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Research Paper

Hosoya index of total graphs and semitotal graphs

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Abstract. The Hosoya index Z(G) of a graph *G* is the total number of matchings in it. In this paper, the recursive formulas of the Hosoya index of semitotal graph Q(G) and total graph T(G) for certain graphs *G* are obtained. Moreover, we obtain the bounds of the Hosoya index of semitotal and total graphs of a connected graph *G*.

Keywords: Hosoya index, semitotal graph, total graph **Mathematics Subject Classification (2010):** Primary 05C90; Secondary 92E10.

1 Introduction

In 1971, Haruo Hosoya introduced the Hosoya index of a graph *G*, denoted by Z(G), and showed that certain Physico-chemical properties of saturated hydrocarbons are corrected with Z(G) [10]. Some papers related to the chemical concepts of the Hosoya index can be found in [7–9].

Let G = (V, E) be a simple connected graph with |V| = n vertices and |E| = m edges. Two edges of *G* are called independent if they don't have a common vertex in *G*. A *k*-matching of

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G is a set of *k* independent edges and the number of *k*-matching in G is denoted by m(G,k). Let m(G,0) = 1 for any graph *G*. Z(G) is defined as follows

$$Z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} m(G,k).$$

More results on the Hosoya index can be found in [1,4,12–15]. There are some derived graphs of a connected graph *G* such as the subdivision graph S(G), the semitotal graph Q(G) and the total graph T(G). In [17], the Hosoya index and matching polynomial of S(G) of a graph *G* are determined in terms of the matchings. Note that S(G) is obtained by putting a path of length two on each edge of the graph *G* [16].

In this paper, we deal with semitotal graphs and total graphs. The semitotal graph Q(G) of the graph *G* is obtained by inserting a new vertex into each edge of *G* and joining these pairs of new vertices on adjacent edges of *G* by an edge [16]. The total graph T(G) is a graph obtained from the graph *G* which its vertex set containing the vertices and edges of *G* and two vertices in T(G) are adjacent if they are either adjacent or incident in *G* [2, 16].

The neighborhood of the vertex $u \in V$ in a graph *G* is defined as $N_G(u) = \{v \in V | uv \in E\}$. The number of edges incident to vertex *u* in *G* is denoted by deg(u). A Hamiltonian cycle in a graph is a cycle that visits each vertex of the graph exactly once. Two graphs G_1 and G_2 which obtain the same number of vertices connected in the same way are said to be isomorphic and denoted as $G_1 \cong G_2$. A subgraph *H* of a graph *G*, denoted by $H \subseteq G$, is a graph with vertex set $V(H) \subseteq V(G)$ and edge set $E(H) \subseteq E(G)$. The corona graph $G_1 \circ G_2$ is obtained of two graphs G_1 and G_2 by determining one copy of G_1 and $|V(G_1)|$ copies of G_2 , in which the *i*th vertex of the graph G_1 is adjacent to every vertex in the *i*th copy of the graph G_2 . The corona $G \circ K_1$, is formed from a copy of *G*, where for each vertex $u \in V(G)$, a new vertex *v* and a pendant edge *uv* are added [3].

In this paper, we study the Hosoya index of Q(G) and T(G). Furthermore, the lower and upper bounds of the Hosoya index of semitotal and total graphs for the connected graph *G* are determined.

2 The Hosoya index of Q(G) and T(G) of certain graphs

In this section, we obtain the results for computing Z(G) of the semitotal graph and the total graph of some certain graphs. First, some lemmas that will be used in the proof of our results are given.

Lemma 2.1. [6] *Let* G = (V, E) *be a graph.*

(*i*) If $uv \in E(G)$, then $Z(G) = Z(G - uv) + Z(G - \{u, v\})$,

Akhbari et al. / Journal of Discrete Mathematics and Its Applications 8 (2023) 23-33

(*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 2.2. [6] Let P_n , S_n and C_n be the path, star and cycle of the order n, respectively. Then

- (*i*) For any n > 0, then $Z(P_n) = F_{n+1}$ and $Z(S_n) = n$,
- (*ii*) For any $n \ge 3$, then $Z(C_n) = F_{n-1} + F_{n+1}$,

where F_n denotes the Fibonacci number, defined by $F_0 = 0$, $F_1 = 1$ and $F_{n+1} = F_n + F_{n-1}$.

The subdivision-related graph R(G) of G is the graph obtained by adding a new vertex corresponding to each edge of G and joining the new vertex to the end vertices of the corresponding edge. In other words, R(G) is obtained by replacing each edge of G with a triangle. The following result is obtained for the Hosoya index on the graph R(G) [2, 16].

Lemma 2.3. [18] Let G be a simple graph with n vertices and R(G) be the graph defined above. Then, the Hosoya index Z(R(G)) is as following

$$Z(R(G)) = \prod_{i=1}^{n} (d_i + 1),$$

where (d_1, d_2, \ldots, d_n) is the degree sequence of vertices of *G*.

Theorem 2.4. For any $n \ge 3$, the Hosoya index of semitotal graph of C_n is equal to

$$Z(Q(C_n)) = 3^n.$$

Proof. Let C_n be a cycle of order n with the vertices set $\{v_1, v_2, ..., v_n\}$. The semitotal of C_n is obtained by adding a new vertex v'_i into each edge $v_i v_{i+1}$ for $1 \le i \le n-1$ and v'_n inserts on edge $v_n v_1$ on cycle C_n . According to the definition the graph Q(G), the new vertices v'_i and v'_{i+1} are adjacent in $Q(C_n)$ for $1 \le i \le n-1$ and the edge $v'_n v'_1 \in E(Q(C_n))$ (see Figure 1.). If we consider the cycle C'_n with the vertices $\{v'_1, ..., v'_n\}$, then Figure 2 shows that $Q(C_n) \simeq R(C'_n)$. Therefore,

$$Z(Q(C_n)) = Z(R(C'_n)).$$

By Lemma 2.3 and since the degree of any vertex v'_i in C'_n equals to 2 for $1 \le i \le n$, we have

$$Z(R(C'_n)) = \prod_{i=1}^n (2+1) = 3^n.$$

Thus, the proof completes.

Now we obtain a recursive formula of the Hosoya index of $K_n \circ K_1$. This result will be used in the next results.



Figure 1. The semitotal graph of C_n .

Proposition 2.5. *For* $n \ge 3$ *,*

$$Z(K_n \circ K_1) = 2Z(K_{n-1} \circ K_1) + (n-1)Z(K_{n-2} \circ K_1),$$
(1)

with the initial conditions $Z(K_1 \circ K_1) = 2$ and $Z(K_2 \circ K_1) = 5$.

Proof. Let $G_n = K_n \circ K_1$ and the complete graph K_n has vertices $v_1, v_2, ..., v_n$ that the vertex u is adjacent to v_1 in $K_n \circ K_1$. Using Lemma 2.1, we have

$$Z(G_n) = Z(G_n - v_1) + Z(G_n - \{v_1, u\}) + \sum_{i=2}^n Z(G_n - \{v_1, v_i\})$$

= Z(G_{n-1}) + Z(G_{n-1}) + (n-1)Z(G_{n-2}).

Therefore, for $n \ge 3$,

$$Z(K_n \circ K_1) = 2Z(K_{n-1} \circ K_1) + (n-1)Z(K_{n-2} \circ K_1).$$

For n = 1, $G_1 = K_1 \circ K_1$ and $G_2 = K_2 \circ K_1$ are isomorphic with paths P_2 and P_4 respectively, that using Lemma 2.2(*i*), $Z(G_1) = 2$ and $Z(G_2) = 5$. So, the result holds.

Theorem 2.6. For star graph S_n of order $n \ge 3$,

$$Z(Q(S_n)) = (n+2)Z(K_{n-1} \circ K_1) + (n-1)Z(K_{n-2} \circ K_1),$$

with the initial conditions $Z(K_1 \circ K_1) = 2$ and $Z(K_2 \circ K_1) = 5$.

Proof. Let S_n be a star graph of order n with the vertices set $\{v_1, v_2, ..., v_n, x\}$ in which x be the central vertex with deg(x) = n. Let v'_i be the new vertices in the graph $Q(S_n)$ for i = 1, 2, ..., n.

According to the structure of the graph $Q(S_n)$, the induces subgraph of vertices $\{v'_1, v'_2, ..., v'_n\}$ is a complete graph in $Q(S_n)$. Therefore, using Lemma 2.1, we have

$$Z(Q(S_n)) = Z(Q(S_n) - x) + \sum_{i=1}^n Z(Q(S_n) - \{x, v'_i\})$$

= $Z(K_n \circ K_1) + nZ(K_{n-1} \circ K_1).$

Using Proposition 2.5, we get

$$Z(Q(S_n)) = Z(K_n \circ K_1) + nZ(K_{n-1} \circ K_1)$$

= $(n+2)Z(K_{n-1} \circ K_1) + (n-1)Z(K_{n-2} \circ K_1).$

Let *u* be the central vertex of degree *n* in S_n and *v* be the vertex of degree *n* in S'_n . The Bistar graph $B_{n,n}$ is obtained by adding an edge joining *u* and *v* of S_n and S'_n .

Corollary 2.7. If $B_{n,n}$ is Bistar graph, then

$$Z(Q(B_{n,n})) = Z(Q(S_n))^2 + 2nZ(Q(S_{n-1}))Z(Q(S_n)).$$

Proof. Assume that Bistar graph $B_{n,n}$ is obtained by adding two central vertices u and v of two stars S_n and S'_n . Let x be the new vertex on the edge uv in the graph $Q(B_{n,n})$ that is adjacent to all of the new inserting vertices. Therefore, using Lemma 2.1,

$$Z(Q(B_{n,n})) = Z(Q(B_{n,n}) - x) + \sum_{v_i \in N_{Q(B_{n,n})}(x)} Z(Q(B_{n,n}) - \{x, v_i\})$$

Since deg(x) = 2n and the graph $Q(B_{n,n}) \setminus \{x\}$ contains two graphs $Q(S_n)$, we have

$$Z(Q(B_{n,n})) = Z(Q(S_n))^2 + 2nZ(Q(S_{n-1}))Z(Q(S_n)).$$

In the next theorem, we give the recursive formula for the Hosoya index of $Q(P_n)$.

Theorem 2.8. Let P_n be a path of order $n \ge 2$. Then

$$Z(Q(P_n)) = 3Z(Q(P_{n-1}))$$

with initial condition $Z(Q(P_1)) = 1$.



Figure 2. The graph G_{n-1} in Theorem 2.8.

Proof. Assume that P_n is the path of order n with vertices set $\{v_1, v_2, ..., v_n\}$ and the new vertices on edges of $Q(P_n)$ be $\{v'_1, v'_2, ..., v'_{n-1}\}$. We denote the graph obtained from deleting vertex v_1 in the semitotal $Q(P_n)$ by G_{n-1} (see Figure 2.). Therefore, using Lemma 2.1(*ii*) and the structure of Figure 2.,

$$Z(Q(P_n)) = Z(Q(P_n) - v_1) + Z(Q(P_n) - \{v_1, v_1'\})$$

= Z(G_{n-1}) + Z(Q(P_{n-1})). (2)

According to Figure 2., we compute $Z(G_{n-1})$ with considering v'_1 and $N_{G_{n-1}}(v'_1) = \{v_2, v'_2\}$ for $n \ge 2$.

Using Lemma 2.1(*ii*), we have

$$Z(G_{n-1}) = Z(G_{n-1} - v'_1) + Z(G_{n-1} - \{v'_1, v_2\}) + Z(G_{n-1} - \{v'_1, v'_2\})$$

= $Z(G_{n-2}) + Z(Q(P_{n-1})) + Z(Q(P_{n-2})),$ (3)

For n = 0, $Z(G_0) = Z(Q(P_0)) = 1$. Clearly, $Z(Q(P_1)) = 1$ and for n = 2, $Z(G_1) = Z(P_2) = 2$ and $Z(Q(P_2)) = Z(P_3) = 3$. For $n \ge 3$, substituting for $Z(G_{n-1})$ in equation (2) by (3) yields

$$Z(Q(P_n)) = Z(G_{n-2}) + 2Z(Q(P_{n-1})) + Z(Q(P_{n-2})).$$

Then, by substituting for $Z(G_{n-2})$ using equation (2), we get

$$Z(Q(P_n)) = 3Z(Q(P_{n-1})).$$

Theorem 2.9. For $n \ge 3$, the Hosoya index of the total graph of S_n is as following

$$Z(T(S_n)) = 2(n+1)Z(K_{n-1} \circ K_1) + (n^2 - 1)Z(K_{n-2} \circ K_1),$$

with the initial conditions $Z(K_1 \circ K_1) = 2$ and $Z(K_2 \circ K_1) = 5$.

Proof. In an analogous manner and labeling in the graph S_n and the new vertices set as Theorem 2.6 and according to the definition of the total graph, the vertex x is adjacent to all vertices v_i and v'_i in $T(S_n)$. Thus, using Lemma 2.1,

$$Z(T(S_n)) = Z(T(S_n) - x) + \sum_{i=1}^n Z(T(S_n) - \{x, v_i\}) + \sum_{i=1}^n Z(T(S_n) - \{x, v'_i\})$$

= $Z(K_n \circ K_1) + nZ(K_{n-1} \circ K_1) + \sum_{i=1}^n Z(T(S_n) - \{x, v'_i\}).$

According to the structure of $T(S_n)$, the graph $G_i = T(S_n) \setminus \{x, v'_i\}$ is the corona graph $K_n \circ K_1$ for $i = 1, 2, \dots, n$ such that pendant edge to the vertex v'_i is deleted. So, with selecting the vertex v_i and since $deg(v'_i) = n - 1$, we have

$$Z(G'_i) = Z(G'_i - v'_i) + \sum_{\substack{i=1\\i\neq j}}^{n-1} Z(G'_i - \{v'_i, v'_j\})$$
$$= Z(K_{n-1} \circ K_1) + (n-1)Z(K_{n-2} \circ K_1)$$

Therefore by applying Proposition 2.5, we get

$$Z(T(S_n)) = Z(K_n \circ K_1) + nZ(K_{n-1} \circ K_1) + nZ(K_{n-1} \circ K_1) + n(n-1)Z(K_{n-2} \circ K_1)$$

= $Z(K_n \circ K_1) + 2nZ(K_{n-1} \circ K_1) + n(n-1)Z(K_{n-2} \circ K_1)$
= $2(n+1)Z(K_{n-1} \circ K_1) + (n^2 - 1)Z(K_{n-2} \circ K_1).$

The following corollary is easily obtained by Lemma 2.1, Proposition 2.5 and Theorem 2.9.

Corollary 2.10. *The Hosoya index of* $T(B_{n,n})$ *, for* $n \ge 3$ *is as following*

$$Z(T(B_{n,n})) = Z(T(S_n))^2 + Z(K_n \circ K_1)^2 + 2Z(K_n \circ K_1)Z(T(S_n)) + 2n \Big[Z(T(S_{n-1}))Z(T(S_n)) + Z(K_{n-1} \circ K_1)Z(K_n \circ K_1) \Big].$$

3 Bounds on Hosoya index of semitotal graphs and total graphs

In this section, we obtain lower and upper bounds on the Hosoya index of semitotal and total graphs of a connected graph *G*. In order to prove our results, we recall the following lemmas.

Lemma 3.1. [11] If *H* is a subgraph of *G*, then $Z(H) \leq Z(G)$ with equality if and only if E(G) = E(H).

Lemma 3.2. [11] Let G be a connected graph of size m. Then

$$m+1 \le Z(G) \le \frac{1}{\sqrt{5}} \left[\left(\frac{1+\sqrt{5}}{2}\right)^{m+2} - \left(\frac{1-\sqrt{5}}{2}\right)^{m+2} \right].$$

It is easy to achieve the following inequality using induction on *n*. If $n \ge 1$ and b < a, then

$$a^n - b^n \le na^{n-1}(a-b). \tag{4}$$

Lemma 3.3. [2] For any connected graph G with n vertices and m edges, $n - 1 \le m \le \frac{n(n-1)}{2}$.

Lemma 3.4. [2] Let T_n , G_k and $K_{r,s}$ be a tree, a k-regular graph and a bipartite graph of order n, respectively. If m(G) denotes the number of edges of graph G, then

- (*i*) $m(T_n) = n 1$,
- (*ii*) $m(G_k) = \frac{nk}{2}$,
- (*iii*) $m(K_{r,s}) \leq \frac{n^2}{4}$.

Lemma 3.5. [5] Let T(G) = (V', E') be a total graph for the given graph G = (V, E). Then

- (i) |V'| = |V| + |E|,
- (*ii*) $|E'| \le |E|(|V|+1)$.

Lemma 3.6. [5] The total graph of a graph G is regular if and only if G is regular.

Theorem 3.7. *Let G be a simple and connected graph with a Hamiltonian cycle of order* $n \ge 3$ *. Then*

$$3^n \le Z(Q(G)) \le (n-1)^n.$$

The first equality holds if and only if G is a cycle of order n.

Proof. Since *G* has the Hamiltonian cycle thus, by definition there exists the cycle C_n in graph *G*. According to the structure semitotal graph of *G*, it is easy to see that $Q(C_n) \subseteq Q(G)$. Therefore, using Lemma 3.1, $Z(Q(C_n)) \leq Z(Q(G))$. Thus, the lower bound holds by Theorem 2.4. Since cycle C_n is the smallest Hamiltonian graph of order *n*, the equality holds. For the upper bound, we can consider $Q \subseteq K_n$ for any connected graph *G* in which K_n is the complete graph. By definition, we can have $Q(G) \subseteq Q(R(K_n))$. Therefore, using Lemma 3.1 and Lemma 2.3

$$Z(Q(G)) \le (n-1)^n.$$

Thus, the proof completes.

Theorem 3.8. *Let G be a connected graph of order* $n \ge 1$ *. Then*

$$2n-1 \le Z(T(G)) \le (a+1)\left(\frac{1+\sqrt{5}}{2}\right)^a,$$

where $a = \frac{n(n^2 - 1)}{2} + 1$.

Proof. Assume that *G* is a connected graph with *n* vertices and of size *m*. Since *G* is a connected graph then, T(G) is a connected graph and by Lemma 3.5(*i*), the number of vertices of T(G) is n' = n + m and for the number of edges of T(G), we have $m' \le m(n + 1)$. By Lemma 3.2,

$$m' + 1 \le Z(T(G)) \le \frac{1}{\sqrt{5}} \left[\left(\frac{1 + \sqrt{5}}{2} \right)^{m' + 2} - \left(\frac{1 - \sqrt{5}}{2} \right)^{m' + 2} \right].$$

By Lemma 3.3, $m' \ge n' - 1$ and $m \ge n - 1$. Thus, $m' \ge 2n - 2$. Therefore,

$$Z(T(G)) \ge m' + 1 \ge 2n - 1.$$

For the upper bound, we use inequality (4). So

$$Z(T(G)) \leq \frac{1}{\sqrt{5}} \left[\left(\frac{1+\sqrt{5}}{2} \right)^{m'+2} - \left(\frac{1-\sqrt{5}}{2} \right)^{m'+2} \right]$$

$$\leq \frac{1}{\sqrt{5}} (m'+2) \left(\frac{1+\sqrt{5}}{2} \right)^{m'+1} \left(\left(\frac{1+\sqrt{5}}{2} \right) - \left(\frac{1-\sqrt{5}}{2} \right) \right)$$

$$= (m'+2) \left(\frac{1+\sqrt{5}}{2} \right)^{m'+1}.$$
 (5)

Using Lemma 3.5(*ii*) and since $m \leq \frac{n(n-1)}{2}$, we have

$$Z(T(G)) \le \left(\frac{n(n^2 - 1)}{2} + 2\right) \left(\frac{1 + \sqrt{5}}{2}\right)^{\frac{n(n^2 - 1)}{2} + 1}$$

By considering $a = \frac{n(n^2-1)}{2} + 1$, the proof completes.

Corollary 3.9. Let G be a Tree T_n of order n. Then

$$2n-1 \le Z(T(G)) \le (n^2+1)\left(\frac{1+\sqrt{5}}{2}\right)^{n^2}.$$

Proof. Let *G* be a tree T_n with *n* vertices. The lower bound follows from Theorem 3.8. For the upper bound, we consider, inequality 5 as following,

$$Z(T(G)) \le (m'+2)\left(\frac{1+\sqrt{5}}{2}\right)^{m'+1},$$

where m' is the number of edges of the total graph of *G*. Using Lemma 3.5(*ii*) and Lemma 3.4(*i*) we have, $m' \le n^2 - 1$. So, $Z(T(G)) \le (n^2 + 1) \left(\frac{1+\sqrt{5}}{2}\right)^{n^2}$.

Corollary 3.10. Let G be a bipartite graph $K_{r,s}$ of order n. Then

$$2n-1 \le Z(T(G)) \le (b+1)\left(\frac{1+\sqrt{5}}{2}\right)^b$$

where $b = \frac{n^2}{4}(n+1)$.

Proof. Let *G* be a bipartite graph $K_{r,s}$. Similar to the proof of the Theorem 3.8, we only prove the upper bound. Since *G* is the bipartite graph of order *n* then, for the graph T(G), we have $m' \leq \frac{n^2}{4}(n+1)$.

Using inequality (5),

$$Z(T(G)) \le \left(\frac{n^2}{4}(n+1) + 2\right) \left(\frac{1+\sqrt{5}}{2}\right)^{\frac{n^2}{4}(n+1)+1}.$$

With considering $b = \frac{n^2}{4}(n+1)$, the result holds.

For a bipartite graph of order $n \ge 2$, the upper bound of Corollary 3.10 is better than Theorem 3.9. Because it is easy to see that $b \le a$.

Corollary 3.11. Let G_k be a k-regular graph of order n. Then

$$c \leq Z(T(G_k)) \leq (c+1)\left(\frac{1+\sqrt{5}}{2}\right)^c,$$

where $c = \frac{nk}{2}(k+2) + 1$.

Proof. Let G_k be a *k*-regular graph of order *n* and size *m*. It is easy to see that the graph $T(G_k)$ is a 2*k*-regular graph of order n' = n + m [5]. Using Lemma 3.5(*ii*), $m = \frac{nk}{2}$ and $m' = \frac{nk}{2}(k+2)$. According to Theorem 3.8, we have

$$m' \le m' + 1 \le Z(T(G_k)) \le (m' + 2) \left(\frac{1 + \sqrt{5}}{2}\right)^{m' + 1}$$

By replacing $m' = \frac{nk}{2}(k+2)$ and considering $c = \frac{nk}{2}(k+2) + 1$, the result completes.

Calculating the Hosoya index of total graphs of path P_n , cycle C_n and complete graph K_n is difficult due to their structure. But, we can find the bound for these graphs. The following corollary is an easy consequence of Theorem 3.8.

Note, The number edges of the total graph of P_n , C_n and K_n is $m'(T(P_n)) = 4n - 5$, $m'(T(C_n)) = 4n$ and $m'(T(K_n)) = \frac{n(n^2-1)}{2}$, respectively [5].

Theorem 3.12. The Hosoya index of total graphs of P_n , C_n and K_n is as follows

- (i) $4n+1 \le Z(T(C_n)) \le (4n+1)\left(\frac{1+\sqrt{5}}{2}\right)^{4n}$, (*ii*) $\alpha \leq Z(T(P_n)) \leq (\alpha + 1) \left(\frac{1+\sqrt{5}}{2}\right)^{\alpha}$, where $\alpha = 4(n-1)$.
- (iii) $\beta \leq Z(T(K_n)) \leq (\beta+1)\left(\frac{1+\sqrt{5}}{2}\right)^{\beta}$, where $\beta = \frac{n(n^2-1)}{2} + 1$.

Theorem 3.13. *Let G be a connected graph of order* $n \ge 1$ *. Then*

$$2n-1 \le Z(Q(G)) \le (\lambda+1)\left(\frac{1+\sqrt{5}}{2}\right)^{\lambda},$$

where $\lambda = \frac{n^2(n-1)}{2}$.

Proof. Let *G* be the connected graph of order *n* and size *m*. According to the definition of the semitotal graph Q(G) and the total graph T(G), the number of edges in Q(G) is equal to m'' = E(T(G)) - m. So using Lemma 3.5(*ii*), $m'' \le mn$.

Similar to the proof of Theorem 3.8, the result completes.

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