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[☆]

Tingzeng Wu[a,*], Hong-Jian Lai[b]

[a] School of Mathematics and Statistics, Qinghai Nationalities University, Xining, Qinghai 810007, PR China
[b] Department of Mathematics, West Virginia University, Morgantown, WV, USA

A R T I C L E I N F O

MSC:
05C31
05C75
15A15
92E10

Keywords:
Permanent
Permanental polynomial
Coefficients
Permanental sum

A B S T R A C T

Let G be a graph and $A(G)$ the adjacency matrix of G. The polynomial $\pi(G, x) = \mathrm{per}(xI - A(G))$ 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

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

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

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

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).

* Corresponding author.
E-mail addresses: mathtzwu@163.com (T. Wu), hjlai@math.wvu.edu (H.-J. Lai).

https://doi.org/10.1016/j.amc.2018.03.026
0096-3003/© 2018 Published by Elsevier Inc.

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.