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The smallest Hosoya index in $(n, n+1)$-graphs

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A $(n, n+1)$-graph G is a connected simple graph with n vertices and $n+1$ edges. In this paper, we determine the lower bound for the Hosoya index in $(n, n+1)$-graphs in terms of the order n, and characterize the $(n, n+1)$-graph with the smallest Hosoya index.

KEY WORDS: $(n, n+1)$-graph, Hosoya index

1. Introduction

The Hosoya index of a simple graph G is defined to be the total number of its matchings [1], where a matching is a subset M of the edge-set of G with the property that no two different edges of M share a common vertex. If $z(G)$ denotes the Hosoya index of G and $m(G, k)$ the number of its k-matchings, matchings consisting of k edges each, then $z(G) = \sum_{k=0}^{\lfloor n/2 \rfloor} m(G, k)$, where n is the order of G, the number of its vertices, and $\lfloor n/2 \rfloor$ is the integer part of $n/2$. It is convenient to set $m(G, 0) = 1$ and $m(G, 1) = m$, the number of the edges of graph G. By its definition, we deduce that $m(G, k) = 0$ when $k > \lfloor n/2 \rfloor$.

The Hosoya index has a close relationship with the total π-electron energy [2], the boiling points, entropies [3]. Many results have been obtained on the Hosoya indices of graphs [4–12], for example, Ref. [7] characterized the acyclic graphs that have the first and the second minimal Hosoya indices; [9] gave the first and the second minimal Hosoya index of unicyclic graphs and the extremal graphs. In this paper, we will determine the lower bound for the Hosoya index in $(n, n+1)$-graphs in terms of the order n, and characterize the $(n, n+1)$-graph with the smallest Hosoya index.

Let $G = (V, E)$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. For any $v \in V$, $N_G(v) = \{u | uv \in E(G)\}$ denotes the neighbors of v, and $d_G(v) = |N_G(v)|$ is the degree of v in G. A leaf is a vertex of degree one. Let $E' \subseteq E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E'. $W \subseteq V(G)$, $G - W$ denotes the subgraph of G obtained by deleting the vertices of W and the edges incident with them. If a graph G has components $G_1, G_2, \ldots, G_t$, then G is denoted by $G_1 \cup G_2 \cup \cdots \cup G_t$. P_n denotes the path on n vertices, C_n is the cycle on n vertices, and S_n is the star consisting of one center vertex adjacent to $n-1$ leaves.

The following basic results will be used and can be found in the references cited.

(i) If $e = uv$ is an edge of G, then $z(G) = z(G - \{e\}) + z(G - \{u, v\})$.

(ii) If v is a vertex of G, then

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

(iii) If G is a graph with components $G_1, G_2, G_3, \ldots, G_k$, then $z(G) = \prod_{i=1}^{k} z(G_i)$.

(iv) $z(S_n) = n$; $\quad z(C_n) = f(n-1) + f(n+1)$.

$$z(P_0) = 0, \qquad z(P_1) = 1, \quad \text{and} \quad z(P_n) = f(n+1) for\ n \geqslant 2,$$

where f(0) = 0, $f(1) = 1$, and $f(n) = f(n-1) + f(n-2)$ for $n \geqslant 2$ denotes the sequence of Fibonacci numbers.

In this paper, we investigate the Hosoya index of $(n, n+1)$-graphs, i.e., connected simple graphs with n vertices and $n+1$ edges. We characterize the $(n, n+1)$-graph with the smallest Hosoya index among all $(n, n+1)$-graphs.

Let $\mathcal{G}(n, n+1)$ be the set of simple connected graphs with n vertices and $n+1$ edges. For any graph $G \in \mathcal{G}(n, n+1)$, there are two cycles C_p and C_q in G. As in [13, 14], we divide all the $(n, n+1)-$graphs with two cycles of lengths p and q into three classes:

(1) $\mathcal{A}(p, q)$ is the set of $G \in \mathcal{G}(n, n+1)$ in which the cycles C_p and C_q have only one common vertex;

(2) $\mathcal{B}(p, q)$ is the set of $G \in \mathcal{G}(n, n+1)$ in which the cycles C_p and C_q have no common vertex;

(3) $\mathcal{C}(p, q, l)$ is the set of $G \in \mathcal{G}(n, n+1)$ in which the cycles C_p and C_q have a common path of length l.

Note that the induced subgraph of vertices on the cycles of $G \in \mathcal{A}(p, q)$ (or $\mathcal{B}(p, q)$, $\mathcal{C}(p, q, l)$) is showed in figure 1(a) (or (b) and (c)) and $\mathcal{C}(p, q, l) = \mathcal{C}(p, p+q-2l, p-l) = \mathcal{C}(p+q-2l, q, q-l)$.

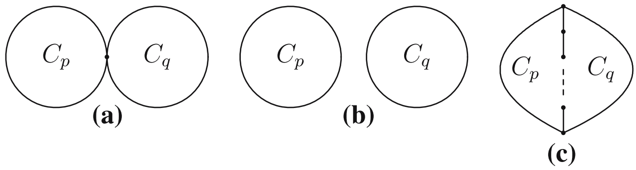

Figure 1. The induced subgraphs of vertices on the cycles of G.

2. Two transformations decreasing the Hosoya index

Before our main results, we give two transformations which will decrease the Hosoya index as follows:

Transformation A: Let uv be an edge G, $N_G(u) = \{v, w_1, w_2, \ldots, w_s\}$, and $w_1, w_2, \ldots, w_s$ are leaves. $G^{'} = G - \{vw_1, vw_2, \ldots, vw_s\} + \{uw_1, uw_2, \ldots, uw_s\}$, as shown in figure 2.

Lemma 2.1. Let G' be obtained from G by transformation A, then $z(G') < z(G)$.

Proof. Let $G_0 = G - \{u, w_1, w_2, \ldots, w_s\}$. By the definition of the Hosoya index, we have

$$\begin{aligned} z(G) &= z(G - \{uv\}) + z(G - \{u, v\}) \\ &= (1+s) \cdot z(G_0) + z(G_0 - \{v\}), \\ z(G') &= z(G_0) + (s+1) \cdot z(G_0 - \{v\}). \end{aligned}$$

Then

$$\begin{aligned} \Delta &= z(G') - z(G) \\ &= s[z(G_0 - \{v\}) - z(G_0)]. \end{aligned}$$

Since $z(G_0 - \{v\}) < z(G_0)$, $z(G') < z(G)$.

Remark. Repeating transformation A, any unicyclic graph can be changed into an unicyclic graph such that all the edges not on the cycles are pendant edges, and the Hosoya index is decreased.

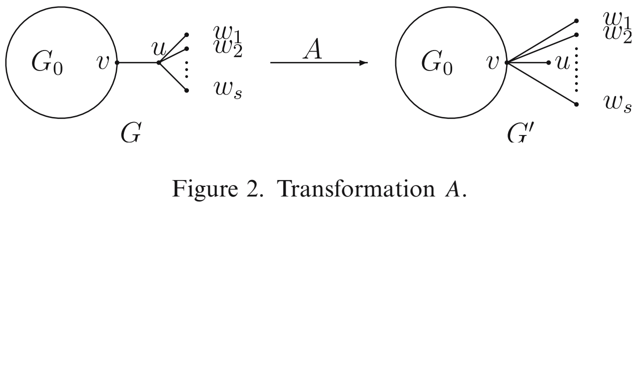

Figure 2. Transformation A.

Transformation B: Let u and v be two vertices in G. $u_1, u_2, \ldots, u_s$ are the leaves adjacent to u, $v_1, v_2, \ldots, v_t$ are the leaves adjacent to v. $G' = G - \{uu_1, uu_2, \ldots, uu_s\} + \{vu_1, vu_2, \ldots, vu_s\}$, $G'' = G - \{vv_1, vv_2, \ldots, vv_t\} + \{uv_1, uv_2, \ldots, uv_t\}$.

Lemma 2.2. Let G' and G'' be obtained from G by transformation B, then either $z(G') < z(G)$ or $z(G'') < z(G)$.

Proof. Let $G_0 = G - \{u_1, u_2, \ldots, u_s, v_1, v_2, \ldots, v_t\}$. Using $z(G) = z(G - \{xy\}) + z(G - \{x, y\})$ repeatedly, we have

$$\begin{aligned} z(G) &= z(G_0) + sz(G_0 - \{u\}) + tz(G_0 - \{v\}) + stz(G_0 - \{u, v\}), \\ z(G') &= z(G_0) + (s+t)z(G_0 - \{v\}), \\ z(G'') &= z(G_0) + (s+t)z(G_0 - \{u\}). \end{aligned}$$

Then

$$\begin{aligned} \Delta_1' &= z(G) - z(G') \\ &= s[z(G_0 - \{u\}) - z(G_0 - \{v\}) + t \cdot z(G_0 - \{u, v\})], \\ \Delta_2' &= z(G) - z(G'') \\ &= t[z(G_0 - \{v\}) - z(G_0 - \{u\}) + s \cdot z(G_0 - \{u, v\})]. \end{aligned}$$

If $z(G) \leqslant z(G')$, then $z(G_0 - \{v\}) \geqslant z(G_0 - \{u\}) + t \cdot z(G_0 - \{u, v\})$. Then

$$\begin{aligned} \Delta_2' &= z(G) - z(G'') \\ &\geqslant t[z(G_0 - \{u\}) + t \cdot z(G_0 - \{u, v\}) - z(G_0 - \{u\}) + s \cdot z(G_0 - \{u, v\})] \\ &= t(s+t) \cdot z(G_0 - \{u, v\}) > 0. \end{aligned}$$

The proof is completed (see figure 3).

Remark. Repeating transformation B, any unicyclic graph can be changed into an unicyclic graph such that all the pendant edges are attached to the same vertex, and the Hosoya index is decreased.

Lemma 2.3. ([8]) Let $G \not\cong P_1$ be a connected graph and choose $u \in V(G)$. $P(n, k, G, u)$ denotes the graph that results from identifying u with the vertex v_k of a path $v_1 v_2 \ldots v_n$ (figure 4(a)). Let $n = 4m + i$, $i = 1, 2, 3, 4$, $m \geqslant 0$. Then

$$\begin{aligned} & z(P(n, 2, G, u)) < z(P(n, 4, G, u)) < \cdots < z(P(n, 2m+2l, G, v)) \\ & \quad < z(P(n, 2m+1, G, v)) < \cdots < z(P(n, 3, G, v)) < z(P(n, 1, G, v)), \end{aligned}$$

where $l = \lfloor \frac{i-1}{2} \rfloor$.

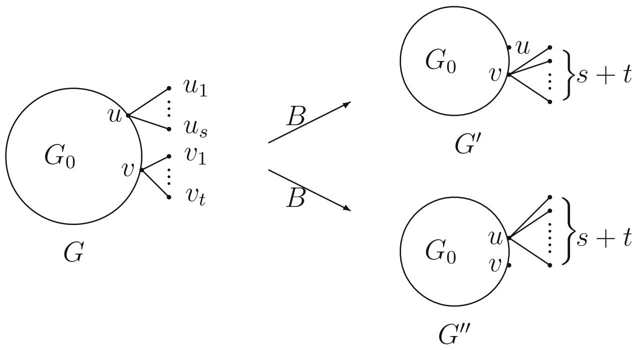

Figure 3. Transformation B.

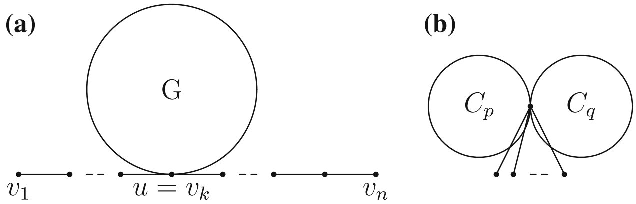

Figure 4. (a) The graph $P(n, k, G, u)$; (b) The graph $S_n(p, q)$.

3. The graph with the smallest Hosoya index in $\mathcal{A}(p, q)$

In this section, we will find the $(n, n+1)-$graph with the smallest Hosoya index in $\mathcal{A}(p, q)$.

Let $S_n(p, q)$ be a graph in $\mathcal{A}(p, q)$ such that $n + 1 - (p + q)$ pendent edges are attached to the common vertex of C_p and C_q (see figure 4(b)).

Theorem 3.1. If $G \in \mathcal{A}(p, q)$, then $z(G) \geqslant z(S_n(p, q)$ with the equality if and only if $G \cong S_n(p, q)$.

Proof. First, repeating the transformations A and B on graph G, we can get a graph G' such that all the edges not on the cycles are the pendant edges attached to the same vertex v. By lemmas 2.1 and 2.2, we have $z(G) \geqslant z(G')$ with the equality if and only if all the edges not on the cycles are also the pendant edges attached to the same vertex in G. If $G' \ncong S_n(p, q)$, then $v \neq u$, where u is the common vertex of C_p and C_q.

Without loss of the generality, we assume that v is on the cycle C_p. H is the graph obtained by deleting all the pendent edges in $S_n(p, q)$, as showed in figure 1(a).

$$\begin{aligned} z(S_n(p,q)) &= z(H) + (n+1-p-q)z(H-\{u\}) \\ &= z(H) + (n+1-p-q)z(P_{p-1})z(P_{q-1}) \\ &= z(H) + (n+1-p-q)f(p)f(q), \end{aligned}$$

$$\begin{aligned} z(G') &= z(H) + (n+1-p-q)z(H-\{v\}) \\ &\geqslant z(H) + (n+1-p-q)z(P(n,2,C_q,u)) \qquad \text{(by lemma 2.3)} \\ &= z(H) + (n+1-p-q)[f(p)f(q) + 2f(p-2)f(q-1)]. \end{aligned}$$

So, $z(S_n(p,q)) \leqslant z(G')$ with the equality if and only if $n = p+q-1$, and $G' \cong S_n(p,q)$.

Given $p \geqslant 3$ and $q \geqslant 3$, from the theorem above, we know $S_n(p,q)$ is the unique graph with the smallest Hosoya index in $\mathcal{A}(p,q)$.

Lemma 3.2. $z(S_n(p,q)) = (n+2-p-q)f(p)f(q)+2f(p-1)f(q)+2f(p)f(q-1)$.

Proof. Let u be the common vertex of C_p and C_q in $S_n(p,q)$. Then we have

$$\begin{aligned} z(S_n(p,q)) &= z(S_n(p,q)-\{u\}) + \sum_{v\in N_{S_n(p,q)}(u)} z(S_n(p,q)-\{u,v\}) \\ &= (n+2-p-q)z(P_{p-1}\cup P_{q-1}) + 2z(P_{p-2}\cup P_{q-1}) \\ &\quad +2z(P_{p-1}\cup P_{q-2}) \\ &= (n+2-p+q)f(p)f(q) + 2f(p-1)f(q) + 2f(p)f(q-1). \end{aligned}$$

Lemma 3.3. (i) If $p > 3$, then $z(S_n(p,q)) > z(S_n(p-1,q))$; (ii) If $q > 3$, then $z(S_n(p,q)) < z(S_n(p,q-1))$.

Proof. From the symmetry of p and q, we only need to prove (i). If $p > 3$, then by lemma 3.2, we have

$$\begin{aligned} \Delta &= z(S_n(p,q)) - z(S(p-1,q)) \\ &= (n+2-p-q)f(p)f(q) + 2f(p-1)f(q) + 2f(p)f(q-1) \\ &\quad -(n+3-p-q)f(p-1)f(q) - 2f(p-2)f(q) - 2f(p-1)f(q-1) \\ &= (n+2-p-q)f(p-2)f(q) + 2f(p-3)f(q) \\ &\quad +2f(p-2)f(q-1) - f(p-1)f(q) \\ &= (n+1-p-q)f(p-2)f(q) + f(p-3)f(q) + 2f(p-2)f(q-1) \\ &> 0. \end{aligned}$$

From theorem 3.1 and lemma 3.3, we know.

Theorem 3.4. $S_n(3,3)$ is the unique graph with the smallest Hosoya index among $\mathcal{A}(p,q)$ for all $p \geqslant 3$ and $q \geqslant 3$.

4. The graph with the smallest Hosoya index in $\mathcal{B}(p, q)$

In this section, we will find the $(n, n+1)-$graph with the smallest Hosoya index in $\mathcal{B}(p, q)$.

Let $T_n^r(p, q)$ be the $(n, n+1)-$graph obtaining from connecting C_p and C_q by a path of length r and the other $n+1-p-q-r$ edges are all attached to the common vertex of the path and C_p (see figure 5(a)). And $T_n^r(q, p)$ is showed in figure 5(b).

Theorem 4.1. If $G \in \mathcal{B}(p, q)$, the length of the shortest path connecting C_p and C_q is r, then either

(i) $z(G) \geqslant z(T_n^r(p, q))$ with the equality if and only if $G \cong T_n^r(p, q)$; or

(ii) $z(G) \geqslant z(T_n^r(q, p))$ with the equality if and only if $G \cong T_n^r(q, p)$; or

(iii) $z(G) \geqslant z(T_n(p, q))$ with the equality if and only if $G \cong T_n(p, q)$, where $T_n(p, q)$ is the $(n, n+1)-$graph obtaining from connecting C_p and C_q by a path uvw of length 3 and the other $n-p-q-1$ edges are all attached to the vertex w of the path, as showed in figure 5(c).

Proof. Let $W = v_1 v_2 \ldots v_r v_{r+1}$ be the shortest path connecting C_p and C_q, and v_1 the common vertex W and C_p, v_{r+1} the common vertex W and C_q.

Repeating the transformations A and B on graph G, we can get a graph G' in figure 5 such that all the edges not on the cycles are the pendant edges

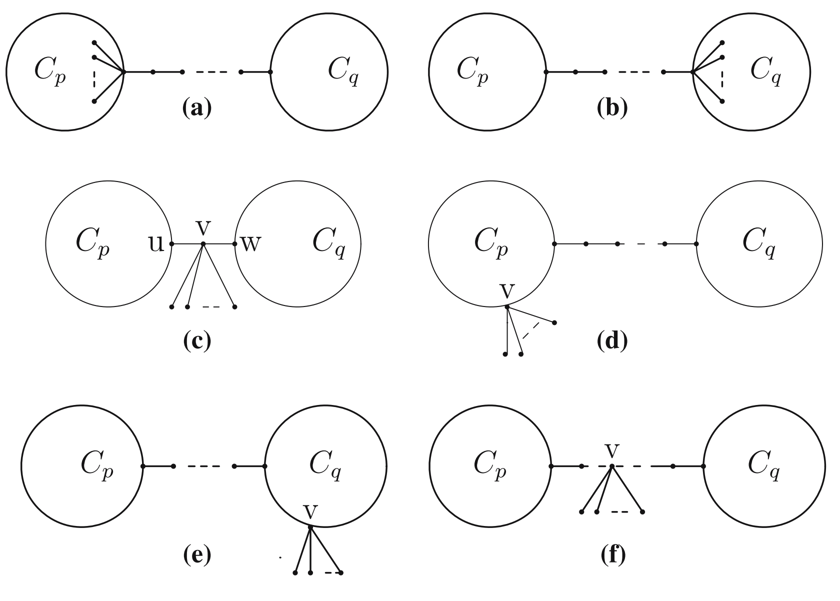

Figure 5. (a) $T_n^r(p, q)$; (b) $T_n^r(q, p)$; (c) $T_n(p, q)$.

attached to the same vertex v. By lemmas 2.1 and 2.2, we have $z(G) \geqslant z(G')$ with the equality if and only if all the edges not on the cycles are also the pendant edges attached to the same vertex in G.

Case I. v is on the cycle C_p (as showed in figure 5(d)) and the distance $d(v_1, v) = k-1$.

(i) If v_1 and v are not adjacent (i.e., $k > 1$), then

$$\begin{aligned}
z(G') - z(T_n^r(p,q)) &= z(G' - \{v\}) + \sum_{x \in N_{G'}(v)} z(G' - \{v, x\}) \\
&\quad - z\left(T_n^r(p,q) - \{v\}\right) - \sum_{x \in N_{T_n^r(p,q)}(v)} z\left(T_n^r(p,q) - \{v, x\}\right) \\
&= z(G' - \{v, v_1\}) + \sum_{y \in N_{G'}(v_1)} z(G' - \{v, v_1, y\}) \\
&\quad + \sum_{x \in N_{G'}(v)} \left[z(G' - \{v, x, v_1\}) + \sum_{y \in N_{G'}(v_1)} z(G' - \{v, x, v_1, y\}) \right] \\
&\quad - z(T_n^r(p,q) - \{v, v_1\}) - \sum_{y \in N_{T_n^r(p,q)}(v_1)} z\left(T_n^r(p,q) - \{v, v_1, y\}\right) \\
&\quad - \sum_{x \in N_{T_n^r(p,q)}(v)} \left[z\left(T_n^r(p,q) - \{v, x, v_1\}\right) \right. \\
&\quad \left. + \sum_{y \in N_{T_n^r(p,q)}(v_1)} z\left(T_n^r(p,q) - \{v, x, v_1, y\}\right) \right].
\end{aligned}$$

Note that

$$\begin{aligned}
z(G' - \{v, v_1\}) &= z(T_n^r(p,q) - \{v, v_1\}), \\
&\sum_{y \in N_{G'}(v_1)} z(G' - \{v, v_1, y\}) - \sum_{y \in N_{T_n^r(p,q)}(v_1)} z(T_n^r(p,q) - \{v, v_1, y\}) \\
&= -(n+1-p-q-r) z(P_{p-k-1} \cup P_{k-1} \cup H_2), \\
&\sum_{x \in N_{G'}(v)} z(G' - \{v, x, v_1\}) - \sum_{x \in N_{T_n^r(p,q)}(v)} z\left(T_n^r(p,q) - \{v, x, v_1\}\right) \\
&= (n+1-p-q-r) z(P_{p-k-1} \cup P_{k-1} \cup H_2), \\
&\sum_{x \in N_{G'}(v)} \sum_{y \in N_{G'}(v_1)} z(G' - \{v, x, v_1, y\}) - \sum_{x \in N_{T_n^r(p,q)}(v)} \sum_{y \in N_{T_n^r(p,q)}(v_1)} \\
&\times z(T_n^r(p,q) - \{v, x, v_1, y\}) \\
&= (n+1-p-q-r) z(P_{p-k-1} \cup P_{k-1} \cup H_1),
\end{aligned}$$

where H_2 is the graph deleting v_1 from the subgraph of $T_n^r(p,q)$ consisting of C_q and W and $H_1 = H_2 - \{v_2\}$. We have

$$\begin{aligned} z(G') - z(T_n^r(p,q)) = &- (n+1-p-q-r) z(P_{p-k-1} \cup P_{k-1} \cup H_2) \\ &+ (n+1-p-q-r) z(P_{p-k-1} \cup P_{k-1} \cup H_2) \\ &+ (n+1-p-q-r) z(P_{p-k-1} \cup P_{k-1} \cup H_2) \\ = &(n+1-p-q-r) z(P_{p-k-1} \cup P_{k-1} \cup H_1) \\ \geqslant &\, 0 \end{aligned}$$

with the equality if and only if $n = p+q+r-1$, and then also $G' \cong T_n^r(p,q)$.

(ii) If v_1 and v are adjacent (i.e., $k=1$), then

$$\begin{aligned} z(G') - z(T_n^r(p,q)) = &\, z(G' - \{v\}) + \sum_{x \in N_{G'}(v)} z(G' - \{v, x\}) \\ &- z(T_n^r(p,q) - \{v\}) - \sum_{x \in N_{T_n^r(p,q)}(v)} z(T_n^r(p,q) - \{v, x\}) \\ = &\, z(G' - \{v, v_1\}) + \sum_{y \in N_{G'}(v_1)} z(G' - \{v, v_1, y\}) \\ &+ \sum_{x \in N_{G'}(v)} \Big[z(G' - \{v, x, v_1\}) + \sum_{y \in N_{G'}(v_1)} z(G' - \{v, x, v_1, y\}) \Big] \\ &- z(T_n^r(p,q) - \{v, v_1\}) - \sum_{y \in N_{T_n^r(p,q)}(v_1)} z\big(T_n^r(p,q) - \{v, v_1, y\}\big) \\ &- \sum_{x \in N_{T_n^r(p,q)}(v)} \Big[z\big(T_n^r(p,q) - \{v, x, v_1\}\big) \\ &+ \sum_{y \in N_{T_n^r(p,q)}(v_1)} z(T_n^r(p,q) - \{v, x, v_1, y\}) \Big]. \end{aligned}$$

Note that

$$\begin{aligned} z(G' - \{v, v_1\}) &= z\big(T_n^r(p,q) - \{v, v_1\}\big), \\ &\sum_{y \in N_{G'}(v_1)} z(G' - \{v, v_1, y\}) - \sum_{y \in N_{T_n^r(p,q)}(v_1)} z(T_n^r(p,q) - \{v, v_1, y\}) \\ &= -(n+1-p-q-r) z(P_{p-2} \cup H_2), \\ &\sum_{x \in N_{G'}(v)} z(G' - \{v, x, v_1\}) - \sum_{x \in N_{T_n^r(p,q)}(v)} z\big(T_n^r(p,q) - \{v, x, v_1\}\big) \end{aligned}$$

$$= (n+1-p-q-r)z(P_{p-2} \cup H_2),$$

$$\sum_{x \in N_{G'}(v)} \sum_{y \in N_{G'}(v_1)} z(G' - \{v, x, v_1, y\}) - \sum_{x \in N_{T_n^r(p,q)}(v)} \sum_{y \in N_{T_n^r(p,q)}(v_1)} \times z\big(T_n^r(p,q) - \{v, x, v_1, y\}\big)$$
$$= (n+1-p-q-r)z(P_{p-2} \cup H_1).$$

We have

$$\begin{aligned} z(G') - z\big(T_n^r(p,q)\big) &= -(n+1-p-q-r)z(P_{p-2} \cup H_2) \\ &\quad +(n+1-p-q-r)z(P_{p-2} \cup H_2) \\ &\quad +(n+1-p-q-r)z(P_{p-2} \cup H_2) \\ &= (n+1-p-q-r)z(P_{p-2} \cup H_1) \\ &\geqslant 0 \end{aligned}$$

with the equality if and only if $n = p+q+r-1$, and then also $G' \cong T_n^r(p,q)$.

Case II. v is on the cycle C_q (as showed in figure 5(e)).

We can prove that $z(G) \geqslant z(T_n^r(q,p))$ with the equality if and only if $G \cong T_n^r(q,p)$ as in the case I.

Case III. v is on the path W (as showed in figure 5(f)). Let $v = v_t$, $1 < t \leqslant r$. $M(G)$ denotes the set of matchings in G. Without loss of the generality, we may assume that $t > 2$.

Let $x_1, x_2, \ldots, x_{n-p-q-1}$ be the leaves attached v in $T_n(p,q)$, $y_1, y_2, \ldots, y_{n-p-q-r+1}$ the leaves attached v_t in G'.

$$\begin{aligned} &e_1 = uv, e_2 = vw, e_3 = vx_1, e_4 = vx_2, \ldots, e_{n-p-q+1} = vx_{n-p-q-1}; \\ &e_1' = v_1v_2, e_2' = v_rv_{r+1}, e_3 = v_2v_3, e_4 = v_3v_4, \ldots, e_t = v_{t-1}v_t, \\ &\quad e_{t+1} = v_ty_1, \ldots, e_{t+n-p-q-r+1} = v_ty_{n-p-q-r+1}, e_{t+n-p-q-r+2} \\ &\quad = v_tv_{t+1}, \ldots, e_{n-p-q+1} = v_{r-1}v_r. \end{aligned}$$

We construct a mapping ξ: $M(T_n(p,q)) \to M(G')$ such that

$$\xi(B) = \begin{cases} (B - \{e_i\}) \cup \{e_i'\}, & \text{if } e_i \in B, \\ B, & \text{otherwise.} \end{cases}$$

The mapping ξ is injective. However, there is no $B \in M(T_n(p,q))$ with $\xi(B) = \{v_1v_2, v_ty_1\}$. So, $z(G') > z(T_n(p,q))$.

Lemma 4.2. (i) If $p > 3$, then $z(T_n(p,q)) > z(T_n(p-1,q))$;

(ii) If $q > 3$, then $z(T_n(p,q)) > z(T_n(p,q-1))$.

Proof. From the symmetry of p and q, we only need to prove (i). Let uvw be the shortest path connecting two cycles in $T_n(p,q)$ or $T_n(p-1,q)$.

$$\begin{aligned}
&z(T_n(p,q)) - z(T_n(p-1,q)) \\
&\quad = z(T_n(p,q) - \{v\}) + \sum_{x\in N_{T_n(p,q)}(v)} z(T_n(p,q) - \{v,x\}) \\
&\qquad - z(T_n(p-1,q) - \{v\}) - \sum_{x\in N_{T_n(p-1,q)}(v)} z(T_n(p-1,q) - \{v,x\}) \\
&\quad = (n-p-q)z(C_p)z(C_q) + z(P_{p-1})z(C_q) + z(C_p)z(P_{q-1}) \\
&\qquad - (n-p-q+1)z(C_{p-1})z(C_q) - z(P_{p-2})z(C_q) - z(C_{p-1})z(P_{q-1}) \\
&\quad = (n-p-q)[f(p-3)+f(p-1)][f(q-1)+f(q+1)] + f(p-2) \\
&\qquad \times [f(q-1)+f(q+1)] + f(q)[f(p-3)+f(p-1)] - [f(p-2)+f(p)] \\
&\qquad \times [f(q-1)+f(q+1)] \\
&\quad = (n-p-q-1)[f(p-3)+f(p-1)][f(q-1)+f(q+1)] \\
&\qquad + f(q)[f(p-3)+f(p-1)] - f(p-4)[f(q-1)+f(q+1)] \\
&\quad = 3(n-p-q-1)f(p-3)[f(q-1)+f(q+1)] + f(q)[f(p-3)+f(p-1)] \\
&\qquad + (n-p-q-2)f(p-4)[f(q-1)+f(q+1)] \\
&\quad > 0.
\end{aligned}$$

And $z(T_n(p,q)) > z(T_n(p-1,q))$.

From lemma 4.2, it is immediately that

Corollary 4.3. $z(T_n(p,q)) \geqslant z(T_n(3,3))$ with the equality if and only if $p=q=3$.

Lemma 4.4. If $r>1$, then $z(T_n^r(p,q)) > z(T_n^1(p,q)$ and $z(T_n^r(q,p)) > z(T_n^1(q,p))$.

Proof. Let $v_1v_2\dots v_{r+1}$ be the shortest path connecting C_p and C_q and $u_1, u_2, \dots, u_{n-p-q-r+1}$ the leaves in $T_n^r(p,q)$, v_1v_{r+1} the edge connecting C_p and C_q and $u_1, u_2, \dots, u_{n-p-q-r+1}$; $v_2, \dots, v_r$ the leaves in $T_n^1(p,q)$.

We construct a mapping ξ: $M(T_n^1(p,q)) \to M(T_n^r(p,q))$ such that

$$\xi(B) = \begin{cases} (B - \{v_1v_{r+1}\}) \cup \{v_rv_{r+1}\}, & \text{if } v_1v_{r+1} \in B, \\ B, & \text{otherwise.} \end{cases}$$

The mapping ξ is injective. However, there is no $B \in M(T_n^1(p,q))$ with $\xi(B) = \{v_1u_1, v_2v_3\}$. So, $z(T_n^r(p,q)) > z(T_n^1(p,q))$.

Similarly, $z(T_n^r(q,p)) > z(T_n^1(q,p))$.

Lemma 4.5. (i) If $p > 3$, then $z(T_n^1(p,q)) > z(T_n^1(p-1,q))$;

(ii) If $q > 3$, then $z(T_n^1(p,q)) > z(T_n^1(p,q-1))$;

(iii) If $p > 3$, then $z(T_n^1(q,p)) > z(T_n^1(q,p-1))$;

(iv) If $q > 3$, then $z(T_n^1(q,p)) > z(T_n^1(q-1,p))$;

(v) $z(T_n^r(p,q)) \geqslant z(T_n^1(3,3))$ and $z(T_n^r(q,p)) \geqslant z(T_n^1(3,3))$ with the equality if and only if $p = q = 3$.

Proof. From the symmetry of p and q, we only need to prove (i).

$$\begin{aligned}
&z(T_n^1(p,q)) - z(T_n^1(p-1,q))\\
&\quad = (n+1-p-q)z(P_{p-1})z(C_q) + 2z(P_{p-2})z(C_q) + z(P_{p-1})z(P_{q-1})\\
&\qquad - (n+2-p-q)z(P_{p-2})z(C_q) - 2z(P_{p-3})z(C_q) - z(P_{p-2})z(P_{q-1})\\
&\quad = (n+1-p-q)f(p)[f(q-1)+f(q+1)] + 2f(p-1)[f(q-1)+f(q+1)]\\
&\qquad + f(p)f(q) - (n+2-(p+q))f(p-1)[f(q-1)+f(q+1)]\\
&\qquad - 2f(p-2)[f(q-1)+f(q+1)] - f(p-1)f(q-1)\\
&\quad = (n+1-p-q)[f(p-1)+f(p-2)][f(q-1)+f(q+1)]\\
&\qquad + 2f(p-3)[f(q-1)+f(q+1)] + f(p)f(q) - f(p-1)f(q-1)\\
&\qquad - (n+2-p-q)f(p-1)[f(q-1)+f(q+1)]\\
&\quad = (n-p-q)f(p-2)[f(q-1)+f(q+1)] + f(p-3)[f(q-1)+f(q+1)]\\
&\qquad + f(p)f(q) - f(p-1)f(q-1)\\
&\quad > 0.
\end{aligned}$$

Now, we compare the Hosoya indices of $T_n^1(3,3)$ and $T_n(3,3)$. It can be computed out easily that

$$z(T_n^1(3,3)) = 8(n-5) + 8,$$
$$z(T_n(3,3)) = 16(n-5).$$
Then $z(T_n(3,3)) > z(T_n(3,3))$.

Theorem 4.6. The $T_n^1(3,3)$ is the unique graph with the smallest Hosoya index among all graphs in $\mathcal{B}(p,q)$ for all $p \geqslant 3$ and $q \geqslant 3$.

5. The graph with the smallest Hosoya index in $\mathcal{C}(p, q, l)$

In this section, we will find the $(n, n+1)-$graph with the smallest Hosoya index in $\mathcal{C}(p,q,l)$.

Let $\theta_n^l(p,q)$ be the graph obtaining from the graph in figure 1(c) by attaching $n+1+l-(p+q)$ to one of its vertices with degree 3 (see figure 6(a)).

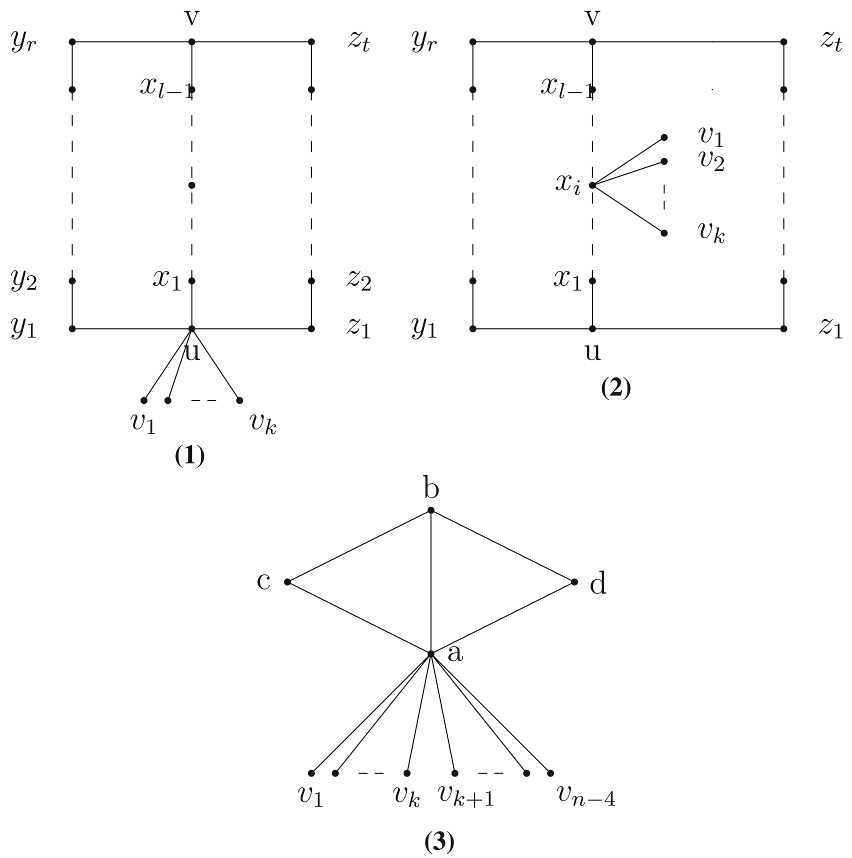

Figure 6. Some graphs in $(n, n+1)$-graphs.

Theorem 5.1. Let $G \in \mathcal{C}(p, q, l)$. Then $z(G) \geqslant z(G_0)$ with the equality if and only if $G \cong G_0$, where $G_0 = \theta_n^1(3, 3)$ is the graph in figure 6(c).

Proof. Let $W_1 = ux_1x_2 \ldots x_{l-1}v$ be the common path of C_p and C_q of the graph G in figure 6, $W_2 = uy_1y_2 \ldots y_rv$ and $W_3 = uz_1z_2 \ldots z_tv$ the other paths from u to v on C_p and C_q, respectively; $r = p - l - 1$, $t = q - l - 1$.

Repeating the transformations A and B on graph G, we can get a graph $G' \in \mathcal{C}(p, q, l)$ such that all the edges not on the cycles are the pendant edges attached to the same vertex v_0. By lemmas 2.1 and 2.2, we have $z(G) \geqslant z(G')$ with the equality if and only if all the edges not on the cycles are also the pendant edges attached to the same vertex in G.

Case I. If $v_0 \neq u, v$, without loss of the generality, we may assume that $v_0 = x_i$ (see figure 6(b)). We show that $z(G') > z(G_0)$ in the following.

Let G' and G_0 have the same edge set E, specially, $av_1 = x_iv_1, \ldots, av_k = x_iv_k$, $ac = uy_1, ad = vy_r, bc = uy_r, bd = vz_t$. We construct a mapping $\xi\colon M(G_0) \to M(G')$ such that

$$\xi(B) = \begin{cases} (B - \{bc\}) \cup \{x_ix_{i+1}\}, & \text{if } B = \{bc, av_j\} \text{ and } av_j \in W_2, \\ (B - \{bc\}) \cup \{x_ix_{i+1}\}, & \text{if } B = \{bc, av_j\},\ av_j \in W_1 \text{ and } av_j \neq x_{i+1}x_{i+2}, \\ (B - \{bd\}) \cup \{x_ix_{i-1}\}, & \text{if } B = \{bd, av_j\} \text{ and } av_j \in W_2, \\ (B - \{bd\}) \cup \{x_ix_{i-1}\}, & \text{if } B = \{bd, av_j\},\ av_j \in W_1 \text{ and } av_j \neq x_{i-1}x_{i-2}, \\ B, & \text{otherwise,} \end{cases}$$

where $j = k+1, \ldots, n-4$. The mapping ξ is injective. However, there is no $B \in M(G_0)$ with $\xi(B) = \{ab, x_iv_1\} \in M(G')$. So, $z(G') > z(G_0)$.

Case II. If $v_0 = u$ or v, without loss of the generality, we may assume that $v_0 = u$ and $l - 1 \leqslant r \leqslant t$. We show that $z(G') \geqslant z(G_0)$ in the following.

Let G' and G_0 have the same edge set E, specially, $av_1 = uv_1, \ldots, av_k = uv_k$, $ac = uy_1, ad = uz_1, ab = ux_1, bc = vy_r, bd = vz_t$. We construct a mapping $\xi\colon M(G_0) \to M(G')$ such that

$$\xi(B) = \begin{cases} (B - \{bc\}) \cup \{uz_1\}, & \text{if } B = \{bc, av_j\} \text{ and } av_j \in W_1, \\ (B - \{bc\}) \cup \{uz_1\}, & \text{if } B = \{bc, av_j\},\ av_j \in W_2, \\ (B - \{bc\}) \cup \{uy_1\}, & \text{if } B = \{bc, av_j\} \text{ and } av_j \in W_3, \\ (B - \{bd\}) \cup \{uy_1\}, & \text{if } B = \{bd, av_j\} \text{ and } av_j \in W_1, \\ (B - \{bd\}) \cup \{uz_1\}, & \text{if } B = \{bd, av_j\},\ av_j \in W_2, \\ (B - \{bd\}) \cup \{uy_1\}, & \text{if } B = \{bd, av_j\} \text{ and } av_j \in W_3, \\ B, & \text{otherwise,} \end{cases}$$

where $j = k+1, \ldots, n-4$. The mapping ξ is injective. ξ is not surjective if $G' \ncong G_0$, and $z(G') > z(G_0)$.

6. Extremal graph in $\mathcal{G}(n, n+1)$

In this section, we give the lower bound for the Hosoya index in $\mathcal{G}(n, n+1)$, and characterize the extremal graph.

Theorem 6.1. Let G be an $(n, n+1)-$graph, then $z(G) \geqslant 3n-4$ with the equality if and only if $G \cong \theta_n^1(3,3)$ (see figure 6(c)).

Proof. From theorems 3.4, 4.6 and 5.1, we only need to compare the Hosoya indices of $S_n(3,3)$, $T_n^1(3,3)$, and $\theta_n^1(3,3)$. Computing immediately, we have

$$z(S_n(3,3)) = 4n - 8,$$
$$z(T_n^1(3,3)) = 8n - 28,$$
$$z(\theta_n^1(3,3)) = 3n - 4.$$

Therefore, $z(G) \geqslant z(\theta_n^1(3,3)) = 3n - 4$ with the equality if and only if $G \cong \theta_n^1(3,3)$.

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