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Trees with m-Matchings and the Third Minimal Hosoya Index *

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Abstract: For a graph G, its Hosoya index is defined as the total number of independent edge sets of G. Hou in Discrete Appl. Math. 119(2002)251–257 characterized the trees with a given size of matching and having minimal and second minimal Hosoya index. In this paper, we determine the trees with m-matchings and the third minimal Hosoya index.

1 Introduction

The Hosoya index of a graph, abbreviated by H-index, was first defined by Hosoya [4] in 1971, which is a topological parameter to study the relation between molecular structure and physical and chemical properties of certain hydrocarbon compound. Much related progress can be found in [2-7]. All graphs considered here are simple, finite and undirect. Undefined notation and terminology conform to those in [1].

Let G be a graph with the vertex set V(G) and the edge set E(G). Two edges of G are said to be *independent* if they possess no vertex in common. Any subset of E(G) containing no two mutually incident edges is called an *independent edge*

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set of G. An independent edge set of k edges in G is said to be an k-matching of G. H-index of a graph G is defined as follows:

$$Z(G) = \sum_{k=0} m(G, k),$$

where m(G, k) denotes the number of k-matchings of G. Recall the m(G, 0) = 1 and m(G, 1) = |E(G)|. Note that if m(G, k) = 0, then m(G, k + 1) = 0. Furthermore, m(G, k) = 0 for $k > \frac{n}{2}$, where n = |V(G)|.

For $n \ge 2$, by P_n and S_n we denote the path and the star of n vertices, respectively. For all trees with n vertices, it was proved that the path P_n and star S_n have maximal and minimal H-index in [4,6], respectively, that is, for any tree T with order n, we have

$$n = Z(S_n) \le Z(T) \le Z(P_n) = F_{n+1}.$$

where F_{n+1} is the (n+1)th Fibonacci number with $F_{n+1} = F_n + F_{n-1}$ and $F_1 = F_2 = 1$. The author in [3] characterized the trees with m-matchings and with the minimal and second minimal H-index. In this paper, we shall characterize the trees with m-matchings and having the third minimal H-index.

Let k and r be two non-negative integers and let n=2k+r+1. The tree S(n,k,r) is defined as follows [3]: S(n,k,r) is the graph obtained from star S_{k+r+1} by attaching a pendent edge to k non-central vertices. Note that S(n,k,r) has a matching of m=k+r' edges, where r'=0 if r=0 and r'=1 if r>0, and the center of S(n,k,r) is the center of the star S_{k+r+1} . For $n\geq 3$, let R(n,k,r) denote the graph obtained from S(n-2,k-1,r) by attaching a path of length 2 to one vertex of degree 2. For example, Graphs S(14,5,3) and R(14,5,3) are the graphs shown in Figure 1:

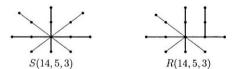


Figure 1. S(14,5,3) and R(14,5,3).

It is obvious that R(n, k, r) also has an m-matching, where m = k + r', r' = 0 if r = 0 and r' = 1 if r > 0. The center of R(n, k, r) is the center of S(n-2, k-1, r). Now we define three new families of graphs: T(n, k, r) is the graph obtained by attaching one vertex of degree 1 of P_3 to the pendant vertex of S(n-2, k, r) that is not adjacent to the center, U(n, k, r) is the graph obtained from R(n-2, k-1, r) by attaching one vertex of degree 1 of P_3 to one vertex of degree 3 which is adjacent to the center, and V(n, k, r) is the graph obtained from R(n-2, k-1, r) by attaching one vertex of degree 1 of P_3 to one vertex of degree 2 which is not adjacent to the center. As some examples, T(14, 4, 3), U(15, 6, 2) and V(14, 6, 1) are the graphs shown in Figure 2.

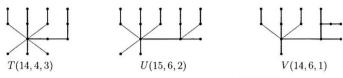


Figure 2. T(14,4,3), U(15,6,2) and V(14,6,1).

2 Preliminaries

Let T be a tree with n vertices and A its adjacent matrix. Let B(T) = A + I, where I is unit matrix of order n. Recall the definition of permanent [8] of a matrix $B = (b_{ij})$:

$$per(B) = \sum_{\sigma} \prod_{i=1}^{n} b_{i\sigma(i)},$$

where the summation is taken over the symmetric group of order n.

Lemma 1([3]). Let T be a tree. Then

$$Z(T) = per(A+I).$$

Let M denote a matching of graph, $v \in M$ means the vertex v is incident to an edge of M and $v \notin M$ means the vertex v is not incident to any edges of M.

Lemma 2([3]). Let T be a tree with a perfect matching. Then T has a pendant edge which is incident to a vertex of degree 2.

Lemma 3([3]). Let T be a tree of n vertices with an m-matching, where n > 2m. Then there exists an m-matching M and a pendant vertex v such that $v \notin M$.

Lemma 4([3]). Let T be a tree of n vertices with an m-matching, where $m \ge 1$. Then

$$Z(T) \ge 2^{m-2}(2n - 3m + 3),$$

where the equality holds if and only if T = S(n, m-1, n-2m+1).

Lemma 5([3]). Let T be a tree of n vertices with an m-matching, where $m \ge 1$. If $T \ne S(n, m-1, n-2m+1)$, then

$$Z(T) \ge 2^{m-4}(10n - 15m + 9),$$

where the equality holds if and only if T = R(n, m-1, n-2m+1).

Remark: There is an error that the original version of Lemma 5 in [3] is $Z(T) \ge 5 \cdot 2^{m-4} (2n-3m)$.

Lemma 6. $Z(T(n, k, r)) = 2^{k-2}(5k + 10r + 11)$.

Proof: We choose an appropriate ordering of the vertices for T(n, k, r), such that

where the unwritten entries are all zeroes. Calculating the permanent by an expansion along the first row, we then obtain

$$Z(T(n,k,r)) = 5 \cdot 2^{k-1} + 3 \cdot 2^{k-1} + 5(k-1)2^{k-2} + 5r2^{k-1} = 2^{k-2}(5k+10r+11).$$

As an analogue to the proof of Lemma 6, we have the following lemma.

Lemma 7. (i)
$$Z(U(n,k,r)) = 2^{k-3}(6k+12r-2)$$
.
(ii) $Z(V(n,k,r)) = 2^{k-3}(6k+12r-1)$.

Lemma 8. Let T be the graph obtained from G by attaching one vertex of degree 1 of P_3 to a vertex of G, where $G \in \{S(n-2,m-2,1),R(n-2,m-2,1),U(n-2,m-2,1),V(n-2,m-2,1)\}$ and $T \notin \{S(n,m-1,1),R(n,m-1,1),U(n,m-1,1),V(n,m-1,1)\}$. Then

$$Z(T) \ge Z(T(n, m-2, 1)).$$

Proof: We only prove the lemma for G = U(n-2, m-2, 1). It is easy to see that n = 2m and

$$Z(U(n, m-1, 1)) = 2^{m-4}(12n - 18m + 4), \ Z(T(n, m-2, 1)) = 2^{m-4}(5m + 11).$$

Note that $m \ge 5$ for U(n-2, m-2, 1) and $U(8, 3, 1) \cong S(8, 3, 1)$ if m=5. By the definition of T, we have that T is one of the following graphs:

S(10,4,1), or $R(10,4,1)\cong U(10,4,1)$, or T(10,3,1), or H_1 , where H_1 is the graph shown in Figure 3.

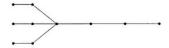


Figure 3. Graph H_1 .

By calculation, we have $Z(H_1) = 76 > Z(T(10, 3, 1)) = 72$. From the condition of the lemma, the result holds.

Now we need only consider the case of $m \ge 6$. For T, v_1 , v_2 and v_3 are the vertices of T shown in Figure 4.

$$v_3$$
 v_2 v_1 $U(n-2,m-2,1)$

Figure 4. Graph T with the vertices v_1 , v_2 and v_3 .

Then

$$B(T) = A + I = \begin{pmatrix} 1 & 1 & 0 & O_{n-3} \\ 1 & 1 & 1 & O_{n-3} \\ 0 & 1 \\ O_{n-3}^T & O_{n-3}^T & B(U(n-2, m-2, 1)) \end{pmatrix},$$

where O_{n-3} is a zero vector of length n-3 and O_{n-3}^T is the transpose of O_{n-3} .

$$perB(T) = 2perB(U(n-2, m-2, 1)) + perB(T'),$$

where T' is the graph obtained from T by deleting v_1, v_2 and v_3 . From the structure of U(n-2, m-2, 1) and the condition of the lemma, we have that $d_T(v_3) = 2$, or 3, or 5. We distinguish the following cases:

Case 1. $d_T(v_3) = 2$. Then T' is a tree of n-3 vertices with (m-2)-matchings. It follows from Lemma 4 that

$$perB(T') \ge 2^{m-4}(2n - 3m + 3)$$

Together with $perB(U(n-2,m-2,1))=2^{m-5}(12n-18m-2)$, we have that $perB(T)\geq$

$$2^{m-4}(14n-21m+1)$$
 and $perB(T)-perT(n,m-2,1)\geq 2^{m-4}(2m-10)$. So

$$perB(T) > perB(T(n, m-2, 1)).$$

Case 2. $d_T(v_3) = 3$. Then T' is the union of K_1 and a tree of n-4 vertices with (m-2)-matchings. From Lemma 4 we have

$$perB(T') \ge 2^{m-4}(2n - 3m + 1).$$

So

$$per B(T) \ge 2^{m-4} (14n - 21m - 1).$$

If m = 5, then T = R(10, 4, 1). If $m \ge 6$, then

$$perB(T) - perB(T(n, m-2, 1)) \ge 2^{m-4}(2m-12),$$

and so

$$perB(T) \ge perB(T(n, m-2, 1)).$$

Case 3. $d_T(v_3) = 5$. Then T is the graph shown in Figure 5.

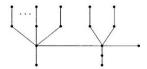


Figure 5. Graph T with $d_T(v_3) = 5$.

If m=6 or 7, then T is R(12,5,1) or U(14,6,1), which contradicts to the condition of the theorem. If $m \geq 8$, by calculation we have $Z(T) = 2^{m-6}(28m - 12)$, and so

$$Z(T) - Z(T(n, m-2, 1)) = 2^{m-6}(28m - 12) - 2^{m-4}(5m + 11) > 0.$$

This completes the proof.

Lemma 9. For $n \ge 2m+1$, let T be the graph obtained from G by attaching one vertex of P_2 to any vertex of G, where $G \in \{S(n-1,m-1,n-2m),R(n-1,m-1,n-2m),U(n-1,m-1,n-2m),V(n-1,m-1,n-2m)\}$ and $T \notin \{S(n,m-1,n-2m+1),R(n,m-1,n-2m+1),U(n,m-1,n-2m+1),V(n,m-1,n-2m+1)\}$. Then

$$Z(T) \ge Z(T(n, m-2, n-2m+1)).$$

Proof: We only prove the lemma for G=U(n-1,m-1,n-2m). For U(n-1,m-1,n-2m), we have $m{\geq}4$. By calculation we have

$$Z(U(n,m-1,n-2m+1)) = 2^{m-4}(12n-18m+4)$$

and

$$Z(T(n, m-2, n-2m+1)) = 2^{m-4}(10n - 15m + 11).$$

For T, v_1 is the vertex of T with $v_1 \in V(P_2)$ and $d_T(v_1) = 1$, and v_2 is the vertex of T with $v_2 \in V(P_2)$ and $d_T(v_2) \ge 2$. Then

$$B(T) = A + I = \begin{pmatrix} 1 & 1 & O_{n-2} \\ 1 & & \\ O_{n-2}^T & B(U(n-1, m-1, n-2m)) \end{pmatrix},$$

where O_{n-2} denotes the zero vector of length of n-2 and O_{n-2}^T is the transpose of O_{n-2} . From the theory of matrix, it follows that

$$perB(T) = perB(U(n-1, m-1, n-2m)) + perB(T'),$$

where T' is the graph obtained from T by deleting v_1 and v_2 . From the structure of U(n-1, m-1, n-2m) and the condition of the lemma, it is easy to see that $d_T(v_2) = 2$, or 3, or 5. We distinguish the following cases:

Case 1. $d_T(v_2) = 2$. Then T' is a tree of n-2 vertices with (m-1)-matchings. From Lemma 4 we have

$$perB(T') \ge 2^{m-3}(2n - 3m + 2)$$

Since

$$perB(U(n-1, m-1, n-2m)) = 2^{m-3}(6n - 9m - 4),$$

we have $per B(T) \ge 2^{m-3}(8n-12m-2)$ and $per B(T) - per T(n, m-2, n-2m+1) \ge 2^{m-4}(6n-9m-15)$. By $n \ge 2m+1$, we have

$$perB(T) \ge perB(T(n, m-2, n-2m+1)).$$

Case 2. $d_T(v_2) = 3$. Then T is the union of K_1 and a tree of n-3 vertices with (m-1)-matching. By Lemma 4, it is not hard get that

$$perB(T') \ge 2^{m-3}(2n - 3m).$$

So

$$perB(T) \ge 2^{m-3}(8n - 12m - 4),$$

$$perB(T) - perB(T(n, m-2, n-2m+1)) \ge 2^{m-4}(6n-9m-19).$$

We arrive that

$$perB(T) \ge perB(T(n, m-2, n-2m+1))$$

for $m \ge 5$. For m = 4, we obtain the result by calculation.

Case 3. $d_T(v_2) = 5$. Then T is the graph shown in Figure 6.

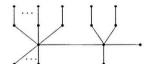


Figure 6. Graph T with $d_T(v_2) = 5$.

If m=5 and n=11, then T=R(11,4,2), contradicting with the condition of the theorem. If m=5 and n>11 or $m\geq 6$, with a similar proof of Lemma 6 we have $Z(T)=2^{m-4}(16n-24m-12)$. It is easy to get that

$$Z(T) - Z(T(n, m-2, n-2m+1)) = 6n - 9m - 23.$$

Note that $n \ge 2m+1$. Thus we have that Z(T)-Z(T(n,m-2,n-2m+1))=6n-9m-23>0 for m=5 and n>11, and Z(T)-Z(T(n,m-2,n-2m+1))=6n-9m-23>3m-17>0 for $m\ge 6$. This completes the proof.

3 Main Results and Proof

Theorem 1. Let T be a tree of n vertices with m-matchings, where $m \ge 1$. If $T \notin \{S(n, m-1, n-2m+1), R(n, m-1, n-2m+1), U(n, m-1, n-2m+1), U(n, m-1, n-2m+1)\}$, then

$$Z(T) \ge 2^{m-4} (10n - 15m + 11)$$

with equality if and only if T = T(n, m-2, n-2m+1), where $n \ge 2m$.

Proof: From the condition of the theorem, we have $n \ge 2m$. Suppose that n = 2m, that is, T has a perfect matching. We prove the theorem by induction on m. When m = 1, $T = P_2 = S(2, 0, 1)$; when m = 2, the tree with perfect 2-matchings is $P_4 = S(4, 1, 1)$; If m = 3, the trees with perfect 3-matchings are S(6, 2, 1), or P_6 . If m = 4, the trees with perfect 4-matchings are P_8 , S(8, 3, 1), R(8, 3, 1), T(8, 2, 1) or the graph H_2 shown in Figure 7:



Figure 7: Graph H_2 .

By calculation, we have that $Z(H_2) = 32 > Z(T(8,2,1)) = 31$.

If m = 5, From the reference [9], we know that the trees with perfect 5—matchings are

 P_{10} , S(10,4,1), R(10,4,1), T(10,3,1), V(10,4,1), $G_i (1 \le i \le 10)$, where G_i are the graphs in Figure 8.

 G_1 G_2 G_3 G_4 G_5 G_6 G_7 G_8 G_9 G_{10}

Figure 8. Some graphs G_i with perfect 5-matchings.

By calculation it is not hard to see that the results holds.

We now suppose that m>5 and proceed by induction. From Lemma 2, it follows that T has a pendant edge uw such that d(u)=1 and d(w)=2.

Then there exists only one another edge wv such that we obtain the graph T' with 2(m-1) vertices and (m-1)-matching, by deleting u and w. Note that $T' \in \{S(n-2,m-2,1), R(n-2,m-2,1), U(n-2,m-2,1), V(n-2,m-2,1)\}$. It follows, from Lemma 8 and the condition of the theorem, that

$$Z(T) > 2^{m-4}(10n - 15m + 11).$$

If $T' \notin \{S(n-2,m-2,1), R(n-2,m-2,1), U(n-2,m-2,1), V(n-2,m-2,1)\}$, by the induction hypothesis we have

$$Z(T') \ge 2^{m-5} (10(n-2) - 15(m-1) + 11) = 2^{m-5} (5(m-1) + 11), \tag{1}$$

with equality if and only if T' = T(2m - 2, m - 3, 1).

Labelling the vertices by the order of u, w and v, we have

$$B(T) = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & X \\ 0 & 0 & X^T & C \end{pmatrix},$$

$$B(T') = \left(\begin{array}{cc} 1 & X \\ X^T & C \end{array}\right)$$

and

$$Z(T) = perB(T) = perC + 2perB(T') = perC + 2Z(T').$$
(2)

Since $T^{'}$ has at least one perfect (m-1)-matching, we label the vertices except for u,w,v such that

$$C = \begin{pmatrix} 1 & 1 & & & & \\ 1 & 1 & & * & & & \\ & & \ddots & & & \\ & & & 1 & 1 & \\ & * & & 1 & 1 & \\ & & & & 1 \end{pmatrix},$$

where there are (m-2) blocks $\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ in C. If the entries in * of C are all 0, then the two entries in X^T of B(T') which have the same rows as some block $\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ in C are not all 1 or 0. If the two entries are all 1, then T contains a cycle; If they are all 0, then T is disconnected. Hence, one of them is 1 and the

other is 0. Noting that the label of T', we have

$$B(T') = \begin{pmatrix} 1 & 1 & 0 & 1 & 0 & 1 & 0 & \dots & 1 & 0 & 1 \\ 1 & 1 & 1 & & & & & & & \\ 0 & 1 & 1 & & & & & & & \\ 1 & 0 & 0 & 1 & 1 & & & * & & & \\ 0 & 0 & 0 & 1 & 1 & & & * & & & \\ 1 & & & & \ddots & & & & & \\ 0 & & * & & & \ddots & & & \\ 1 & & & & & & 1 \end{pmatrix}$$

Obviously, T'=S(2m-2,m-2,1) which is a contradiction. So the number of 1's in * of C is at least 2(C is symmetric). We choose two blocks $\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$, which have the same row or column as that of some 1. By expanding perC along the four rows in which the two blocks lie, we have

$$PerC \ge perD \cdot perE,$$
 (3)

where D is one of the following four matrices,

$$\begin{pmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}$$

and E is obtained from C by deleting the row and column in which the entries of D lie. It is obvious that $perE \ge 2^{m-4}$ and perD = 5. Thus

$$perC > 5 \cdot 2^{m-4}, \tag{4}$$

$$Z(T) = perC + 2Z(T') \ge 5 \cdot 2^{m-4} + 2 \cdot 2^{m-5} (5(m-1) + 11) = 2^{m-4} (5m + 11)$$
 (5)

with equality in (5) holds if and only if $Z(T') = 2^{m-5}(5(m-1)+11)$, that is, T' = T(2m-2, m-3, 1) and $perC = 5 \cdot 2^{m-4}$. Then there exists only one minor like as D in C, the other entries is 0, the minor like as D implies that there is path P_4 contained in T'. Since T is a tree, there is only one 1 of the entries in X^T which have the same rows as D. The degree of all vertices in T' = T(2m-2, m-3, 1) is less than 3 except the vertex v. Thus, the number of 1's in every row of C is not more than 4. So the entries in X^T , which have the same row as one of the rows in which the two 1's of D lie, are 1, then one of pendant vertex of P_4 is adjacent to v of T'.

2m), V(n-1, m-1, n-2m)}, by the condition of the theorem and Lemma 9 we have

$$Z(T) > 2^{m-4}(10n - 15m + 11).$$

If $T'\not\in\{S(n-1,m-1,n-2m),R(n-1,m-1,n-2m),U(n-1,m-1,n-2m),V(n-1,m-1,n-2m)\}$, by the induction hypothesis we have

$$Z(T') \ge 2^{m-4}(10(n-1) - 15m + 11) \tag{6}$$

with equality if and only if T' = T(n-1, m-2, n-2m).

Ordering the vertices of T as v, w, \dots , we have

$$B(T) = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & X \\ 0 & X^T & C \end{pmatrix}, \quad B(T') = \begin{pmatrix} 1 & X \\ X^T & C \end{pmatrix}.$$

By expanding the permanent along the first row, we have

$$Z(T) = perB(T) = perB(T') + perC.$$

As an analogue to the above proof, we can obtain

$$perC \ge 5 \cdot 2^{m-3},\tag{7}$$

$$Z(T') \ge 2^{m-4} (10(n-1) - 15m + 11).$$
 (8)

Thus

$$Z(T) \ge 5 \cdot 2^{m-3} + 2^{m-4} (10(n-1) - 15m + 11) = 2^{m-4} (10n - 15m + 11). \tag{9}$$

If the equality holds in (9), so do (6) and (7). By induction hypothesis, we have T' = T(n-1, m-2, n-2m).

Similarly, by induction on m, we can show the case of n=2m, and w is the center of T'=T(n-1,m-2,n-2m) and

$$T = T(n, m-2, n-2m+1).$$

This completes the proof.

Remark: From Lemma 7, if $m \ge 6$, then

$$Z(U(n, m-1, n-2m+1)) \ge Z(T(n, m-2, n-2m+1)).$$

If $m \geq 7$, then

$$Z(V(n, m-1, n-2m+1)) > Z(T(n, m-2, n-2m+1)).$$

We only characterize the tree with m-matchings and having the third minimal Hosoya index when the number of matchings is more than 6.

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