MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **66** (2011) 743-750

ISSN 0340 - 6253

Remarks on the Relations Between the Permanental and Characteristic Polynomials of Fullerenes*

Qiang Chou   Heng Liang †   Fengshan Bai

Department of Mathematical Sciences,
Tsinghua University,
Beijing, 100084, P.R.CHINA.

(Received January 10, 2011)

Abstract

Several relations between the coefficients of the permanental and characteristic polynomials were given by Gutman and Cash [*MATCH Commun. Math. Comput. Chem.* **45** (2002) 55-70]. In this paper, some more and general connections between those coefficients are presented.

1 Introduction

Graph polynomials were among the most popular objects of research in chemical graph theory (see, for example, refs [1–4]). The most extensively examined one is the characteristic polynomial.

Let G be a graph with n vertices and A be its (0-1) adjacency matrix. Thus A is a square matrix with order n. The characteristic polynomial of the graph G is defined as

$$\phi(G,\lambda) = det(\lambda I - A) = \sum_{k=0}^{n} a_k \lambda^{n-k}, \tag{1}$$

where *det* denotes the determinant of a matrix.

Replacing the determinant in (1) with another matrix operator permanent [5–7], the permanental polynomial of a graph G, which is also of interest in chemical graph theory [8–14], is given as

$$\pi(G,x) = per(xI - A) = \sum_{k=0}^{n} b_k x^{n-k}, \tag{2}$$

*Supported by National Science Foundation of China 10871115.

†E-mail address: hliang@math.tsinghua.edu.cn

where *per* denotes the permanent of a matrix. Some efficient methods were developed for the computation of the coefficients a_k of the characteristic polynomial [15, 16]. The computation of permanental polynomial is much harder than that of characteristic polynomial [9, 11].

The formulas for the first several coefficients of characteristic polynomial of fullerene graph are proposed by Balasubramanian [17]. Then some relations between the coefficients of characteristic polynomial and permanental polynomial are presented by Gutman and Cash [11]. In this paper, some more formulas on a_k and b_k and the relations between them are given for fullerene graph.

2 The Relations Between the Permanental and Characteristic Polynomials of Fullerenes

A fullerene C_n is a convex polyhedral carbon cage with n atoms arranged in 12 pentagonal and $\frac{n}{2}-10$ hexagonal faces. The coefficients a_k of the characteristic polynomial and b_k of the permanental polynomial can be represented through the structure of the graph G by Sachs Theorem [18].

A Sachs graph S is a graph whose components are cycles and/or the complete graphs with two vertices [1]. Let $p(S)$ and $c(S)$ denote the number of components and cycles in a Sachs graph S. Then the Sachs theorem reads

$$a_k = \sum_S (-1)^{p(S)} 2^{c(S)}, \tag{3}$$

where the summation goes over all k-vertex Sachs graphs of G.

For the coefficients of the permanental polynomial, the result is given by [8],

$$b_k = (-1)^k \sum_S (+1)^{p(S)} 2^{c(S)} = (-1)^k \sum_S 2^{c(S)}. \tag{4}$$

Equations (3) and (4) provide a general connection between the structure of a graph and the coefficients of its characteristic and permanental polynomials respectively.

By Sachs theorem, Gutman, Cash and Balasubramanian give the following results on the coefficients of characteristic and permanental polynomials for fullerene graph.

Theorem 2.1 ([11]). *Let G be a molecular graph of a fullerene in which $p > 0$. Then for $k = 0, 1, \cdots, 7$, $|a_k| = |b_k|$ and $|a_8| = b_8 - 4p$, where p is the number of edges common to two pentagons.*

Theorem 2.2 ([11]). *Let G be a molecular graph of an IPR fullerene, Then for $k = 0, 1, \cdots, 9$, $|a_k| = |b_k|$ and $|a_{10}| = b_{10} - 528$.*[1]

Theorem 2.3 ([17]). *For all the fullerenes, the values of a_k and $b_k (k = 0, 1, \cdots, 7)$ are depend on the number of the vertices n of the graph only.*

$a_0 = b_0 = 1;$

$a_1 = b_1 = 0;$

$-a_2 = b_2 = \frac{3}{2}n;$

$a_3 = b_3 = 0;$

$a_4 = b_4 = \frac{9}{8}n^2 - \frac{15}{4}n;$

$a_5 = b_5 = -24;$

$-a_6 = b_6 = \frac{9}{16}n^3 - \frac{45}{8}n^2 + \frac{31}{2}n - 20;$

$a_7 = -b_7 = 36n - 240.$

In this paper, we give more discussions on a_k and b_k with some structural parameters of fullerene graph by using equations (3) and (4) extensively. Besides the parameter p, which is appeared in Theorem 2.1, two more parameters q and r will be also used, where q enumerates the number of vertices common to three pentagons respectively, r counts the number of pairs of nonadjacent pentagon edges shared with two other pentagons. These parameters are discussed in many references [19–22]. Figure 1 shows the local structures that contribute to the values p, q and r respectively.

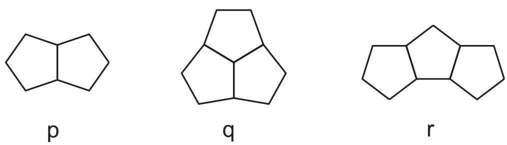

Figure 1: Substructures that contribute to the p, q and r counts

Two new parameters are introduced here. The parameters s and t count the number of pairs of nonadjacent hexagon edges shared with two other pentagons, whose local structures are shown in Figure 2.

[1]The equation given by Gutman and Cash [11] was $|a_{10}| = b_{10} - 264$.

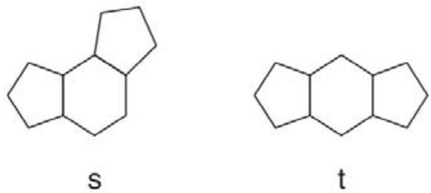

Figure 2: Substructures that contribute to the s and t counts

There are three possible 8-vertex Sachs graphs of fullerene graph, which are shown in Figure 3. Similarly Figure 4 shows all 9-vertex Sachs graphs of fullerene graph. These lead to the Proposition 2.1 and 2.2.

Proposition 2.1. *Let G be a molecular graph of a fullerene with n atoms. Then*

$$a_8 = \frac{27}{128}n^4 - \frac{135}{32}n^3 + \frac{969}{32}n^2 - \frac{879}{8}n + 240 - 2p \ ;$$

$$b_8 = \frac{27}{128}n^4 - \frac{135}{32}n^3 + \frac{969}{32}n^2 - \frac{879}{8}n + 240 + 2p \ .$$

Hence $b_8 - a_8 = 4p$ and $b_8 = a_8$ in IPR case.

Proposition 2.2. *Let G be a molecular graph of a fullerene with n atoms. Then*

$$-a_9 = -b_9 = 27n^2 - 450n + 2040 + 2(q - 2p) \ .$$

For IPR fullerenes, b_9 and a_9 are only dependent on n.

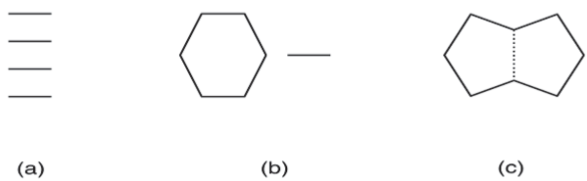

Figure 3: 8-vertex Sachs graphs of fullerene graph

Proposition 2.3. *Let G be a molecular graph of a fullerene with n atoms. Then*

$$|b_{10}| - |a_{10}| = 528 + 2p(3n - 34).$$

For IPR fullerene, $|b_{10}| - |a_{10}| = 528$.

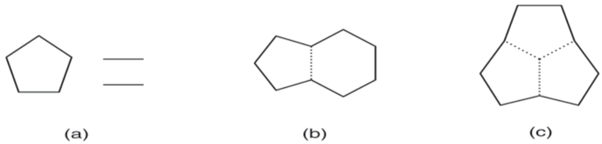

Figure 4: 9-vertex Sachs graphs of fullerene graph

According to equations (3) and (4), the difference between b_{10} and a_{10} comes from 10-vertex Sachs graphs with even components. All possible structures are shown in Figure 5.

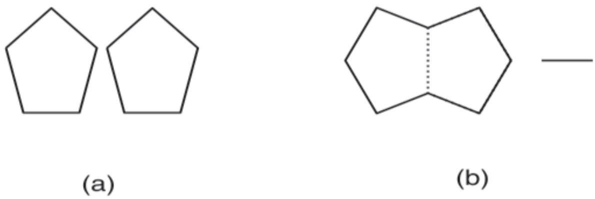

Figure 5: 10-vertex Sachs graphs with even components of fullerene graph

For the cases of $k = 11$ and $k = 12$, only IPR fullerenes are considered here. All 11-vertex Sachs graphs of IPR fullerene graph are shown in Figure 6. Hence we have the following results.

Proposition 2.4. *Let G be a molecular graph of a IPR fullerene with n atoms. Then*

$$a_{11} = \frac{27}{2}n^3 - 405n^2 + 4332n - 17280 \ ,$$

and $|b_{11}| - a_{11} = 240$.

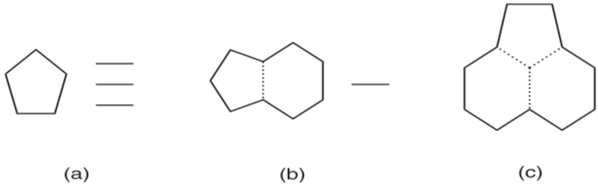

Figure 6: 11-vertex Sachs graphs of IPR fullerene graph

The difference between b_{12} and a_{12} comes from 12-vertex Sachs graphs with odd components, which are shown in Figure 7.

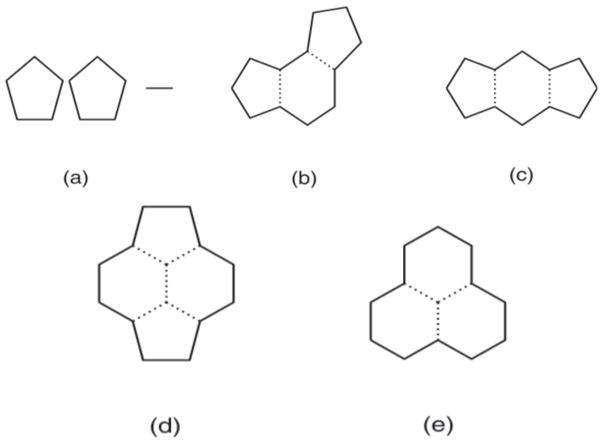

Figure 7: 12-vertex Sachs graphs with odd components of IPR fullerene graph

Proposition 2.5. *Let G be a molecular graph of a IPR fullerene with n atoms. Then*

$$|b_{12}| - |a_{12}| = 796n - 10800 + 8p - 4q + 10s + 4t.$$

3 Conclusions

Gutman and Cash asked the following question in [11]. *For the system studied here, can profitable comparison be made for a_k vs b_k for larger k?* In this paper, the fullerene graph is considered. For fullerenes with (5,5)-edges ($p > 0$), we give a general formulas of a_k and b_k for $k = 8$ and $k = 9$ and a formula of $|b_k| - |a_k|$ for $k = 10$. For IPR fullerenes ($p = 0$), we give a general formula of a_k and b_k for $k = 11$ and a formula of $|b_k| - |a_k|$ for $k = 12$.

For larger k's, numerical results show that $|a_k|$ and $|b_k|$ are very close before they reach their maximums and the differences between them are more and more distinct thereafter. The maximums appear at about $k \approx 2n/3$ [12]. Hence it might be possible to investigate the relations between a_k and b_k for little larger k's that are not very far from 12.

References

[1] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer–Verlag, Berlin, 1986.

[2] D. Bonchev, D. H. Rouvray, *Chemical Graph Theory – Introduction and Fundamentals*, Gordon Breach, New York, 1991.

[3] N. Trinajstić, *Chemical Graph Theory*, 2nd ed., CRC Press, Boca Raton, 1992.

[4] J. R. Dias, *Molecular Orbital Calculations Using Chemical Graph Theory*, Springer–Verlag, Berlin, 1993.

[5] D. M. Cvetković, I. Gutman, N. Trinajstić, Kekulé structures and topology, *Chem. Phys. Lett.* **16** (1972) 614–616.

[6] H. Minc, *Permanents*, Addison–Wesley, Reading, 1978.

[7] I. Gutman, Permanents of adjacency matrices and their dependence on molecular structure, *Polyc. Arom. Comp.* **12** (1998) 281–287.

[8] D. Kasum, N. Trinajstić, I. Gutman, Chemical graph theory. 3. On the permanental polynomial, *Croat. Chem. Acta* **54** (1981) 321–328.

[9] G. G. Cash, The permanental polynomial, *J. Chem. Inf. Comput. Sci.* **40** (2000) 1203–1206.

[10] G. G. Cash, Permanental polynomials of the smaller fullerenes, *J. Chem. Inf. Comput. Sci.* **40** (2000) 1207–1209.

[11] I. Gutman, G. G. Cash, Relations between the permanental and characteristic polynomials of fullerenes and benzenoid hydrocarbons, *MATCH Commun. Math. Comput. Chem.* **45** (2002) 55–70.

[12] H. Tong, H. Liang, F. Bai, Permanental polynomials of the larger fullerenes, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 141–152.

[13] H. Liang, H. Tong, F. Bai, Computing the permanental polynomial of C_{60} in parallel, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 349–358.

[14] F. Belardo, V. Filippis, S. K. Simić, Computing the permanental polynomial of a matrix from a combinatorial viewpoint, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 381–396.

[15] G. G. Cash, A simple program for computing characteristic polynomials with Mathematica, *J. Chem. Inf. Comput. Sci.* **39** (1999) 833–834.

[16] M. V. Diudea, I. Gutman, L. Jäntschi, *Molecular Topology*, Nova, Huntington, 2001.

[17] K. Balasubramanian, Graph–theoretical characterization of fullerene cages, *Polyc. Arom. Comp.* **3** (1993) 247–259.

[18] H. Sachs, Beziehungen zwischen den in einem Graphen entaltenen Kreisen und seinem charakteristischen Polynom, *Publ. Math. (Debrecen)* **11** (1964) 119–134.

[19] G. G. Cash, Permanents of adjacency matrices of fullerenes, *Polyc. Arom. Comp.* **12** (1997) 61–69.

[20] A. T. Balaban, X. Liu, D. J. Klein, D. Babić, T. G. Schmalz, W. A. Seitz, M. Randić, Graph invariants for fullerenes, *J. Chem. Inf. Comput. Sci.* **35** (1995) 396–404.

[21] S. Jiang, H. Liang, F. Bai, New structural parameters and permanents of adjacency matrices of fullerenes, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 131–139.

[22] Y. Ju, H. Liang, J. Zhang, F. Bai, A note on Fowler–Manolopoulos predictor of fullerene stability, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 419–424.