

Research Article

## On quasi-tree graphs attaining the three largest Zagreb spectral radii

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### Abstract

Let  $G$  be a simple undirected graph with vertex set  $V(G) = \{v_0, v_1, \dots, v_{n-1}\}$ . Let  $d_i$  be the degree of the vertex  $v_i$  in  $G$  for  $i = 0, 1, \dots, n-1$ . The Zagreb matrix of  $G$  is the square matrix of order  $n$  whose  $(i, j)$ -entry is equal to  $d_i + d_j$  if the vertices  $v_i$  and  $v_j$  are adjacent, and 0 otherwise. The Zagreb spectral radius of  $G$  is the largest eigenvalue of the Zagreb matrix of  $G$ . In [P. Das, K. C. Das, S. Mondal, A. Pal, First zagreb spectral radius of unicyclic graphs and trees, *J. Comb. Optim.* **48** (2024) #5], extremal problems concerning the Zagreb spectral radius of trees were investigated. In this paper, we determine the quasi-tree graphs with the first three largest Zagreb spectral radii.

**Keywords:** Zagreb matrix; Zagreb spectral radius; quasi-tree graph.

**2020 Mathematics Subject Classification:** 05C05, 05C50.

## 1. Introduction

Let  $G$  be a simple undirected graph with vertex set  $V(G) = \{v_0, v_1, \dots, v_{n-1}\}$  and edge set  $E(G)$ . For  $v_i \in V(G)$ , we use  $d_G(v_i)$  and  $N_G(v_i)$  to denote the degree and the set of neighbors of  $v_i$  in  $G$ . The minimum degree and maximum degree of  $G$  are denoted by  $\delta(G)$  and  $\Delta(G)$ , respectively. If there is no confusion, we simply denote the above notation as  $d_i$ ,  $N_i$ ,  $\delta$  and  $\Delta$ . A connected graph  $G$  is called a quasi-tree graph if there exists a vertex  $v_0 \in V(G)$  such that  $G - v_0$  is a tree.

The adjacency matrix of the graph  $G$  is the  $n \times n$  symmetric matrix  $A(G) = (a_{ij})$  where

$$a_{ij} = \begin{cases} 1, & \text{if } v_i v_j \in E(G), \\ 0, & \text{otherwise.} \end{cases}$$

Since  $A(G)$  is symmetric, its eigenvalues  $\lambda_1(G), \lambda_2(G), \dots, \lambda_n(G)$  are real and can be written in descending order; that is,  $\lambda_1(G) \geq \lambda_2(G) \geq \dots \geq \lambda_n(G)$ . The largest eigenvalue  $\lambda_1(G)$  is called the spectral radius of  $G$ . On the basis of successful analyses of the adjacency matrix, the spectral radii of extended adjacency matrices (often constructed from topological indices) have been proposed and extensively studied. For example, the spectral radii of matrices such as the Randić matrix [4], the geometric–arithmetic matrix [10], the harmonic matrix [5], the ABC matrix [3], and the ABS matrix [8] have been thoroughly investigated.

Based on the classical first Zagreb index, Rad, Jahanbani, and Gutman [9] replaced the entry 1 in the adjacency matrix with the sum of the degrees of the corresponding vertices,  $d_i + d_j$ , thereby introducing the Zagreb matrix  $Z(G) = (z_{ij})$ , where

$$z_{ij} = \begin{cases} d_i + d_j, & \text{if } v_i v_j \in E(G), \\ 0, & \text{otherwise.} \end{cases}$$

The eigenvalues of the Zagreb matrix  $Z(G)$  are denoted by  $\rho_1(G) \geq \rho_2(G) \geq \dots \geq \rho_n(G)$ , where  $\rho_1(G)$  is called the Zagreb spectral radius of  $G$ . Subsequently, the study of the Zagreb spectral radius quickly attracted significant attention and stimulated extensive research within the research community.

In [1], Das established both lower and upper bounds for the Zagreb spectral radius in terms of the maximum and minimum degrees of graphs. Jahanbani, Khoelilar, and Shooshtari [6] derived a relation between the spectral radius of the Zagreb matrix and its trace. Shetty and Bhat [11] identified a novel correlation between the density and refractive index of  $n$ -alkanes and the Zagreb spectral radius. From the perspective of spectral extremal problems (an active and cutting-edge topic in graph theory), Das et al. [2] investigated the extremal values of the Zagreb spectral radius. They [2]

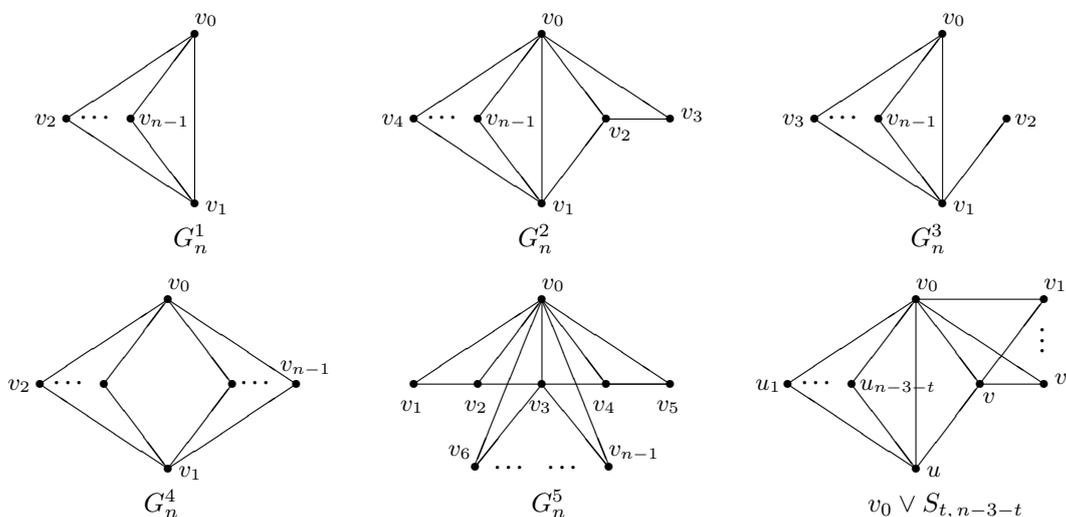
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established both upper and lower bounds for the Zagreb spectral radius of trees and unicyclic graphs, and characterized the extremal graphs that attain these bounds. Inspired by this, we investigate the extremal problems concerning the Zagreb spectral radius of quasi-tree graphs. Specifically, we characterize the graphs with the first three largest Zagreb spectral radii among all quasi-tree graphs on  $n$  vertices.

The remainder of this paper is organized as follows. In Section 2, we introduce essential concepts and notation, and establish several lemmas that will be used in the subsequent proofs. Section 3 provides the quasi-tree graphs with the three largest Zagreb spectral radii.

## 2. Preliminaries

We use  $G - u$  and  $G - e$  to denote the graphs that arise from  $G$  by deleting the vertex  $u \in V(G)$  and the edge  $e \in E(G)$ , respectively. Let  $QT(n, d_0)$  denote the set of all quasi-tree graphs on  $n$  vertices in which the degree of vertex  $v_0$  is  $d_0$ . Let  $K_{1, n-1}$  denote the star with  $n$  vertices. Denote by  $\text{diam}(G)$  the diameter of a graph  $G$ . The join of two graphs  $G$  and  $H$ , denoted by  $G \vee H$ , is a graph obtained from  $G$  and  $H$  by joining each vertex of  $G$  to all vertices of  $H$ . A double star graph  $S_{a, n-2-a}$  is a tree consisting of two central vertices connected by an edge, where these vertices have  $a$  and  $n - 2 - a$  neighbors of degree 1, respectively, with  $n - 3 \geq a \geq 1$ . The graph  $v_0 \vee S_{t, n-3-t}$  is shown in Figure 2.1.



**Figure 2.1:** The graph  $G_n^1, G_n^2, G_n^3, G_n^4, G_n^5$ , and  $v_0 \vee S_{t, n-3-t}$ .

**Lemma 2.1** (see [7]). *Let  $f(x, y)$  be an increasing function in both  $x$  and  $y$  for  $x \geq 1$  and  $y \geq 1$ . Define a matrix  $Af(G) = (w_{ij})$ , called the weighted adjacency matrix of a connected graph  $G$ , whose  $(i, j)$ -entry is  $w_{ij} = f(d_i, d_j)$  if  $v_i v_j \in E(G)$  and  $w_{ij} = 0$  otherwise. Let  $\theta_1(G)$  be the largest eigenvalue of  $Af(G)$ . Then  $\theta_1(G) > \theta_1(G - v_i v_j)$  and  $\theta_1(G) > \theta_1(G - v_i)$ .*

Let  $M$  be a complex matrix of order  $n$  described in the following block form:

$$M = \begin{pmatrix} M_{11} & \cdots & M_{1t} \\ \vdots & \ddots & \vdots \\ M_{t1} & \cdots & M_{tt} \end{pmatrix}, \tag{1}$$

where the blocks  $M_{ij}$  are  $n_i \times n_j$  matrices for any  $1 \leq i, j \leq t$  and  $n = \sum_{k=1}^t n_k$ . For  $1 \leq i, j \leq t$ , let  $b_{ij}$  denote the average row sum of  $M_{ij}$ , i.e.  $b_{ij}$  is the sum of all entries in  $M_{ij}$  divided by the number of rows. Then,  $B(M) = (b_{ij})$  is called the quotient matrix of  $M$ . In addition, if for each pair  $i, j$ , the block  $M_{ij}$  has a constant row sum, i.e.,  $M_{ij} \vec{e}_{n_i} = b_{ij} \vec{e}_{n_i}$ , then  $B(M)$  is called the equitable quotient matrix of  $M$ , where  $\vec{e}_k = (1, 1, \dots, 1)^T \in \mathbb{C}^k$  and  $\mathbb{C}$  denotes the field of complex numbers. Let  $\sigma(M)$  denote the spectrum of a square matrix  $M$  including algebraic multiplicity.

**Lemma 2.2** (see [13]). *Let  $M$  be the matrix defined via (1) such that  $M_{ij} = s_{ij} J_{n_i, n_j}$ , for  $i \neq j$ , and  $M_{ii} = s_{ii} J_{n_i, n_i} + p_i I_{n_i}$ . Then the equitable quotient matrix of  $M$  is  $B(M) = (b_{ij})$  with  $b_{ij} = s_{ij} n_j$  if  $i \neq j$ , and  $b_{ii} = s_{ii} n_i + p_i$ . Moreover,*

$$\sigma(M) = \sigma(B) \cup \left\{ p_1^{[n_1-1]}, \dots, p_t^{[n_t-1]} \right\},$$

where  $p_1^{[k]}$  indicates that  $p_1$  is an eigenvalue with algebraic multiplicity  $k$ .

**Lemma 2.3.** *Let  $n \geq 5$ ,  $G \in QT(n, n - 1)$ , and  $X$  be the unique positive unit eigenvector of  $\mathcal{Z}(G)$  corresponding to  $\rho_1(G)$ , and denote by  $x_v$  the entry of  $X$  corresponding to vertex  $v$ . Let  $u, v \in V(G - v_0)$ ,  $uv \in E(G)$  and  $G^* = G - vv_j + uv_j$ ,  $v_j \in N_G(v) - \{v_0\}$ . If  $d_G(u) \geq 3$ ,  $d_G(v) \geq 3$ , and  $x_u \geq x_v$ , then  $\rho_1(G) < \rho_1(G^*)$ .*

**Proof.** Let  $X$  be the unique positive unit eigenvector of  $\mathcal{Z}(G)$  corresponding to  $\rho_1(G)$ . Since  $d_G(u) \geq 3$ ,  $d_G(v) \geq 3$  and  $x_u \geq x_v$ , by Rayleigh’s principle, we have

$$\begin{aligned} \rho_1(G^*) - \rho_1(G) &\geq X^T(\mathcal{Z}(G^*) - \mathcal{Z}(G))X \\ &= 2x_u x_0(d_u + d_v + n - 3) + 2x_v x_0(n + 1) \\ &\quad + 2x_u \sum_{u_i \in N_G(u) - \{v, v_0\}} (d_u + d_v + d_i - 2)x_i + 2x_u \sum_{v_j \in N_G(v) - \{u, v_0\}} (d_u + d_v + d_j - 2)x_j \\ &\quad - \left[ 2x_u x_0(d_u + n - 1) + 2x_v x_0(d_v + n - 1) \right. \\ &\quad \left. + 2x_u \sum_{u_i \in N_G(u) - \{v, v_0\}} (d_u + d_i)x_i + 2x_v \sum_{v_j \in N_G(v) - \{u, v_0\}} (d_v + d_j)x_j \right] \\ &= 2(x_u - x_v) \left[ x_0(d_v - 2) + \sum_{v_j \in N_G(v) - \{u, v_0\}} (d_v + d_j)x_j \right] \\ &\quad + 2x_u \left[ (d_u - 2) \sum_{v_j \in N_G(v) - \{u, v_0\}} x_j + (d_v - 2) \sum_{u_i \in N_G(u) - \{v, v_0\}} x_i \right] \\ &> 0. \end{aligned}$$

Thus,  $\rho_1(G^*) - \rho_1(G) > 0$ . □

**Lemma 2.4.** *Consider the graph  $v_0 \vee S_{t, n-3-t}$  shown in Figure 2.1 for  $n \geq 7$  and  $1 \leq t \leq \lfloor \frac{n-4}{2} \rfloor$ . Then,*

$$\rho_1\left(v_0 \vee S_{\lfloor \frac{n-4}{2} \rfloor, \lceil \frac{n-2}{2} \rceil}\right) < \dots < \rho_1(v_0 \vee S_{2, n-5}) < \rho_1(v_0 \vee S_{1, n-4}).$$

**Proof.** Let  $G_t = v_0 \vee S_{t, n-3-t}$  for  $1 \leq t \leq \lfloor \frac{n-4}{2} \rfloor$  and  $n \geq 7$ . Then, we have

$$\mathcal{Z}(G_t) = \begin{pmatrix} 0 & n+t+1 & 2n-2-t & n+1 & \cdots & n+1 & n+1 & \cdots & n+1 \\ n+t+1 & 0 & n+1 & t+4 & \cdots & t+4 & 0 & \cdots & 0 \\ 2n-2-t & n+1 & 0 & 0 & \cdots & 0 & n-t+1 & \cdots & n-t+1 \\ n+1 & t+4 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & 0 \\ n+1 & t+4 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ n+1 & 0 & n-t+1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ n+1 & 0 & n-t+1 & 0 & \cdots & 0 & 0 & \cdots & 0 \end{pmatrix}.$$

It can be written in the form of the following block matrix:

$$\mathcal{Z}(G_t) = \begin{pmatrix} 0 & n+t+1 & 2n-2-t & (n+1)J_{1,t} & (n+1)J_{1, n-t-3} \\ n+t+1 & 0 & n+1 & (t+4)J_{1,t} & 0_{1, n-t-3} \\ 2n-2-t & n+1 & 0 & 0_{1,t} & (n-t+1)J_{1, n-t-3} \\ (n+1)J_{t,1} & (t+4)J_{t,1} & 0_{t,1} & 0_t & 0_{t, n-t-3} \\ (n+1)J_{n-t-3,1} & 0_{n-t-3,1} & (n-t+1)J_{n-t-3,1} & 0_{n-t-3,t} & 0_{n-t-3} \end{pmatrix}.$$

Then, the corresponding quotient matrix of  $\mathcal{Z}(G_t)$  is

$$B(G_t) = \begin{pmatrix} 0 & n+t+1 & 2n-2-t & (n+1)t & (n+1)(n-t-3) \\ n+t+1 & 0 & n+1 & (t+4)t & 0 \\ 2n-2-t & n+1 & 0 & 0 & (n-t+1)(n-t-3) \\ n+1 & t+4 & 0 & 0 & 0 \\ n+1 & 0 & n-t+1 & 0 & 0 \end{pmatrix}.$$

By Lemma 2.2, we have  $\sigma(G_t) = \sigma(B(G_t)) \cup \{0^{[n-5]}\}$ . Thus, the characteristic polynomial of  $G_t$  is

$$\begin{aligned} \Phi(G_t, x) &= x^{n-5} \det(xI - B(G_t)) \\ &= x^{n-5} [x^5 - [2n^3 + (4 - 3t)n^2 + (3t^2 - 14)n + 9t^2 + 27t]x^3 \\ &\quad - 2(n+1)[2n^3 - (4 + 5t)n^2 + (5t^2 + 15t - 2)n + 4]x^2 \\ &\quad + t(n-t-3)[n^4 - (2t-5)n^3 + (3t^2 + 7t + 29)n^2 \\ &\quad - (2t^3 + 7t^2 - 12t - 95)n + t^4 + 6t^3 - 6t^2 - 45t + 6]x \\ &\quad + 4t(t+4)(n+1)(4n-3t+nt-t^2-4)(n-t-3)(n-t+1)]. \end{aligned}$$

Let  $\Phi(G_t, x) = x^{n-5} f_t(x)$ . Since

$$\begin{aligned} f_{t+1}(x) - f_t(x) &= 3(n+3)(n-2t-4)x^3 + 10n(n+1)(n-2t-4)x^2 \\ &\quad + (n-2t-4)[n^4 + (3-4t)n^3 + (7t^2 + 21t + 39)n^2 \\ &\quad - (6t^3 + 29t^2 + 3t - 98)n + 3t^4 + 24t^3 + 31t^2 - 68t - 38]x \\ &\quad + 4(n+1)(n-2t-4)[(3t^2 + 19t + 25)n^2 \\ &\quad - (6t^3 + 43t^2 + 89t + 40)n + 3t^4 + 24t^3 + 61t^2 + 52t] \\ &> 3(n+3)(n-2t-4)x^3 + 10n(n+1)(n-2t-4)x^2 \\ &\quad + (n-2t-4)[n^2(n-2t)^2 + (3t^2n + 21tn + 39n)(n-2t) + (98n - 68t - 38)]x \\ &\quad + 4(n+1)(n-2t-4)^2(3t^2n + 19tn + 25n) \\ &> 0 \end{aligned}$$

for  $x > 0$ , we have  $\rho_1(G_{t+1}) < \rho_1(G_t)$  for  $1 \leq t \leq \lfloor \frac{n-4}{2} \rfloor$ . This implies that the Zagreb spectral radius of  $G_t$  is a decreasing function of  $t$ . Therefore, we have

$$\rho_1 \left( v_0 \vee S_{\lfloor \frac{n-4}{2} \rfloor, \lceil \frac{n-2}{2} \rceil} \right) < \dots < \rho_1(v_0 \vee S_{2,n-5}) < \rho_1(v_0 \vee S_{1,n-4}).$$

This completes the proof. □

### 3. Main results

**Theorem 3.1.** *Let  $n \geq 5$  and  $G \in QT(n, d_0)$ . Consider the graph  $G_n^1$  shown in Figure 2.1. Then,*

$$\rho_1(G) \leq \rho_1(G_n^1)$$

with equality if and only if  $G \cong G_n^1$ .

**Proof.** For any  $G \in QT(n, d_0)$ , by Lemma 2.1, we can conclude that there exist  $G' \in QT(n, n-1)$  such that  $\rho_1(G) \leq \rho_1(G')$ . For  $G' \in QT(n, n-1) \setminus \{G_n^1\}$ , by Lemma 2.2, we have  $\rho_1(G') < \rho_1(G_n^1)$ . Thus, we have  $\rho_1(G) \leq \rho_1(G_n^1)$  with equality if and only if  $G \cong G_n^1$ . □

**Theorem 3.2.** *Let  $n \geq 7$  and  $G \in QT(n, d_0) \setminus \{G_n^1\}$ . Then,  $\rho_1(G) \leq \rho_1(G_n^2)$  with equality if and only if  $G \cong G_n^2$ .*

**Proof.** Since  $G_n^2 \cong v_0 \vee S_{1,n-4}$ , by the proof of Lemma 2.4, we conclude that  $\rho_1(G_n^2)$  is the largest real root of the following polynomial:

$$f_1(x) = x^5 - (2n^3 + n^2 - 11n + 36)x^3 - (4n^4 - 14n^3 + 18n^2 + 44n + 8)x^2 + (n^5 - n^4 + 27n^3 - 58n^2 - 430n + 152)x + 100n^4 - 460n^3 + 80n^2 + 640n.$$

Now, we discuss the following three cases based on the diameter of  $G - v_0$  to prove that  $\rho_1(G_n^2)$  is the largest among  $G \in QT(n, d_0) \setminus \{G_n^1\}$ .

**Case 1.**  $\text{diam}(G - v_0) = 2$ .

In this case,  $G - v_0 \cong K_{1,n-2}$ . By Lemma 2.1, we only need to consider the Zagreb spectral radii of graphs  $G_n^3$  and  $G_n^4$ . Since  $G_n^4$  is the complete bipartite graph, by using Theorem 2.3 of [12], we have  $\rho_1(G_n^4) = n\sqrt{2n-4}$ . Using calculations similar to the ones done in the proof of Lemma 2.4, we obtain the characteristic polynomial of  $G_n^3$ , given as follows:

$$\Phi(G_n^3, x) = x^{n-4}[x^4 + (-2n^3 - n^2 + 17n - 6)x^2 + (-4n^4 + 14n^3 - 18n)x + n^5 - 3n^4].$$

Let  $\Phi(G_n^3, x) = x^{n-4}g(x)$ . Then  $\rho_1(G_n^3)$  is the largest root for  $g(x) = 0$ . By taking the derivative,  $g(x)$  is an increasing function on the interval  $[n\sqrt{2n-4}, +\infty)$ . Since

$$g(n\sqrt{2n-4}) = (-4\sqrt{2n-4} - 9)n^5 + (14\sqrt{2n-4} + 51)n^4 - 80n^3 + (24 - 18\sqrt{2n-4})n^2 < 0,$$

we have

$$\rho_1(G_n^3) > \rho_1(G_n^4) > n\sqrt{n-1}.$$

Next, we will prove that  $\rho_1(G_n^2) > \rho_1(G_n^3)$ . Note that  $K_{1,n-1}$  is a subgraph of  $G_n^2$ . By Lemma 2.1, we have

$$\rho_1(G_n^2) > \rho_1(K_{1,n-1}) = n\sqrt{n-1}.$$

Let

$$\begin{aligned} h(x) &= xg(x) - f_1(x) \\ &= (6n + 30)x^3 + (18n^2 + 26n + 8)x^2 + (-2n^4 - 27n^3 + 58n^2 + 430n - 152)x - 100n^4 + 460n^3 - 80n^2 - 640n. \end{aligned}$$

By taking the derivative, we observe that  $h(x)$  is an increasing function on the interval  $[n\sqrt{n-1}, +\infty)$ . Since

$$h(n\sqrt{n-1}) = n[18n^4 - 92n^3 + 442n^2 - 88n - 640 + (4n^4 - 3n^3 + 28n^2 + 430n - 152)(n-1)^{1/2}] > 0,$$

we have  $\rho_1(G_n^2) > \rho_1(G_n^3)$ .

**Case 2.**  $\text{diam}(G - v_0) = 3$ .

Here, we have  $G - v_0 \cong S_{t,n-3-t}$ . By Lemmas 2.1 and 2.4, we have

$$\rho_1(G_n^2) = \rho_1(v_0 \vee S_{1,n-4}) > \rho_1(G)$$

for  $G \in QT(n, d_0) \setminus \{G_n^2\}$ .

**Case 3.**  $\text{diam}(G - v_0) \geq 4$ .

Let  $G - v_0 = T$ . By Lemma 2.1, we have  $\rho_1(G) \leq \rho_1(v_0 \vee T)$ . By Lemma 2.2, we have  $\rho_1(v_0 \vee T) < \rho_1(G_n^2)$ .

Combining the above arguments, we have  $\rho_1(G) \leq \rho_1(G_n^2)$  with equality if and only if  $G \cong G_n^2$ . □

**Theorem 3.3.** *Let  $n \geq 9$  and  $G \in QT(n, d_0) \setminus \{G_n^1, G_n^2\}$ . Then,  $\rho_1(G) \leq \rho_1(G_n^3)$  with equality holds if and only if  $G \cong G_n^3$ .*

**Proof.** We discuss the following four cases based on the diameter of  $G - v_0$  to prove that  $\rho_1(G_n^3)$  is the largest among  $G \in QT(n, d_0) \setminus \{G_n^1, G_n^2\}$ .

**Case 1.**  $\text{diam}(G - v_0) = 2$ .

In this case,  $G - v_0 \cong K_{1,n-2}$ . By the proof of Theorem 3.2, we have  $\rho_1(G) < \rho_1(G_n^3)$ .

**Case 2.**  $\text{diam}(G - v_0) = 3$ .

By Lemma 2.4, we have  $\rho_1(G_n^2) > \rho_1(v_0 \vee S_{2,n-5})$ . Next, we will prove that  $\rho_1(G_n^3) > \rho_1(v_0 \vee S_{2,n-5})$ . Since  $K_{1,n-1}$  is a subgraph of  $G_n^3$ , by Lemma 2.1, we have  $\rho_1(G_n^3) > \rho_1(K_{1,n-1}) = n\sqrt{n-1}$ . By the proof of Lemma 2.4 and Theorem 3.2, we obtain

$$\begin{aligned} \Phi(v_0 \vee S_{2,n-5}, x) - \Phi(G_n^3, x) &= x^{n-5}[(3n^2 - 15n - 84)x^3 + (10n^3 - 68n^2 - 86n - 8)x^2 \\ &\quad + (n^5 - 5n^4 + 100n^3 - 400n^2 - 838n + 440)x \\ &\quad + 288n^4 - 2112n^3 + 3072n^2 + 2112n - 3360]. \end{aligned}$$

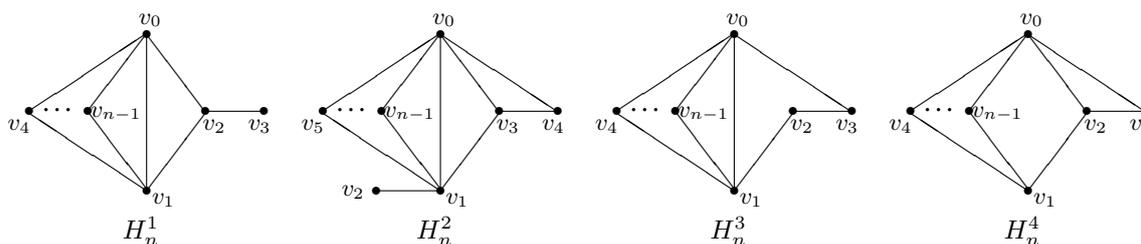
Let

$$\begin{aligned} p(x) &= (3n^2 - 15n - 84)x^3 + (10n^3 - 68n^2 - 86n - 8)x^2 + (n^5 - 5n^4 + 100n^3 - 400n^2 - 838n + 440)x \\ &\quad + 288n^4 - 2112n^3 + 3072n^2 + 2112n - 3360. \end{aligned}$$

Then  $p(x) > 0$  for  $x > 0$  and  $n \geq 9$ . Thus,  $\Phi(v_0 \vee S_{2,n-5}, x) - \Phi(G_n^3, x) > 0$ , that is,  $\rho_1(G_n^3) > \rho_1(v_0 \vee S_{2,n-5})$ .

It is evident that removing edge  $e$  from graph  $G_n^2$  yields a subgraph  $G_n^2 - e$  with exactly four possible configurations:  $H_n^1, H_n^2, H_n^3$  and  $H_n^4$ , as illustrated in Figure 3.1. By Lemma 2.2, we obtain the characteristic polynomials of  $H_n^1, H_n^2, H_n^3$  and  $H_n^4$  as follows:

$$\begin{aligned} \Phi(H_n^1, x) &= x^{n-5}[x^5 + (-2n^3 + 2n^2 + 12n - 34)x^3 + (-4n^4 + 20n^3 - 32n^2 + 12n + 8)x^2 \\ &\quad + (32n^3 - 64n^2 - 256n + 256)x + 64n^4 - 384n^3 + 512n^2], \\ \Phi(H_n^2, x) &= x^{n-6}[x^6 + (-2n^3 + 2n^2 + 14n - 44)x^4 \\ &\quad + (-4n^4 + 24n^3 - 50n^2 + 2n + 8)x^3 + (2n^5 - 9n^4 + 41n^3 - 110n^2 - 410n + 426)x^2 \\ &\quad + (110n^4 - 710n^3 + 990n^2 + 10n)x - 25n^5 + 175n^4 - 275n^3 + 125n^2], \\ \Phi(H_n^3, x) &= x^{n-5}[x^5 + (-2n^3 + 2n^2 + 16n - 32)x^3 + (-4n^4 + 24n^3 - 32n^2)x^2 \\ &\quad + (2n^5 - 7n^4 + 16n^3 - 32n^2 - 256n + 256)x - 8n^5 + 96n^4 - 384n^3 + 512n^2], \\ \Phi(H_n^4, x) &= x^{n-5}[x^5 + (-2n^3 + 7n^2 - 11n - 22)x^3 + (-10n^2 - 10n)x^2 \\ &\quad + (n^5 - 5n^4 + 59n^3 - 254n^2 + 226n - 104)x - 10n^3 + 50n^2 - 40n]. \end{aligned}$$



**Figure 3.1:** The graphs  $H_n^1, H_n^2, H_n^3$ , and  $H_n^4$ .

Next, we will prove that  $\rho_1(G_n^3) > \rho_1(H_n^i)$  for  $i = 1, 2, 3, 4$ . Note that  $K_{1,n-1}$  is a subgraph of  $G_n^3$ . By Lemma 2.1, we have

$$\rho_1(G_n^3) > \rho_1(K_{1,n-1}) = n\sqrt{n-1}.$$

Let

$$\begin{aligned} \Phi(H_n^1, x) - \Phi(G_n^3, x) &= x^{n-5}h_1(x), \\ \Phi(H_n^2, x) - \Phi(G_n^3, x) &= x^{n-6}h_2(x), \\ \Phi(H_n^3, x) - \Phi(G_n^3, x) &= x^{n-5}h_3(x), \\ \Phi(H_n^4, x) - \Phi(G_n^3, x) &= x^{n-5}h_4(x), \end{aligned}$$

where

$$\begin{aligned}
 h_1(x) &= (3n^2 - 5n - 28)x^3 + (6n^3 - 32n^2 + 30n + 8)x^2 \\
 &\quad + (-n^5 + 3n^4 + 32n^3 - 64n^2 - 256n + 256)x + 64n^4 - 384n^3 + 512n^2, \\
 h_2(x) &= (3n^2 - 3n - 38)x^4 + (10n^3 - 50n^2 + 20n + 8)x^3 \\
 &\quad + (n^5 - 6n^4 + 41n^3 - 110n^2 - 410n + 426)x^2 \\
 &\quad + (110n^4 - 710n^3 + 990n^2 + 10n)x - 25n^5 + 175n^4 - 275n^3 + 125n^2, \\
 h_3(x) &= (3n^2 - n - 26)x^3 + (10n^3 - 32n^2 + 18n)x^2 \\
 &\quad + (n^5 - 4n^4 + 16n^3 - 32n^2 - 256n + 256)x - 8n^5 + 96n^4 - 384n^3 + 512n^2, \\
 h_4(x) &= (8n^2 - 28n - 16)x^3 + (4n^4 - 14n^3 - 10n^2 + 8n)x^2 \\
 &\quad + (-2n^4 + 59n^3 - 254n^2 + 226n - 104)x - 10n^3 + 50n^2 - 40n.
 \end{aligned}$$

By taking the derivative, we note that  $h_i(x)$  ( $i = 1, 2, 3, 4$ ) is an increasing function on the interval  $[n\sqrt{n-1}, +\infty)$ , and

$$\begin{aligned}
 h_1(n\sqrt{n-1}) &= n(n-4)[6n^4 - 14n^3 + 70n^2 - 126n + (2n^4 + 3n^3 + 21n^2 + 48n - 64)(n-1)^{1/2}] > 0 \\
 h_2(n\sqrt{n-1}) &= n^2[4n^6 - 16n^5 + 18n^4 - 103n^3 - 163n^2 + 561n - 301 \\
 &\quad + (10n^4 - 50n^3)(n-1)^{3/2} + (130n^3 - 722n^2 + 982n + 10)(n-1)^{1/2}] > 0 \\
 h_3(n\sqrt{n-1}) &= n[10n^5 - 50n^4 + 146n^3 - 402n^2 + 512n \\
 &\quad + (4n^5 - 8n^4 - 9n^3 - 6n^2 - 256n + 256)(n-1)^{1/2}] > 0 \\
 h_4(n\sqrt{n-1}) &= n(n-4)[4n^5 - 2n^4 - 4n^3 + 2n^2 - 10n + 10 \\
 &\quad + 8n^3(n-1)^{3/2} + (2n^3 + 47n^2 - 50n + 26)(n-1)^{1/2}] > 0.
 \end{aligned}$$

Thus, we have  $\rho_1(G_n^3) > \rho_1(H_n^i)$  for  $i = 1, 2, 3, 4$ .

**Case 3.**  $\text{diam}(G - v_0) = 4$ .

By Lemma 2.1, we have  $\rho_1(G) \leq \rho_1(G^*)$  for  $G^* \in QT(n, n-1) \setminus \{G_n^5\}$  and  $\text{diam}(G^* - v_0) = 4$ . By Lemmas 2.3 and 2.4, we have

$$\rho_1(G^*) < \rho_1(v_0 \vee S_{t, n-3-t}) \leq \rho_1(v_0 \vee S_{2, n-5})$$

for  $t \geq 2$ . By Case 2, we have  $\rho_1(v_0 \vee S_{2, n-5}) < \rho_1(G_n^3)$ . Next, we will prove that  $\rho_1(G_n^3) > \rho_1(G_n^5)$ . Note that  $K_{1, n-1}$  is a subgraph of  $G_n^3$ . By Lemma 2.1, we have

$$\rho_1(G_n^3) > \rho_1(K_{1, n-1}) = n\sqrt{n-1}.$$

Also, we have

$$\begin{aligned}
 \Phi(G_n^5, x) - \Phi(G_n^3, x) &= x^{n-7} \left[ (3n^2 - 15n - 58)x^5 + (10n^3 - 64n^2 - 42n + 8)x^4 \right. \\
 &\quad + (n^5 - 5n^4 + 64n^3 - 182n^2 - 310n + 1015)x^3 \\
 &\quad + (200n^4 - 1440n^3 + 2940n^2 + 2340n - 1640)x^2 \\
 &\quad + (-50n^5 + 200n^4 - 350n^3 + 3300n^2 + 6500n - 1000)x \\
 &\quad \left. - 2500n^4 + 21000n^3 - 33500n^2 - 21000n + 36000 \right].
 \end{aligned}$$

Let

$$\Phi(G_n^5, x) - \Phi(G_n^3, x) = x^{n-7} h_5(x).$$

By taking the derivative, we observe that  $h_5(x)$  is an increasing function on the interval  $[n, +\infty)$ . Since

$$h_5(n) = n^8 + 8n^7 + 135n^6 - 1522n^5 - 212n^4 + 27655n^3 - 28640n^2 - 22000n + 36000 > 0,$$

for  $n \geq 8$ , we have  $\rho_1(G_n^3) > \rho_1(G_n^5)$ . Thus,  $\rho_1(G) < \rho_1(G_n^3)$  for  $G \in QT(n, d_0)$ .

**Case 4.**  $\text{diam}(G - v_0) \geq 5$ .

By Lemma 2.1, we have  $\rho_1(G) \leq \rho_1(G^\#)$  for  $G^\# \in QT(n, n-1)$  and  $\text{diam}(G^\# - v_0) \geq 5$ . From Lemmas 2.3 and 2.4, and Case 3, it follows that  $\rho_1(G^\#) < \rho_1(G_n^3)$ .

Combining the conclusions obtained in all four cases, we have  $\rho_1(G) \leq \rho_1(G_n^3)$  with equality if and only if  $G \cong G_n^3$ .  $\square$

## 4. Conclusion

In this work, we characterize quasi-tree graphs possessing the three largest Zagreb spectral radii. This finding naturally leads to a promising direction for further investigation: ordering specific families of graphs (particularly, chemical graphs) according to their Zagreb spectral radii.

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