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The second Zagreb index of acyclic conjugated molecules *

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Abstract

The second Zagreb index $M_2(G)$ of a (molecule) graph G is the sum of the weights $d(u)d(v)$ of all edges uv in G, where $d(u)$ denotes the degree of the vertex u. In this paper, we give a sharp upper bound on the second Zagreb index of conjugated trees (trees with a perfect matching) in terms of the number of vertices. A sharp upper bound on the second Zagreb index of trees with a given size of matching is also given.

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1 Introduction

For a molecular graph G, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined in [6] as

$$M_1(G) = \sum_{u \in V(G)} (d(u))^2, \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v),$$

where $d(u)$ denotes the degree of the vertex u of G. The research background of Zagreb index together with its generalization appears in chemistry or mathematical chemistry. The readers is referred to literatures [1] [4] [5] [8] [9] [12] [14] and the references therein.

Recently, finding bounds for the topological index of graphs, as well as related problem of finding the graphs with maximum or minimum value of the respective index, attracted the attention of many researchers and many results were obtained (see [3] [10] [16]–[18]). Zhou [17] presented sharp upper bounds for the Zagreb indices M_1 and M_2 of a graph, especially for triangle-free graphs, in terms of the number of vertices and the number of edges. Additionally, sharp upper and lower bounds on the second Zagreb index of trees and unicyclic graphs with n vertices and k pendant vertices were respectively given in [11] and [15], in terms of n and k.

In this paper we confined ourselves to conjugated trees (trees with a perfect matching). A sharp upper bound on the second Zagreb index of trees with a given size of matching is given, and the corresponding extremal graphs are characterized.

2 Definitions and notations

We only consider finite, undirected and simple graphs. For undefined terminology and notations, the readers are referred to [2]. A connected acyclic graph is called a *tree*. The sets of vertices and edges of a tree T are denoted by $V(T)$ and $E(T)$, respectively. For a vertex x of a tree T, we denote the *neighborhood* and the *degree* of x by $N_T(x)$ and $d_T(x)$, respectively. The *maximum degree* of T is denoted by $\Delta(T)$. A *pendant vertex* is a vertex with degree one. We denote the set of pendant vertices in T by $PV(T)$. We will use $T - xy$ ($T - x$, respectively) to denote the graph that arises from T by deleting the edge $xy \in E(T)$ (the vertex $x \in V(G)$, respectively).

Let $P_T(u, v)$ be the path in T starting from u to v. The *distance* between u and v in T, denoted by $d_T(u, v)$, is the length of $P_T(u, v)$. Namely, $d_T(u, v) = |E(P_T(u, v))|$. The *diameter* of T is the maximum distance between two vertices of T, denoted by $diam(T)$. If $u \in V(T)$ satisfies $d_T(w, u) = \max\{d_T(v, u) : v \in V(T)\} = diam(T)$, we call u a *peripheral vertex* of T. It is easy to see that a peripheral vertex of T must be a pendant vertex. A subset $M \subseteq E(T)$ is called a *matching* in T if no two elements in M are adjacent. If some edge of M is incident with a vertex v, v is said to be *M-saturated*, or *M saturates v*. If every vertex of T is M-saturated, the matching M is *perfect*. A matching M is said to be an *m-matching*, if $|M| = m$ and for every matching M' in T, $|M'| \leq m$. From this definition, it is evident that if M is an m-matching, then M is a maximum matching in T.

Let n and m be positive integers with $n \geq 2m$. Let T_m^n be a tree on n vertices obtained from the star graph S_{n-m+1} by attaching a pendant edge to each of certain $m-1$ non-central vertices of S_{n-m+1}. Obviously, T_m^n is a tree on n vertices with an m-matching.

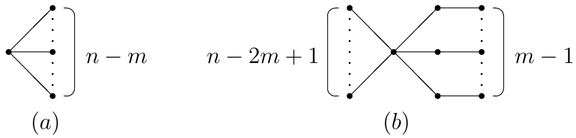

Figure 1. (a) the star graph S_{n-m+1}; (b) T_m^n

3 Main results

We first give some lemmas that will be used in the proof of our theorems.

Lemma 3.1 *Let T be a tree. If $u, w \in V(T)$ and $d_T(w,u)$ is maximum, then w is a pendant vertex.*

Proof. By contradiction. If w is not a pendant vertex, then there exists $z \in N_T(w)$ such that $d_T(z,u) = d_T(w,u) + 1 > d_T(w,u)$, contradicting that $d_T(w,u)$ is maximum. $\square$

Lemma 3.2 *Let T be a tree with a perfect matching. If $u, w \in V(T)$ and $d_T(w,u)$ is maximum, then w is adjacent to a vertex with degree two.*

Proof. By Lemma 3.1, we have that w is a pendant vertex, so w has the unique neighbor x. If $d_T(x) \neq 2$, then we have $d_T(x) \geq 3$, which means that there exists $y \in N_T(x)$ such that $d_T(y,u) = d_T(w,u)$. By Lemma 3.1, we have that y is a pendant vertex. Since T has a perfect matching and both w and y are pendant vertices, we have $wx, yx \in M$, which yields a contradiction. $\square$

From the proof above, we also have the following simple result.

Lemma 3.3 *Let T be a tree with a perfect matching and $v \in V(T)$. Then $|N_T(v) \cap PV(T)| \leq 1$.*

Denote

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

Theorem 3.4 *Let T be a tree on $2m$ vertices with a perfect matching. Then*

$$M_2(T) \leq f(2m, m)$$

with equality holds if and only if $T \cong T_m^{2m}$.

Proof. By induction on m. If $m = 1$, $M_2(T) = 1 \leq f(2,1)$.

Suppose the theorem true for all trees on fewer than $2m$ vertices with a perfect matching. Let T be a tree on $2m \geq 4$ vertices with a perfect matching M. Let u be a peripheral vertex and $d_T(w,u) = \max\{d_T(v,u) : v \in V(T)\}$. Since T has a perfect matching and $n \geq 4$, we have $d_T(w,u) \geq 3$ (Note that $d_T(w,u) = 3$ only if $T = P_4 = T_2^4$ holds). By Lemma 3.1, we have that w is a pendant vertex. Let $wx \in E(T)$. By lemma 3.2, let $N_T(x) = \{y, w\}$, where $y \in P_T(u,x)$, and $N_T(y) = \{y_1, y_2, \ldots, y_s, z\}$, where $z \in P_T(u,y)$ and $y_1 = x$ (Note that if $z = u$, then $T = P_4 = T_2^4$).

We distinguish two cases:

Case 1. $yz \in M$.

Then $N_T(y) \setminus \{z\} \cap PV(T) = \emptyset$. Otherwise, there exists a vertex $v \in N_T(y) \setminus \{z\} \cap PV(T)$ such that v is not M-saturated, which contradicts that M is a perfect matching of T. Then we have $d_T(y_i) \geq 2$, $1 \leq i \leq s$. By Lemma 3.1, we have $N_T(y_i) \setminus \{y\} \subset PV(T)$, $1 \leq i \leq s$. Combined with Lemma 3.3, we have $d_T(y_i) = 2$, $1 \leq i \leq s$. Let $N(y_i) \setminus \{y\} = \{w_i\}$, $1 \leq i \leq s$, where $w_1 = w$. Note that $y_i w_i \in M$, $1 \leq i \leq s$. Let $T^* = T - y_1 - w_1$. Then T^* is a tree on $2m-2$ vertices with a perfect matching. By induction hypothesis, we have $M_2(T^*) \leq f(2m-2, m-1)$. Moreover,

$d_T(z) + d_T(y) + \sum\limits_{i=1}^{s}(d_T(y_i) + d_T(w_i)) = d_T(z) + (1+s) + 3s \leq \sum\limits_{i=1}^{n} d_T(v_i) = 2(n-1) = 4m-2$. Then

$$\begin{aligned} M_2(T) &= M_2(T^*) + d_T(z) + \sum_{i=2}^{s} d_T(y_i) + 2d_T(y) + 2 \\ &= M_2(T^*) + d_T(z) + 2(s-1) + 2(s+1) + 2 \\ &\leq f(2m-2, m-1) + d_T(z) + 2(s-1) + 2(s+1) + 2 \\ &= f(2m, m) - 4m + 1 + d_T(z) + 4s + 2 \\ &\leq f(2m, m), \end{aligned}$$

with the equality holds only if $M_2(T^*) = f(2m-2, m-1)$ and $V(T) = \{z, y\} \cup \bigcup\limits_{i=1}^{s} \{y_i, w_i\}$, which implies that $z = u$, $s = 1$ and $T^* = T_1^2$. So we have $T \cong T_2^4$.

Case 2. $yz \notin M$.

Then there exists $z' \in N_T(z)$ and $y_i \in N_T(y)$ ($i \neq 1$) such that $zz' \in M$ and $yy_i \in M$. Without loss of generality, we may assume that $yy_s \in M$. Then we claim that y_s is a pendant vertex. Otherwise, there exists vertex $y_s' \in N_T(y_s) \setminus \{y\}$. By Lemma 3.1, y_s' is a pendant vertex. Since T has a perfect matching, we have $y_s' y_s \in M$, which contradicts $yy_s \in M$. By Lemma 3.3 and a similar reasoning as in the proof of case 1, we have $d_T(y_i) = 2$, $1 \leq i \leq s-1$. Let $N(y_i) \setminus \{y\} = \{w_i\}$, $1 \leq i \leq s-1$, where $w_1 = w$. Note that $y_i w_i \in M$, $1 \leq i \leq s-1$. Let $T^* = T - y_1 - w_1$. Then T^* is a tree on $2m-2$ vertices with a perfect matching. By induction hypothesis, we have $M_2(T^*) \leq f(2m-2, m-1)$. Moreover, $1 + d_T(z) + (1+s) + 3(s-1) + 1 \leq d_T(z') + d_T(z) + d_T(y) + \sum\limits_{i=1}^{s-1}(d_T(y_i) + d_T(w_i)) + d_T(y_s) \leq \sum\limits_{i=1}^{n} d_T(v_i) = 2(n-1) = 4m-2$. Then

$$\begin{aligned} M_2(T) &= M_2(T^*) + d_T(z) + \sum_{i=2}^{s-1} d_T(y_i) + d_T(y_s) + 2d_T(y) + 2 \\ &= M_2(T^*) + d_T(z) + 2(s-2) + 1 + 2(s+1) + 2 \\ &\leq f(2m-2, m-1) + d_T(z) + 4s + 1 \\ &= f(2m, m) - 4m + 1 + d_T(z) + 4s + 1 \\ &\leq f(2m, m), \end{aligned}$$

with the equality holds only if $M_2(T^*) = f(2m-2, m-1)$, $d_T(z') = 1$ and $V(T) = \{z', z, y, y_s\} \cup \bigcup_{i=1}^{s-1} \{y_i, w_i\}$, which implies that $T^* \cong T_{m-1}^{2m-2}$ and $T \cong T_m^{2m}$. $\square$

In the following, by $\mathcal{T}_{n,m}$ we denote the set of trees on n vertices with an m-matching, i.e., $\mathcal{T}_{n,m} = \{T : T \text{ is a tree on } n \text{ vertices with an } m\text{-matching}\}$.

Theorem 3.5 *Let $T \in \mathcal{T}_{n,m}$. Then*

$$M_2(T) \leq f(n, m),$$

with equality holds if and only if $T \cong T_m^n$.

Proof. By induction on n. If $n = 2m$, then the theorem is true by Theorem 3.4.

Now suppose the theorem true for all trees on fewer than n vertices and $n > 2m$. Let T be a tree on n vertices with an m-matching M. Let u be a peripheral vertex satisfying $d_T(w, u) = \max\{d_T(v, u) : v \in V(T)\}$. If $d_T(w, u) \leq 2$, then $T = T_1^n$, which means $M_2(T) = f(n, 1)$. Thus we may assume $d_T(w, u) \geq 3$. By Lemma 3.1, we have that w is a pendant vertex. Let $wx \in E(T)$ and $N_T(x) = \{y, x_1, x_2, \ldots, x_s\}$ $(s \geq 1)$, where $y \in P_T(u, x)$ and $x_1 = w$. Note that x_i is a pendant vertex, $1 \leq i \leq s$.

We distinguish two cases.

Case 1. $xy \in M$.

Then x_1 is not M-saturated. Since let $T^* = T - x_1$. Then $T^* \in \mathcal{T}_{n-1,m}$. By induction hypothesis, we have $M_2(T^*) \leq f(n-1, m)$. Moreover, we have $2(n-1) = \sum_{i=1}^{n} d_T(v_i) > d_T(y) + d_T(x) + \sum_{i=1}^{s} d_T(x_i) + m - 1 = d_T(y) + (1+s) + s + m - 1 = d_T(y) + 2s + m$ (Note that for each matching in $T - \{y, x, x_1, x_2, \ldots, x_s\}$, there are at least $m-1$ edges). Then

$$\begin{aligned} M_2(T) &= M_2(T^*) + d_T(y) + \sum_{i=2}^{s} d_T(x_i) + d_T(x) \\ &= M_2(T^*) + d_T(y) + (s-1) + (s+1) \\ &\leq f(n-1, m) + d_T(y) + 2s \\ &= f(n, m) - 2(n-1) + m + d_T(y) + 2s \\ &< f(n, m). \end{aligned}$$

Case 2. $xy \notin M$.

Since M is the maximum matching in T, there exists $x_i \in N_T(x)$ such that $xx_i \in M$. Without loss of generality, we may assume that $xx_1 \in M$.

Subcase 2.1. $s = 1$.

If $d_T(y) = 2$, let $N_T(y) = \{x, z\}$, where $z \in P_T(u, y)$. Note that if $z = u$, then $T = P_4 = T_2^4$. So we may assume that $z \neq u$. Let $T^* = T - \{x_1, x\}$. Then $T^* \in \mathcal{T}_{n-2,m-1}$. By induction hypothesis, we have $M_2(T^*) \leq f(n-2, m-1)$. Moreover, we have $2(n-1) =$

$\sum_{i=1}^{n} d_T(v_i) > d_T(z) + d_T(y) + d_T(x) + d_T(x_1) = d_T(z) + 5$, since $d_T(w, u) \geq 4$. Then

$$\begin{aligned} M_2(T) &= M_2(T^*) + d_T(z) + 4 + 2 \\ &\leq f(n-2, m-1) + d_T(z) + 6 \\ &= f(n, m) - 2(n-1) - n + 2m - 1 + d_T(z) + 6 \\ &= f(n, m) - 2(n-1) - (n - 2m) + d_T(z) + 5 \\ &< f(n, m). \end{aligned}$$

Now suppose that $d_T(y) \geq 3$. Let $N_T(y) = \{x, z, y_1, \ldots, y_t\}$ $(t \geq 1)$, where $z \in P_T(u, y)$. Note that if $z = u$, then y_i is a pendant vertex, $1 \leq i \leq t$. Then $T = T_2^n$. So we may assume that $z \neq u$ and $zz' \in E(T)$. Let $T^* = T - \{x_1, x\}$. Then $T^* \in \mathcal{T}_{n-2,m-1}$. By induction hypothesis, we have $M_2(T^*) \leq f(n-2, m-1)$. Moreover, we have $2(n-1) = \sum_{i=1}^{n} d_T(v_i) \geq d_T(z') + d_T(z) + d_T(y) + \sum_{i=1}^{t} d_T(y_i) + d_T(x) + d_T(x_1) + m - 3 \geq 1 + d_T(z) + (2 + t) + \sum_{i=1}^{t} d_T(y_i) + 2 + 1 + m - 3 = d_T(z) + \sum_{i=1}^{t} d_T(y_i) + t + m + 3$, since there are at least $m - 3$ M-saturated vertices in $V(T) - \{x_1, x, y, z, z', y_1, y_2, \ldots, y_t\}$. We also have $n = |V(T)| \geq |\{x_1, x, y, z, z', y_1, y_2, \ldots, y_t\}| + m - 3 = t + m + 2$. Then

$$\begin{aligned} M_2(T) &= M_2(T^*) + d_T(z) + \sum_{i=1}^{t} d_T(y_i) + 2(t+2) + 2 \\ &\leq f(n-2, m-1) + d_T(z) + \sum_{i=1}^{t} d_T(y_i) + 2t + 6 \\ &= f(n, m) - 2(n-1) - n + 2m - 1 + d_T(z) + \sum_{i=1}^{t} d_T(y_i) + 2t + 6 \\ &= f(n, m) - 2(n-1) + d_T(z) + \sum_{i=1}^{t} d_T(y_i) + t + m + 3 + (t + m + 2 - n) \\ &\leq f(n, m)\ . \end{aligned}$$

Equalities in the above expressions hold only if $M_2(T^*) = f(n-2, m-1)$, $d_T(z') = 1$ and $n = |\{x_1, x, y, z, z', y_1, y_2, \ldots, y_t\}| + m - 3$, which implies that $T^* \cong T_{m-1}^{n-2}$ and $T \cong T_m^n$.

Subcase 2.2. $s \geq 2$.

Then x_i is not M-saturated, $2 \leq i \leq s$. Since $d_T(w, u) \geq 3$, we have $yz \in E(T)$, where $z \in P_T(u, x_1)$. Let $T^* = T - x_2$. Then $T^* \in \mathcal{T}_{n-1,m}$. By induction hypothesis, we have $M_2(T^*) \leq f(n-1, m)$. Moreover, we have $2(n-1) = \sum_{i=1}^{n} d_T(v_i) > d_T(z) + d_T(y) + d_T(x) + \sum_{i=1}^{s} d_T(x_i) + 2(m-2) = 1 + d_T(y) + (s+1) + s + 2m - 4 \geq d_T(y) + 2s + m$, since for each matching in $T - \{y, x, x_1, x_2, \ldots, x_s\}$, there are at least $m-2$ edges. Then

$$\begin{aligned} M_2(T) &= M_2(T^*) + d_T(y) + \sum_{i=3}^{s} d_T(x_i) + 1 + (s+1) \\ &\le f(n-1,m) + d_T(y) + s - 2 + 1 + s + 1 \\ &= f(n,m) - 2(n-1) + m + d_T(y) + 2s \\ &< f(n,m). \end{aligned}$$

This completes the proof of the theorem. □

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