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The (n, m)–Graphs of Minimum Hosoya Index*

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Abstract

The Hosoya index of a graph is defined as the total number of matchings of the graph. In this paper, we characterize the graphs with the minimum Hosoya index among all graphs of n vertices and m edges, where $n + 2 \leq m \leq 2n - 3$.

1 Introduction

We only consider finite and simple graphs here. The reader is referred to [1] for undefined terminology and notation. Let $G = (V(G), E(G))$ denote graph with vertex-set $V(G)$ and edge-set $E(G)$. Two edges of G are said to be independent if they are not adjacent in G. A k-matching of G is a set of k mutually independent edges. Denote by $z(G, k)$ the number of the k-matchings of G. For convenience, let $z(G, 0) = 1$ for any graph G. The Hosoya index of G, denoted by $z(G)$, is defined as $z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} z(G, k)$, where $n = |V(G)|$. Obviously, $z(G)$ is equal to the total number of matchings of the graph G. The Hosoya index of a graph was introduced by Hosoya in 1971 [2] and was shown to correlate with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures (see [3, 4]). Since then, many authors have investigated the Hosoya index and many results have been obtained. Among all n-vertex trees, the

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path P_n has the maximum Hosoya index and the star S_n has the minimum Hosoya index [3]. The unicyclic graphs with prescribed girth and minimum Hosoya index, and the unicyclic molecular graphs with maximum Hosoya index are characterized in [5] and [6], respectively. In addition, the minimum Hosoya index of bicyclic graphs is also determined in [7].

In this paper, we characterize the graphs with minimum Hosoya index among all graphs of n vertices and m edges, where $n+2 \leq m \leq 2n-3$. The extremal graphs are analogous to those with maximum Merrifield-Simmons index among all graphs of n vertices and m edges (see [8]), where the Merrifield-Simmons index of a graph is the total number of its independent sets.

A (n, m)-graph is a connected graph of n vertices and m edges. In particular, $(n, n-1)$-graphs, (n, n)-graphs and $(n, n+1)$-graphs are well-known trees, unicyclic graphs and bicyclic graphs, respectively. Let $\mathscr{G}_{n,m}$ denote the set of all (n, m)-graphs. A pendent vertex is a vertex of degree 1. A pendent edge is an edge incident with a pendent vertex. Suppose that $V' \subseteq V(G)$. Let $G - V'$ denote the subgraph obtained from G by deleting the vertices in V' together with their incident edges. If $V' = \{v\}$, we write $G - v$ for $G - \{v\}$. Let $G - uv$ denote the graph that arises from G by deleting the edge $uv \in E(G)$. For a vertex u of a graph G, we denote the neighborhood and degree of u by $N_G(u) = \{v | uv \in E(G)\}$ and $d_G(u)$, respectively. Denote by P_n, C_n and S_n the path, cycle and star of order n, respectively. There are occasions when it is convenient to select a vertex of a tree T under discussion and designate this vertex as the root of T. The tree T then becomes a rooted tree. Often the rooted tree T is drawn with the root r at the top and the other vertices of T drawn below, in levels, according to their distance from r.

2 Lemmas

In this section, we give some lemmas that will be used in the proof of our result.

Lemma 1([3]). *Let $G = (V(G), E(G))$ be a graph.*

(i) If $uv \in E(G)$, then

$$z(G) = z(G - uv) + z(G - \{u, v\});$$

(ii) If $v \in V(G)$*, then*

$$z(G) = z(G - v) + \sum_{u \in N_G(v)} z(G - \{u, v\});$$

(iii) If $G_1, G_2, \ldots, G_t$ *are all components of* G*, then*

$$z(G) = \prod_{i=1}^{t} z(G_i).$$

Lemma 2([9]). *Let* G *be a connected graph and* $u, v \in V(G)$*. Suppose that* $G_{s,t}$ *is a graph obtained from* G *by attaching* s, t *pendent vertices to* u, v*, respectively. Then*

$$z(G_{s+i,t-i}) < z(G_{s,t}) \quad \text{for } 1 \le i \le t \qquad \text{or} \qquad z(G_{s-i,t+i}) < z(G_{s,t}) \qquad \text{for } 1 \le i \le s.$$

Lemma 3([10]). *Let* H_1, H_2 *be two connected graphs with* $V(H_1) \cap V(H_2) = \{v\}$*. Let* $G = H_1 v H_2$ *be a graph defined by* $V(G) = V(H_1) \cup V(H_2), E(G) = E(H_1) \cup E(H_2)$*. Let* H *be a connected graph and* T_l *be a tree of order* l *with* $V(H) \cap V(T_l) = \{v\}$*, then* $z(HvT_l) \geqslant z(HvS_l)$ *with equality holding if and only if* $HvT_l \cong HvS_l$*, where* v *is identified with the center of the star* S_l *in* HvS_l*.*

By the definition of the Hosoya index, it is easy to obtain the following lemma.

Lemma 4. *If* H *is a subgraph of* G*, then* $z(H) \le z(G)$ *with equality holding if and only if* $E(H) = E(G)$*.*

By Lemma 4, any connected graph G of order n contains a spanning tree T_n such that $z(G) \ge z(T_n) \ge z(S_n)$ with equalities holding if and only if the corresponding graphs are isomorphic. Then we have the following conclusion.

Lemma 5. S_n *has the minimum Hosoya index among all connected graphs of order* n*.*

Lemma 6. *Let* G, H *be two disjoint connected graphs of order at least* 2 *with* $v \in V(G)$ *and* $u \in V(H)$*. Denote by* G' *(see Figure 1) the graph obtained from the union of* G *and* H *by adding a new edge* uv*. Let* G'' *(see Figure 1) denote the graph obtained from* G' *by deleting the edge* uv *and identifying* v *with* u *to form a new vertex* w*, and attaching a pendent vertex* i *to* w*. Then* $z(G'') < z(G')$*.*

Figure 1.

Proof. By Lemma 1,

$$\begin{aligned} z(G') &= z(G'-uv)+z(G'-\{u,v\}) \\ &= z(G)z(H)+z(G-v)z(H-u), \end{aligned}$$

where $z(G)=z(G-v)+\sum_{v'\in N_G(v)} z(G-\{v,v'\})$ and $z(H)=z(H-u)+\sum_{u'\in N_H(u)} z(H-\{u,u'\})$.

So we have

$$\begin{aligned} z(G') &= 2z(G-v)z(H-u) \\ &+ z(G-v)\sum_{u'\in N_H(u)} z(H-\{u,u'\}) \\ &+ z(H-u)\sum_{v'\in N_G(v)} z(G-\{v,v'\}) \\ &+ \sum_{v'\in N_G(v)} z(G-\{v,v'\})\sum_{u'\in N_H(u)} z(H-\{u,u'\}). \end{aligned} \tag{1}$$

Similarly,

$$z(G'')=z(G''-w)+\sum_{w'\in N_{G''}(w)} z(G''-\{w',w\}).$$

Note that

$$N_{G''}(w)=N_H(u)\bigcup N_G(v)\bigcup\{i\}.$$

So

$$\begin{aligned} z(G'') &= z(G''-w)+\sum_{w'\in N_{G''}(w)} z(G''-\{w',w\}) \\ &= z(G''-w)+z(G''-\{w,i\})+\sum_{w'\in N_{G''}(w)\setminus\{i\}} z(G''-\{w',w\}) \\ &= 2z(G-v)z(H-u) \\ &+ \sum_{w'\in N_G(v)} z(G''-\{w',w\})+\sum_{w'\in N_H(u)} z(G''-\{w',w\}), \end{aligned}$$

where

$$\sum_{w' \in N_G(v)} z(G'' - \{w, w'\}) = z(H - u) \sum_{v' \in N_G(v)} z(G - \{v, v'\})$$

and

$$\sum_{w' \in N_H(u)} z(G'' - \{w, w'\}) = z(G - v) \sum_{u' \in N_H(u)} z(H - \{u, u'\}).$$

Then we have

$$\begin{aligned} z(G'') &= 2z(G - v)z(H - u) \\ &+ z(H - u) \sum_{v' \in N_G(v)} z(G - \{v, v'\}) \\ &+ z(G - v) \sum_{u' \in N_H(u)} z(H - \{u, u'\}). \end{aligned} \tag{2}$$

By comparing (1) and (2), we have

$$z(G') - z(G'') = \sum_{v' \in N_G(v)} z(G - \{v, v'\}) \sum_{u' \in N_H(u)} z(H - \{u, u'\}) > 0$$

that is $z(G'') < z(G')$. The proof of the lemma is complete. ■

Lemma 7. *Suppose that $G \in \mathscr{G}_{n,m}$, where $n + 2 \leq m \leq 2n - 3$, and all cut edges are pendent edges incident with the same vertex. Then there exists an edge uv in G such that the subgraphs $G - uv$ and $G - \{u, v\}$ are still connected.*

Proof. Suppose that all the pendent vertices $v_1, v_2, \ldots, v_t$ of G are attached to the vertex v_0. Then there exists a spanning tree T of G rooted at v_0 and besides $v_1, v_2, \ldots, v_t$, there exist other pendent vertices in T. We have to distinguish two cases according to whether there are edges in G between these pendent vertices or not.

Case 1. There exist two pendent vertices u and v other than $v_1, v_2, \ldots, v_t$ in the spanning tree T with $uv \in E(G)$. Then both $G - uv$ and $G - \{u, v\}$ are connected, since T and $T - \{u, v\}$ are spanning trees of $G - uv$ and $G - \{u, v\}$, respectively. Thus the edge uv is as required.

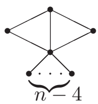
Case 2. Each pair of two pendent vertices of the spanning tree T are not adjacent in G. Then T is not a star and there exists at least a vertex u which is a pendent vertex in T but not a pendent vertex in G. Without loss of generality, assume u is one of the farthest vertices from itself to the root v_0. Suppose that the adjacent vertex of u in T is

v. Then $v \neq v_0$, since T is not a star and u is one of the farthest vertices from itself to the root v_0. There are two subcases according to the degree of v in T.

Subcase 2.1. $d_T(v) = 2$. Then the edge uv is as required. In fact, since u has neighbours in G other than v, $G - uv$ is still connected. In addition, $G - \{u, v\}$ is still connected, since $T - \{u, v\}$ is a spanning tree of $G - \{u, v\}$.

Subcase 2.2. $d_T(v) > 2$. Suppose that $u, u'_1, u'_2, \ldots, u'_l$ are all adjacent pendent vertices of v in T. Then $u, u'_1, u'_2, \ldots, u'_l$ are not pendent vertices in graph G, since $v \neq v_0$. Consequently, by the hypothesis in Case 2, $u, u'_1, u'_2, \ldots, u'_l$ are not adjacent to one another in G. Thus, in G, each of $u, u'_1, u'_2, \ldots, u'_l$ is adjacent to at least one of those vertices which are not pendent vertices of T. Then $G - uv$ is connected, since u has another adjacent vertex other than v in G. In addition, $T - \{u, v\}$ is connected except for isolated vertices $u'_1, u'_2, \ldots, u'_l$, which however, must have neighbours in $G - \{u, v, v_1, \ldots, v_t, u'_1, \ldots, u'_l\}$. Then $G - \{u, v\}$ still connected. So the edge uv is as required. ■

Lemma 8([7]). *$B_{n,n+1}$ (see Figure 2) has the minimum Hosoya index among all $(n, n+1)$-graphs.*



$B_{n,n+1}$
Figure 2.

3 The (n, m)- Graphs of Minimum Hosoya Index

Theorem 9. *Let $G \in \mathscr{G}_{n,m}$.*

(i) If $m = n + 2$, then $z(G) \geq z(T_{n,n+2}) = z(T'_{n,n+2})$ with equality holding if and only if either $G \cong T_{n,n+2}$ or $G \cong T'_{n,n+2}$, where $T_{n,n+2}$ and $T'_{n,n+2}$ are shown in Figure 3;

(ii) If $n + 3 \leq m \leq 2n - 3$, then $z(G) \geq z(G^*_{n,m})$ with equality holding if and only if $G \cong G^*_{n,m}$, where $G^*_{n,m}$ is shown in Figure 3.

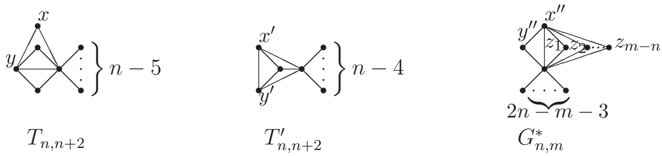


Figure 3.

Proof. For any $G \in \mathscr{G}_{n,m}$ $(n+2 \leq m \leq 2n-3)$, by Lemmas 3, 6 and 2, we can obtain a graph G' from G such that all cut edges are pendent edges incident with the same vertex and $z(G') \leq z(G)$ with equality holding if and only if $G' \cong G$. By Lemma 7, there exists an edge uv in G' such that $G' - uv \in \mathscr{G}_{n,m-1}$ and $G' - \{u, v\}$ is a connected graph of order $n-2$.

(i) Assume $m = n+2$.

Firstly, it is easy to see that

$$\begin{aligned}
z(T_{n,n+2}) &= z(T_{n,n+2} - xy) + z(T_{n,n+2} - \{x, y\}) \\
&= z(B_{n,n+1}) + z(S_{n-2}) \\
&= z(T'_{n,n+2} - x'y') + z(T'_{n,n+2} - \{x', y'\}) \\
&= z(T'_{n,n+2}),
\end{aligned}$$

where x, y, x', y' are shown in Figure 3.

Secondly, since $G' - uv \in \mathscr{G}_{n,n+1}$ and $G' - \{u, v\}$ is a connected graph of order $n-2$, we have

$$\begin{aligned}
z(G) \geq z(G') &= z(G' - uv) + z(G' - \{u, v\}) \\
&\geq z(B_{n,n+1}) + z(S_{n-2}) \\
&= z(T_{n,n+2}) = z(T'_{n,n+2}),
\end{aligned}$$

where the last inequality is obtained from Lemmas 8 and 5. In order for the equalities to hold, all inequalities in the above argument should be equalities. Thus we have $G' - uv \cong B_{n,n+1}$, $G' - \{u, v\} \cong S_{n-2}$ and $G' \cong G$. Then it is not difficult to check that either $G \cong G' \cong T_{n,n+2}$ or $G \cong G' \cong T'_{n,n+2}$.

(ii) When $m \geq n+3$, we apply induction on m.

Firstly, let $m = n+3$. On the one hand,

$$\begin{aligned} z(G^*_{n,n+3}) &= z(G^*_{n,n+3} - x''y'') + z(G^*_{n,n+3} - \{x'', y''\}) \\ &= z(T_{n,n+2}) + z(S_{n-2}), \end{aligned}$$

where x'', y'' are shown in Figure 3. On the other hand, since $G' - uv \in \mathscr{G}_{n,n+2}$ and $G' - \{u, v\}$ is a connected graph of order $n-2$,

$$\begin{aligned} z(G) \geq z(G') &= z(G' - uv) + z(G' - \{u, v\}) \\ &\geq z(T_{n,n+2}) + z(S_{n-2}) \\ &= z(T'_{n,n+2}) + z(S_{n-2}) \\ &= z(G^*_{n,n+3}) \end{aligned}$$

where the last inequality is obtained from the result (i) of this theorem and Lemma 5.

In order for the equalities to hold, all inequalities in the above argument should be equalities. Then $G' - uv \cong T_{n,n+2}$ or $T'_{n,n+2}$, $G' - \{u, v\} \cong S_{n-2}$ and $G' \cong G$. To begin with, we claim $G' - uv \ncong T'_{n,n+2}$. In fact, assume $G' - uv \cong T'_{n,n+2}$. Let u' and v' denote the images of u and v, respectively, under the isomorphism from $G' - uv$ to $T'_{n,n+2}$. Then $u'v' \notin E(T'_{n,n+2})$, since $uv \notin G' - uv$, and $T'_{n,n+2} - \{u', v'\} \cong (G' - uv) - \{u, v\} = G' - \{u, v\} \cong S_{n-2}$. However, for all pairs of $u', v' \in V(T'_{n,n+2})$ with $u'v' \notin E(T'_{n,n+2})$, $T'_{n,n+2} - \{u', v'\} \ncong S_{n-2}$, a contradiction. So the claim is true. Then $G' - uv \cong T_{n,n+2}$ and $G' - \{u, v\} \cong S_{n-2}$. Thus it is not difficult to check that $G \cong G' \cong G^*_{n,n+3}$. So the result holds for $k = 3$.

Secondly, assume the result holds for $m-1$ $(m \geq n+4)$, we are going to prove that it is true for m in the following. On the one hand,

$$\begin{aligned} z(G^*_{n,m}) &= z(G^*_{n,m} - x''y'') + z(G^*_{n,m} - \{x'', y''\}) \\ &= z(G^*_{n,m-1}) + z(S_{n-2}) \end{aligned}$$

where x'', y'' are shown in Figure 3.

On the other hand, since $G' - uv \in \mathscr{G}_{n,m-1}$ and $G' - \{u, v\}$ is a connected graph of order $n-2$,

$$z(G) \geq z(G') = z(G' - uv) + z(G' - \{u, v\})$$

$$
\begin{aligned}
&\geq z(G^*_{n,m-1}) + z(S_{n-2}) \\
&= z(G^*_{n,m})
\end{aligned}
$$

where the last inequality is obtained from the inductive hypothesis and Lemma 5. In order for the equalities to hold, all inequalities in the above argument should be equalities. Then $G' - uv \cong G^*_{n,m-1}$, $G' - \{u, v\} \cong S_{n-2}$ and $G \cong G'$. Then it is not difficult to check that $G \cong G' \cong G^*_{n,m}$. Thus the result holds for m. Consequently, it holds for all $n + 3 \leq m \leq 2n - 3$.

The proof of the theorem is complete. ■

4 Remark

Although we characterized the graphs with the minimum Hosoya index among all (n, m)-graphs, where $n + 2 \leq m \leq 2n - 3$, the same problem for $m > 2n - 3$ deserves further study.

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