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Applied Mathematics Letters 19 (2006) 652–656
Applied Mathematics Letters
www.elsevier.com/locate/aml

Maximal Hosoya index and extremal acyclic molecular graphs without perfect matching

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Received 13 September 2004; received in revised form 15 July 2005; accepted 1 August 2005

Abstract

Let T be an acyclic graph without perfect matching and $Z(T)$ be its Hosoya index; let F_n be the nth Fibonacci number. It is proved in this work that $Z(T) \leq 2F_{2m}F_{2m+1}$ when T has order $4m$ with the equality holding if and only if $T = T_{1,2m-1,2m-1}$, and that $Z(T) \leq F_{2m+2}^2 + F_{2m}F_{2m+1}$ when T has order $4m+2$ with the equality holding if and only if $T = T_{1,2m+1,2m-1}$, where m is a positive integer and $T_{1,s,t}$ is a graph obtained by joining an isolated vertex with an edge to the $(s+1)$-th vertex (according to its natural ordering) of path P_{s+t+1}.

MSC: 05C90

Keywords: Hosoya index; Acyclic graph; Matching; Molecular; Fibonacci

1. Introduction

A molecular graph is the topology of some molecule or potential molecule (which has not been compounded but possibly), so it is connected with small maximum degree. The Hosoya index of a molecular graph T is defined to be the total number of its matchings [1], where a matching is a subset M of the edge-set of T with the property that no two different edges of M share a common vertex. If denote by $Z(T)$ the Hosoya index of T and $m(T,k)$ the number of its k-matchings, matchings consisting of k edges each, then

$$Z(T) = \sum_{k=0}^{\lfloor n/2 \rfloor} m(T,k)$$

where n stands for the order of T, the number of its vertices, and $\lfloor n/2 \rfloor$ is the integer part of $n/2$. It is convenient to set $m(T,0) = 1$ and $m(T,1) = \varepsilon$, the number of the edges of graph T. By its definition, we deduce that $m(T,k) = 0$ when $k > \lfloor n/2 \rfloor$. The Hosoya index has a close relationship with the total π-electron energy; when T is an acyclic

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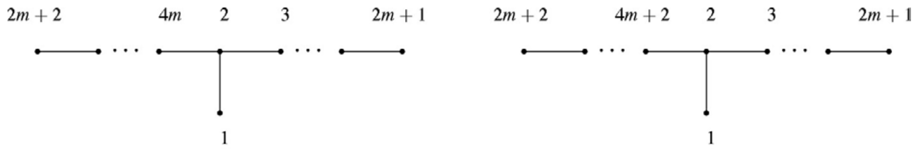
0893-9659/$ - see front matter © 2005 Published by Elsevier Ltd
doi:10.1016/j.aml.2005.08.017



$T_{1,2m-1,2m-1}$ $T_{1,2m+1,2m-1}$

Fig. 1.

molecular graph, according to [2] its total π-electron energy can be expressed as (within the framework of the HMO approximation)

$$E(T) = \frac{2}{\pi}\int_0^{+\infty} x^{-2}\ln\left(1 + \sum_{k=1}^{\lfloor n/2\rfloor} m(T,k)x^{2k}\right)\mathrm{d}x.$$

And so, for acyclic graphs, those that have extremal Hosoya indices are the same ones as have extremal total π-electron energy. Applications of the extremal Hosoya index to the inverse structure–property problem have been observed by many chemists [3]. Many results have also been obtained on the acyclic molecular graphs with minimal Hosoya index [4–7], but very few on the other extremal case that can be reached although it was established long ago that the path P_n is the unique graph that has maximal Hosoya index among acyclic graphs [8]. Furthermore, almost all of these known results focus on graphs that have perfect matching. In this work, we study the maximal Hosoya index of acyclic graphs that contain no perfect matchings and the extremal topology.

To state the main results, we need to define a class of graphs first. Let $T_{1,s,t}$ be the acyclic graph obtained by joining an isolated vertex with an edge to the $(s+1)$-th vertex of the $(s+t+1)$-vertex path P_{s+t+1}, so $T_{1,s,t}$ and $T_{1,t,s}$ are one and the same. For clarity, graphs $T_{1,2m-1,2m-1}$ and $T_{1,2m+1,2m-1}$ are depicted in Fig. 1.

Let F_n stand for the nth Fibonacci number. Since path P_n is the unique extremal acyclic graph that has maximal Hosoya index and P_n contains no perfect matchings when n is odd, when studying the extremal acyclic graphs with maximal Hosoya index and without perfect matchings one need only consider the case where these graphs both have even order. We present explicit expressions for the maximal Hosoya indices and characterize the extremal topology by showing the following two theorems.

Theorem 1. *Let m be a positive integer and T be an acyclic graph of order $4m$. If T contains no perfect matching, then $Z(T) \le 2F_{2m}F_{2m+1}$ with the equality holding if and only if $T = T_{1,2m-1,2m-1}$.*

Theorem 2. *Let m be a positive integer and T be an acyclic graph of order $4m+2$. If T contains no perfect matching, then $Z(T) \le F_{2m+2}^2 + F_{2m}F_{2m+1}$ with the equality holding if and only if $T = T_{1,2m+1,2m-1}$.*

For an n-vertex graph T, let $A(T)$ stand for its adjacency matrix. Define $B(T) = A(T) + I$ to be the neighbor matrix of graph T, where I is the unit matrix of order n. For other graph theoretical notation and terminology not defined here, we follow that of [9].

2. Proofs

Let G and T be two graphs of the same order. G is called *m-smaller* than T if $m(G,k) \le m(T,k)$ holds for every nonnegative integer k, written as $G \preceq T$ or $T \succeq G$; G is strictly m-smaller than T if G is m-smaller than T and $m(G,k) < m(T,k)$ holds for some integer k [4,5].

Lemma 1 ([6]). *Let P_n be a path of order $n = 4s + r$, $0 \le r \le 3$. Then*

$$\begin{aligned} P_n &\succeq P_2 \cup P_{n-2} \succeq P_4 \cup P_{n-4} \succeq \cdots \succeq P_{2s} \cup P_{2s+r} \succeq P_{2s+1} \cup P_{2s+r-1} \\ &\succeq P_{2s-1} \cup P_{2s+r+1} \succeq \cdots \succeq P_3 \cup P_{n-3} \succeq P_1 \cup P_{n-1}. \end{aligned}$$

Lemma 2 ([8]). *Let T be an n-vertex tree (connected acyclic graph). Then $Z(T) \le Z(P_n) = F_{n+1}$, with the equality holding if and only if $T = P_n$.*

Lemma 3. *If m is a positive integer, then $Z(T_{1,2m-1,2m-1}) = 2F_{2m}F_{2m+1}$ and $Z(T_{1,2m+1,2m-1}) = F_{2m+2}^2 + F_{2m}F_{2m+1}$.*

Proof. Label the vertices of $T_{1,2m-1,2m-1}$ just as in Fig. 1. Then its neighbor matrix $B(T_{1,2m-1,2m-1})$ is a square matrix of order $4m$ that has the following form:

$$\begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ \\ 2m \\ \\ \\ \\ \\ \\ \\ \end{array}
\begin{array}{c}
\begin{array}{cccccccc} 1 & 2 & 3 & 4 & 5 & 6 & \cdots & 2m-1 \end{array} \\
\begin{pmatrix}
1 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
1 & 1 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 \\
0 & 1 & 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 1 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 1 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 1 & 1 \\
0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 1
\end{pmatrix}
\end{array}$$

where the $\binom{1,2,\ldots,2m+1}{1,2,\ldots,2m+1}$-minor is the neighbor matrix of path P_{2m+1}, and the $\binom{2m+2,2m+3,\ldots,4m}{2m+2,2m+3,\ldots,4m}$-minor is the neighbor matrix of path P_{2m-1}. In order to prove the lemma, we shall expand the permanent $Per(B(T_{1,2m-1,2m-1}))$ in two different ways. Firstly, we expand it along the first two rows and obtain

$$\begin{aligned}
&Per(B(T_{1,2m-1,2m-1})) \\
&= 2Per\begin{pmatrix}
1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
1 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & 1 & 1 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & 1 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & 1 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 1
\end{pmatrix}_{4m-2} \\
&+ Per\begin{pmatrix}
1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 1 & 1 & 1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & 1 & 1 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & 1 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & 1 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 1 & 1 \\
1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 1
\end{pmatrix}_{4m-2}
\end{aligned}$$

$$+ Per\begin{pmatrix} 1 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & 1 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 \end{pmatrix}_{4m-2}.$$

Noting that the entries lie in the intersections of the first $2m-1$ rows and the first $2m-1$ columns of the first permanent form $B(P_{2m-1})$, from Lemma 2 we deduce that the first permanent equals to $F_{2m}F_{2m}$. Similarly, expanding the second and third permanents along the first column, we get $F_{2m-1}F_{2m}$ and $F_{2m}F_{2m-1}$, respectively. Consequently,

$$Per(B(T_{1,2m-1,2m-1})) = 2F_{2m}F_{2m} + 2F_{2m}F_{2m-1} = 2F_{2m}F_{2m+1}. \tag{1}$$

Secondly, we expand $Per(B(T_{1,2m-1,2m-1}))$ according to the definition of the permanent and get

$$Per(B(T_{1,2m-1,2m-1})) = \sum_{\sigma} b_{1,\sigma(1)}, \ldots, b_{4m,\sigma(4m)}$$

where b_{ij} stands for the element in the ith row and jth column of $B(T_{1,2m-1,2m-1})$ and σ goes over the symmetric group of order $4m$. Since $T_{1,2m-1,2m-1}$ is acyclic, the term $\prod_{i=1}^{4m} b_{i,\sigma(i)} = 0$ if and only if either σ contains a cycle of length more than 2 or, for some $i \neq \sigma(i)$, vertex v_i is not adjacent to vertex $v_{\sigma(i)}$. Therefore, every non-zero term of $Per(B(T_{1,2m-1,2m-1}))$ corresponds to a matching of $T_{1,2m-1,2m-1}$. And so

$$Per(B(T_{1,2m-1,2m-1})) = Z(T_{1,2m-1,2m-1}). \tag{2}$$

The first part of Lemma 3 follows from the combination of Eqs. (1) and (2). With a similar technique one can get

$$\begin{aligned} Z(T_{1,2m+1,2m-1}) &= 2F_{2m}F_{2m+2} + F_{2m-1}F_{2m+2} + F_{2m}F_{2m+1} \\ &= F_{2m+2}^2 + F_{2m}F_{2m+1}. \end{aligned}$$

The second part also follows. □

Lemma 4. *Let T be a $4m$-vertex tree and k be a nonnegative integer. If T contains no perfect matching, then $m(T,k) \leq m(T_{1,2m-1,2m-1}, k)$ with equality holding if and only if $T = T_{1,2m-1,2m-1}$.*

Proof. Since T contains no perfect matching, it is not a path and so has maximum vertex degree $\Delta(T) \geq 3$. Let w be one of its maximum degree vertices and u a 1-degree vertex nearest to w, denote by v the unique neighbor of u. If vertex w has degree $d(w) \geq 4$, then $T \setminus u$, the graph obtained by deleting vertex u and the edge incident with u from T, has a vertex of degree at least 3. And so $T \setminus u \neq P_{4m-1}$. From Lemma 1 we deduce that when $k \geq 1$

$$\begin{aligned} m(T,k) &= m(T \setminus \{u,v\}, k-1) + m(T \setminus u, k) \\ &\leq m(P_{2m-1} \cup P_{2m-1}, k-1) + m(P_{4m-1}, k) \\ &= m(T_{1,2m-1,2m-1}, k). \end{aligned} \tag{3}$$

And so Lemma 4 follows in this case from the combination of (3) and the well-known result that if the n-vertex tree $T \neq P_n$ then $m(P_n, k) \geq m(T,k)$ holds for every nonnegative integer k and the inequality strictly holds for some integer k. Since $T \setminus u \neq P_{4m-1}$ is also true when either $d(w) = 3$ and T contains another vertex of degree 3 or w is the unique vertex with maximum degree 3 but $v \neq w$, Lemma 4 follows in every case. □

By a similar technique to that employed in the proof of Lemma 4, one can prove with ease the following

Lemma 5. *Let T be a $4m+2$-vertex tree and k be a nonnegative integer. If T contains no perfect matching, then $m(T,k) \leq m(T_{1,2m+1,2m-1}, k)$ with equality holding if and only if $T = T_{1,2m+1,2m-1}$.* □

Now, Theorem 1 follows from the combination of Lemma 4 and the first part of Lemma 3 and Theorem 2 follows from the combination of Lemma 5 and the second part of Lemma 3.

Acknowledgements

The author is grateful to the referees for their valuable suggestions which made this work more readable. The author was supported by the National Natural Science Foundation of China (10271105); the Natural Science Foundation of Fujian (2003J036); the Education Ministry of Fujian (JA03147).

References

[1] H. Hosoya, Topological index, a newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, Bull. Chem. Soc. Japan 44 (1971) 2332–2339.
[2] I. Gutman, O.E. Polansky, Mathematical Concepts in Organic Chemistry, Springer, Berlin, 1986.
[3] M.I. Skvortsova, K.S. Fedyaev, V.A. Palyulin et al., Inverse structure–property relationship problem for the case of a correlation equation containing the Hosoya index, Dokl. Chem. 379 (1–3) (2002) 209–213.
[4] H. Li, On minimal energy ordering of acyclic conjugated molecules, J. Math. Chem. 25 (1999) 145–169.
[5] F. Zhang, H. Li, On acyclic conjugated molecules with minimal energies, Discrete Appl. Math. 92 (1999) 71–84.
[6] I. Gutman, F. Zhang, On the ordering of graphs with respect to their matching numbers, Discrete Appl. Math. 15 (1986) 25–33.
[7] Y. Hou, On acyclic systems with minimal Hosoya index, Discrete Appl. Math. 119 (2002) 251–257.
[8] I. Gutman, Acyclic systems with extremal Hückel π-electron energy, Theor. Chim. Acta 45 (1977) 79–87.
[9] J.A. Bondy, U.S.R. Murty, Graph Theory with Applications, Macmillan Press, London, 1976.