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ESTIMATING THE MODIFIED HOSOYA INDEX

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Abstract

A modified version of Hosoya index of a graph G is defined as $Z^\dagger(G) = \prod_{j=1}^{n} \sqrt{1+\lambda_j^2}$, where λ_j , $j = 1, 2, \ldots, n$, are the eigenvalues of G. If G is bipartite, then $Z^\dagger$ coincides with two previously considered modification of the Hosoya index. If G is acyclic, then $Z^\dagger(G)$ coincides also with the ordinary Hosoya index. We find an upper bound for $Z^\dagger(G)$ in terms of the number of vertices, number of edges and the first Zagreb index, and characterize those graphs for which the upper bound is attained. Similar results for bipartite graphs are also obtained.

INTRODUCTION

The *Hosoya index* of a graph G is $Z = Z(G) = \sum_{k\geq 0} m(G,k)$, where $m(G,k)$ is the number of k-matchings (i. e., number of k-element independent edge sets) of G, with the convention that $m(G,0) = 1$ [1,2]. In the attempt to extend the applicability of the index Z to conjugated π-electron systems, Hosoya et al. [3] put forward its modified version, denoted by $\tilde{Z}$.

Let the characteristic polynomial of the graph G be of the form

$$\phi(G,\lambda) = \sum_{k\geq 0} a_k \, \lambda^{n-k}$$

and let $i = \sqrt{-1}$. Then it is easy to show that

$$\phi(G,i) = i^n \left[\sum_{k\geq 0} (-1)^k \, a_{2k} - i \sum_{k\geq 0} (-1)^k \, a_{2k+1} \right] . \tag{1}$$

According to [3], the modified Hosoya index (originally called "*modified topological index*") is defined as

$$\tilde{Z} = \tilde{Z}(G) = \sum_{k\geq 0} (-1)^k \, a_{2k} .$$

In view of (1),

$$\tilde{Z} = Re\left[(-i)^n \, \phi(G,i)\right]$$

and, if $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the graph eigenvalues (and therefore the zeros of the characteristic polynomial),

$$\tilde{Z} = Re\left[\prod_{j=1}^{n} (1 + i\,\lambda_j) \right] .$$

In the above formulas, $Re[\zeta]$ stands for the real part of the complex number ζ.

If G is a bipartite graph, then all odd coefficients of the characteristic polynomial are equal to zero, and then

$$\tilde{Z} = (-i)^n \, \phi(G,i) .$$

If, in addition, G is acyclic, then $(-1)^k \, a_{2k} = m(G,k)$ and $\tilde{Z}$ reduces to the ordinary Hosoya index Z.

Short time after the introduction of the modified Hosoya index $\tilde{Z}$, Aihara [4] proposed a closely related "*total π-electron energy index*" Z^*, defined as

$$Z^* = Z^*(G) = |\phi(G,i)| = \sqrt{\left[\sum_{k\geq 0}(-1)^k a_{2k}\right]^2 + \left[\sum_{k\geq 0}(-1)^k a_{2k+1}\right]^2} \ .$$

In the case of bipartite graphs, Z^* and $\tilde{Z}$ are identical, but they differ for non-bipartite graphs. Aihara [4] was first to report the expression

$$\sqrt{\prod_{j=1}^{n}(1+\lambda_j^2)}$$

for the calculation of Z^* or $\tilde{Z}$ of bipartite graphs. Eventually, the same expression was much used in the theory of the (ordinary) Hosoya index [5–9].

Aihara used Z^* in connection with the total π-electron energy E_π, and established the relation $E_\pi \approx 6.0846 \log Z^*$. Except the work [4] there seems to be no other chemical application of Z^*. Hosoya used the difference $\Delta Z = \tilde{Z} - Z$ for predicting and rationalizing aromaticity of polycyclic conjugated molecules; he refers to ΔZ as to the "*aromaticity index*"; for details see [10].

GRAPH THEORETICAL PREPARATIONS

Let G be a graph of order n. We define an invariant of G, denoted $Z^\dagger(G)$, by

$$Z^\dagger = Z^\dagger(G) = \prod_{j=1}^{n} \sqrt{1+\lambda_j^2}, \tag{2}$$

where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of G. As explained in the preceding section, if G is bipartite, then the right–hand side of Eq. (2) coincides with both $\tilde{Z}(G)$ and $Z^*(G)$. If G is acyclic, then $Z^\dagger$ coincides also with Z.

The *first Zagreb index* of a graph G is defined as $\delta = \sum_{j=1}^{n}(d_j)^2$, where $d_1, d_2, \ldots, d_n$ are the vertex degrees of G; for details see the book [11] and the recent works [12,13].

A graph G is *semiregular bipartite* (of degrees r_1 and r_2) if it is bipartite, and if each vertex in the same part of its bipartition has the same degree (each vertex in one part of the bipartition has degree r_1 and each vertex in the other part of the bipartition has degree r_2). Clearly a regular bipartite graph is a semiregular bipartite graph ($r_1 = r_2$). Let G be a graph of order n and let its first Zagreb index be δ. It is known [14] that $\lambda_1 \geq \sqrt{\delta/n}$, and that equality holds if and only if G is a regular graph or a semiregular bipartite graph.

In this paper we report an upper bound for the modified Hosoya index $Z^\dagger$ in terms of the number of vertices, number of edges and the first Zagreb index, and characterize those graphs for which the upper bound is attained. For this we employ techniques closely analogous to those used in the recent paper [15] and elsewhere [16,17]. Similar results on a bipartite graph are also obtained.

We first consider general graphs.

BOUNDS FOR $Z^\dagger$ FOR A GENERAL GRAPH

A *strongly regular graph* G with parameters (n, k, ρ, σ) is a k-regular graph on n vertices, each pair of adjacent vertices having ρ common neighbors, and each pair of non-adjacent vertices having σ common neighbors. If $\sigma \geq 1$ and G is non-complete, then the eigenvalues of G are k, s, and t, with multiplicities 1, m_s, and m_t, where s and t are the roots of the equation $x^2 + (\sigma - \rho)x + (\sigma - k) = 0$, while m_s and m_t can be determined from the equalities $m_s + m_t = n - 1$ and $k + s\,m_s + t\,m_t = 0$.

Theorem 1. *If G is a graph with $n \geq 2$ vertices, $m \geq 1$ edges and first Zagreb index δ, then*

$$Z^\dagger(G) \leq \left(1 + \frac{\delta}{n}\right)^{1/2} \left(1 + \frac{2mn - \delta}{n(n-1)}\right)^{(n-1)/2} . \qquad (3)$$

Equality in (3) holds if and only if G is either $\frac{n}{2} K_2$ or K_n or a non-complete connected strongly regular graph with two non-trivial eigenvalues both with absolute value $\sqrt{(2m - 4m^2/n^2)/(n-1)}$.

Proof. By the arithmetic-geometric-mean inequality and $\sum_{j=1}^{n} \lambda_j^2 = 2m$, we have

$$\prod_{j=2}^{n}(1 + \lambda_j^2) \leq \left(\frac{1}{n-1}\sum_{j=2}^{n}(1 + \lambda_j^2)\right)^{n-1} = \left(1 + \frac{2m - \lambda_1^2}{n-1}\right)^{n-1} .$$

Hence

$$Z^\dagger(G) \leq (1 + \lambda_1^2)^{1/2} \left(1 + \frac{2m - \lambda_1^2}{n-1}\right)^{(n-1)/2} .$$

Note that the function

$$F(x) = (1+x^2)^{1/2}\left(1+\frac{2m-x^2}{n-1}\right)^{(n-1)/2}$$

decreases for $\sqrt{2m/n} \le x \le \sqrt{2m}$, and that $\sqrt{2m/n} \le \sqrt{\delta/n} \le \lambda_1$ .Therefore $F(\lambda_1) \le F\left(\sqrt{\delta/n}\right)$. This proves (3).

It is easy to check that if G is one of the graphs specified in the second part of Theorem 1, then equality in (3) holds.

Conversely, if equality in (3) holds, then by the above argument, $\lambda_1 = \sqrt{\delta/n}$. It follows that G is a regular graph or a semiregular bipartite graph. If G is regualr, then $\lambda_1 = \sqrt{\delta/n} = 2m/n$. Then, according to [17], G is either $\frac{n}{2}K_2$ or K_n or a non-complete connected strongly regular graph with two non-trivial eigenvalues, both with absolute value $\sqrt{(2m-(2m/n)^2)/(n-1)}$. Suppose now that G is a semiregular bipartite graph. Since equality holds in the above arithmetic–geometric–mean inequality, we have $\sqrt{\delta/n} = \lambda_1 = -\lambda_n = \sqrt{(2m-\lambda_1^2)/(n-1)}$, from which it follows that $\delta = 2m$. Thus the degree of any vertex of G is 1 , i. e., G is $\frac{n}{2}K_2$. □

Remark 2. By the Cauchy–Schwartz inequality,

$$4\,m^2 = \left(\sum_{j=1}^{n} d_j\right)^2 \le n\delta\ .$$

Therefore $\sqrt{\delta/n} \ge 2m/n$ and $F(x)$ decreases for $\sqrt{2m/n} \le x \le \sqrt{2m}$. We have

$$Z^\dagger(G) \le F\left(\sqrt{\delta/n}\right) \le F(2m/n)$$

which is an (n,m)-type upper bound for $Z^\dagger$.

BOUNDS FOR $Z^\dagger$ FOR A BIPARTITE GRAPH

In order to estimate the modified Hosoya index of a bipartite graph, we need the following:

Lemma 3. *Let G be a connected bipartite graph with n vertices and m edges and the first Zagreb index δ. Then $\delta \le mn$, and equality holds if and only if G is a complete bipartite graph.*

Proof. Let $\mathcal{E}$ be the edge set of G. For any edge $uv \in \mathcal{E}$, $d_u + d_v \le n$. Then $\delta = \sum_{j=1}^{n} (d_j)^2 = \sum_{uv \in \mathcal{E}} (d_u + d_v) \le mn$. Equality holds if and only if $d_u + d_v = n$ for any $uv \in \mathcal{E}$, i. e., if G is a complete bipartite graph. □

A 2-(v, k, λ)-design is a collection of k-subsets or blocks of a set of v points, such that each 2-set of the points lies in exactly λ blocks. If $b = v$, then the design is called *symmetric*. The *incidence matrix* of a 2-(v, k, λ)-design is a $v \times b$ matrix $B = [b_{ij}]$, where $b_{ij} = 1$ if the i-th point is contained in the j-th block, and $b_{ij} = 0$ otherwise. The *incidence graph* of a design is defined to be the graph with adjacency matrix $\left[\begin{smallmatrix} O & B \\ B^T & O \end{smallmatrix}\right]$. If $v > k > \lambda > 0$ (when, by Fisher's inequality, $b \ge v$), then the incidence graph of a 2-(v, k, λ)-design has eigenvalues $\sqrt{rk}$, $\sqrt{r-\lambda}$, 0, $-\sqrt{r-\lambda}$, $-\sqrt{rk}$ with multiplicities $1, v-1, b-v, v-1$ and 1, respectively, where $r = bk/v$; for more details see [18].

Recall that the spectrum of a bipartite graph is symmetric w. r. t. the origin.

Theorem 4. *If G is a bipartite graph with $n \ge 3$ vertices, $m \ge 1$ edges and first Zagreb index δ, then*

$$Z^{\dagger}(G) \le \left(1 + \frac{\delta}{n}\right) \left(1 + \frac{2mn - 2\delta}{n(n-2)}\right)^{(n-2)/2} . \tag{4}$$

Equality in (4) holds if and only if G is either $\frac{n}{2} K_2$ or $K_{r,n-r}$ with $1 \le r \le n/2$ or the incidence graph of a symmetric 2-(v, k, λ)-design with $v > k = 2m/n$ and $\lambda = k(k-1)/(v-1)$.

Proof. By the arithmetic–geometric–mean inequality and $2\lambda_1^2 + \sum_{j=2}^{n-1} \lambda_j^2 = 2m$, we have

$$\prod_{j=2}^{n-1} (1 + \lambda_j^2) \le \left(\frac{1}{n-2} \sum_{j=2}^{n-1} (1 + \lambda_j^2)\right)^{n-2} = \left(1 + \frac{2m - 2\lambda_1^2}{n-2}\right)^{n-2} .$$

Hence

$$Z^{\dagger}(G) \le (1 + \lambda_1^2) \left(1 + \frac{2m - 2\lambda_1^2}{n-2}\right)^{(n-2)/2} .$$

Note that the function

$$H(x) = (1 + x^2) \left(1 + \frac{2m - 2x^2}{n-2}\right)^{(n-2)/2}$$

decreases for $\sqrt{2m/n} \le x \le \sqrt{m}$, and that $\sqrt{2m/n} \le \sqrt{\delta/n} \le \lambda_1$. Therefore, $H(\lambda_1) \le H\left(\sqrt{\delta/n}\right)$. This proves (4).

It is easy to check that if G is one of the graphs given in the second part of Theorem 4, then equality in (4) holds.

Conversely, if equality in (4) holds, then by the above argument, we see that $\lambda_1 = \sqrt{\delta/n}$. It follows that G is a semiregular bipartite graph. Since equality holds in the arithmetic–geometric–mean inequality given above, we have $|\lambda_j| = \sqrt{(2m - 2\lambda_1^2)/(n-2)}$ for $2 \le j \le n-1$. Hence we have the following possibilities: either

(i) G has two eigenvalues with equal absolute values and then $G = m\,K_2$, or

(ii) G has three distinct eigenvalues, i. e., $\lambda_j = 0$ for $2 \le j \le n-1$, and then $\delta/n = \lambda_1^2 = m$ and by Lemma 3, $G = K_{r,n-r}$ with $1 \le r \le n/2$, or

(iii) G has four distinct eigenvalues, in which case, since 0 is not an eigenvalue and G is bipartite semiregular, G is regular and connected, $\lambda_1 = 2m/n > \sqrt{(2m - 2\lambda_1^2)/(n-2)}$ and therefore G is the incidence graph of a symmetric 2-$(v, 2m/n, \lambda)$-design [19]. □

Remark 5. As in Remark 2, $\sqrt{\delta/n} \ge 2m/n$ and $H(x)$ decreases for $\sqrt{2m/n} \le x \le \sqrt{m}$. Then for a bipartite graph G,

$$Z^{\dagger}(G) \le H\left(\sqrt{\delta/n}\right) \le H(2m/n)\ .$$

Hence for bipartite graphs a better (n,m)-type upper bound for $Z^{\dagger}(G)$ is obtained.

When the number of vertices is odd, we have the following improvement of Theorem 4:

Theorem 6. *Let G be a bipartite graph with $n \ge 5$ vertices, $m \ge 1$ edges and first Zagreb index δ, where n is odd.*

1. *If $\delta/n \ge 2m/(n-1)$, then*

$$Z^{\dagger}(G) \le \left(1 + \frac{\delta}{n}\right)\left(1 + \frac{2mn - 2\delta}{n(n-3)}\right)^{(n-3)/2} \tag{5}$$

and equality holds if $G = K_{r,n-r}$ with $1 \le r < n/2$ or G is the incidence graph of a 2-(v,k,λ)-design with $k > \lambda = \dfrac{k(k-1)}{v(v-1)}(v+1)$.

2. *If $\delta/n < 2m/(n-1)$, then $Z^{\dagger}(G) \le 2^m$, and equality holds if G is the disjoint union of mK_2 and $(n-2m)K_1$ with $1 \le m < n/2$.*

Proof. Let $p = (n-1)/2$. Then $\lambda_{p+1} = 0$ and $\sum_{j=1}^{p} \lambda_j^2 = m$. By the arithmetic-geometric-mean inequality and $\sum_{j=1}^{p} \lambda_j^2 = m$,

$$Z^\dagger(G) \leq (1+\lambda_1^2)\left(\frac{1}{p-1}\sum_{j=2}^{p}(1+\lambda_j^2)\right)^{p-1} = (1+\lambda_1^2)\left(1+\frac{2m-2\lambda_1^2}{n-3}\right)^{(n-3)/2}.$$

There are two cases:

Case 1: $\delta/n \geq 2m/(n-1)$. Since the function

$$I(x) = (1+x^2)\left(1+\frac{2m-2x^2}{n-3}\right)^{(n-3)/2}$$

decreases for $\sqrt{2m/(n-1)} \leq x \leq \sqrt{m}$ and $\sqrt{2m/(n-1)} \leq \sqrt{\delta/n} \leq \lambda_1$, we see that $I(\lambda_1) \leq I\left(\sqrt{\delta/n}\right)$. This proves (5), and equality in (5) holds if and only if G is a semiregular bipartite graph with $\lambda_2 = \cdots = \lambda_p$. Hence equality in (5) holds if $G = K_{r,n-r}$ with $1 \leq r < n/2$ or G is the incidence graph of a 2-(v,k,λ)-design with $k > \lambda = \dfrac{k(k-1)}{v(v-1)}(v+1)$.

Case 2: $\delta/n < 2m/(n-1)$. Then $2m \leq n-1$ [15]. Delete any $n-2m$ isolated vertices from G to get a graph G_1. We have $Z^\dagger(G) = Z^\dagger(G_1) \leq H(1) = 2^m$, and it is easy to see that $Z^\dagger(G) = 2^m$ if G is the disjoint union of $m\,K_2$ and $(n-2m)\,K_1$ with $1 \leq m < n/2$. □

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