ with the equality if and only if $G \cong D_{r,n-r}$.*

Acknowledgment

We would like to thank the referees for their helpful recommendations.

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