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MAXIMIZING THE SPECTRAL RADIUS OF GENERALIZED CACTUS GRAPHS

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Abstract. For an integer $k \geq 0$, a connected graph G is called a k-cactus graph if each edge $e \in E(G)$ is contained in at most k cycles of G. Inspired by the Brualdi–Solheid problem, in this paper, we address the problem of determining the maximum spectral radius of k-cactus graphs. Lovász and Pelikán [*Period. Math. Hungar.* **3** (1973) 175–182], Borovićanin and Petrović [*Publ. Inst. Math. (Beograd) (N.S.)* **79** (2006) 13–18] resolved the cases of $k = 0$ and $k = 1$, respectively. We solve this problem for the cases of $k = 2$ and $k = 3$, that is the graphs with the maximum spectral radius among all 2-cactus graphs and 3-cactus graphs are determined, respectively.

Mathematics Subject Classification. 05C50.

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1. Introduction

Let $G = (V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. Its order is $|V(G)|$, denoted by n, and its size is $|E(G)|$, denoted by m. For a vertex $v \in V(G)$, its neighborhood $N_G(v)$ (or simply $N(v)$) is the set $\{u : uv \in E(G)\}$. For a cycle C, a chord of a cycle C is an edge between two non-consecutive vertices of C. A *block* of a graph G is a maximal connected subgraph of G containing no cut-vertices. A block is called an H-*block*, if it is isomorphic to a graph H. For integer $k \geq 0$, a connected graph G is called a k-cactus graph if each edge $e \in E(G)$ is contained in at most k cycles. Let $\mathscr{G}_n^k$ be the sets of all k-cactus graphs of order n. In particular, $\mathscr{G}_n^0$ and $\mathscr{G}_n^1$ are the sets of trees and cacti of order n, respectively.

The adjacency matrix of a simple graph G is a $(0, 1)$-matrix $A(G) = [a_{i,j}]_{n\times n}$, where $a_{i,j} = 1$ if and only if v_i and v_j are adjacent in G. Note that $A(G)$ is a real symmetric matrix. Then the eigenvalues of $A(G)$ (also called the eigenvalues of G) are real. The largest eigenvalue of $A(G)$ is called the spectral radius of G, denoted by $\rho(G)$.

Brualdi and Solheid [4] posed a classic spectral extremal problem: "*Given a set $\mathscr{G}$ of graphs, find an upper bound for the spectral radius of graphs in $\mathscr{G}$ and characterize the graphs in which the maximal spectral radius is attained.*" This problem is known as Brualdi–Solheid problem and was well studied in the literature for various classes of graphs, such as graphs with a given matching number [6], diameter [8], independence number [11] and a fixed girth [17], *etc.* For more results in this direction, readers are referred to a survey [9] and a book [13].

Keywords. Spectral radius, k-cactus, extremal graph.

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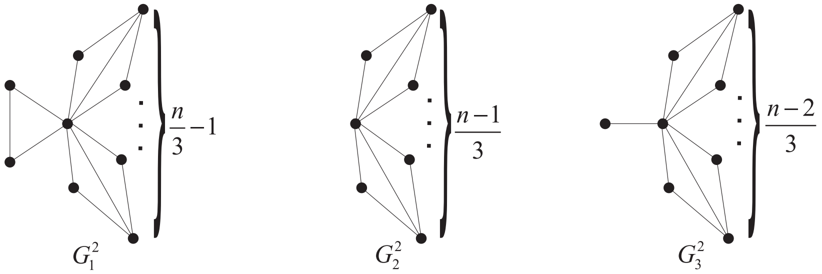


FIGURE 1. Graphs G_1^2, G_2^2 and G_3^2.

The Brualdi–Solheid problem have also been explored within the classes of k-cactus graphs. Previous studies have partially investigated the spectral radius for $\mathscr{G}_n^0$ and $\mathscr{G}_n^1$, which are trees and cacti, respectively. Lovász and Pelikán [12], Borovićanin and Petrović [2] determined the graphs with the maximum spectral radius among all graphs in $\mathscr{G}_n^0$ and $\mathscr{G}_n^1$, respectively. In [1,5,7,10,16], trees and cacti have been extensively studied. However, for $\mathscr{G}_n^k$ with $k \geq 2$ remain relatively underexplored. Recently, Zhang and Huang [18] studied the number of edges for $\mathscr{G}_n^k$, and respectively established the maximum values of the number of edges for $\mathscr{G}_n^k$ when $k = 2, 3, 4$ and also provided the characterizations for the corresponding extremal graphs. Inspired by their results, in this paper, we consider the problem of determining the graphs with the maximum spectral radius among graphs in $\mathscr{G}_n^k$. The graphs with the maximum spectral radius among all graphs in $\mathscr{G}_n^k$ when $k = 2, 3$ are determined, respectively. Our results in this paper can be read as follows.

Theorem 1.1. *For any $G \in \mathscr{G}_n^2$ with $n \geq 2$, we have*

$$\rho(G) \leq \begin{cases} \rho(G_1^2), \, n \equiv 0 \pmod 3, \\ \rho(G_2^2), \, n \equiv 1 \pmod 3, \\ \rho(G_3^2), \, n \equiv 2 \pmod 3, \end{cases}$$

with equality if and only if

$$G \cong \begin{cases} G_1^2, \, n \equiv 0 \pmod 3, \\ G_2^2, \, n \equiv 1 \pmod 3, \\ G_3^2, \, n \equiv 2 \pmod 3, \end{cases}$$

where G_1^2, G_2^2 and G_3^2 are shown in Figure 1, respectively.

Theorem 1.2. *For any $G \in \mathscr{G}_n^3$ with $n \geq 2$, we have*

$$\rho(G) \leq \begin{cases} \rho(G_1^3), \, n \equiv 0 \pmod 4, \\ \rho(G_2^3), \, n \equiv 1 \pmod 4, \\ \rho(G_3^3), \, n \equiv 2 \pmod 4, \\ \rho(G_4^3), \, n \equiv 3 \pmod 4, \end{cases}$$

with equality if and only if

$$G \cong \begin{cases} G_1^3, \, n \equiv 0 \pmod 4, \\ G_2^3, \, n \equiv 1 \pmod 4, \\ G_3^3, \, n \equiv 2 \pmod 4, \\ G_4^3, \, n \equiv 3 \pmod 4, \end{cases}$$

where G_1^3, G_2^3, G_3^3 and G_4^3 are shown in Figure 2, respectively.

The remainder of the paper is organized as follows. In Section 2, we present some preliminary results and structural properties for graphs in $\mathscr{G}_n^2$ (or $\mathscr{G}_n^3$) with the maximum spectral radius, which will be used in the subsequent. In Sections 3 and 4, we present the proofs of Theorems 1.1 and 1.2, respectively.

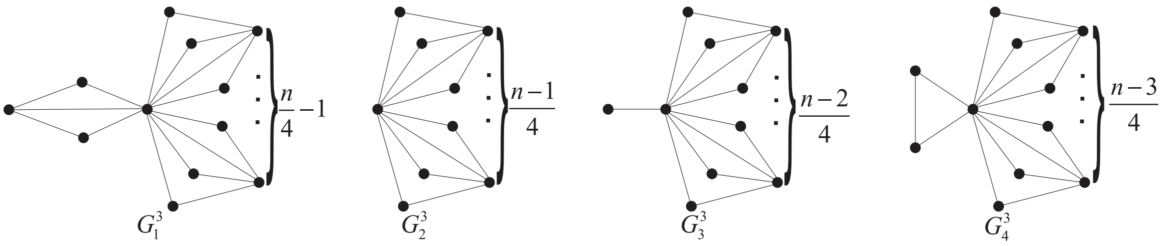


Figure 2. Graphs G_1^3, G_2^3, G_3^3 and G_4^3.

2. Preliminaries

In this section, we present some useful lemmas. Note that when G is connected, then by the Perron–Frobenius Theorem, there exists a positive unit eigenvector $\boldsymbol{x}$ of $A(G)$ corresponding to $\rho(G)$, which is also called the Perron vector of $A(G)$. Clearly, the Perron vector $\boldsymbol{x}$ of $A(G)$ satisfies the eigenvalue equation $A(G)\boldsymbol{x} = \rho(G)\boldsymbol{x}$, that is

$$\rho(G)x_v = \sum_{u \in N(v)} x_u \qquad \text{for all } v \in V(G). \tag{1}$$

where x_u is the entry of $\boldsymbol{x}$ corresponding to the vertex $u \in V(G)$. In addition, we have

$$\rho(G) = \boldsymbol{x}^T A(G)\boldsymbol{x} = 2\sum_{uv \in E(G)} x_u x_v. \tag{2}$$

Lemma 2.1 ([3]). *Let H be a subgraph of a graph G. Then $\rho(H) \leq \rho(G)$. Moreover, if G is connected, then the equality holds if and only if $G \cong H$.*

Lemma 2.2 ([15]). *For a connected graph G and $u, v \in V(G)$, let $W \subseteq N_G(v) \setminus (N_G(u) \cup \{u\})$. Let $G' = G - \{vw : w \in W\} + \{uw : w \in W\}$. Let $\boldsymbol{x}$ be the Perron vector of $A(G)$ corresponding to $\rho(G)$. If $x_v \leq x_u$ and $W \neq \emptyset$, then $\rho(G) < \rho(G')$.*

For an integer $t \geq 3$, a θ_t-graph, denoted by $\theta(l_1, l_2, \ldots, l_t)$, is a graph obtained from two distinct vertices u and v joined by t pairwise internally disjoint paths of lengths $l_1, l_2, \ldots, l_t$, respectively. Note that each block in a 0-cactus is an edge and each block in a 1-cactus graph is either an edge or a cycle. Moreover, for 2-cactus and 3-cactus graphs, Zhang *et al.* [18] established the following structural properties, respectively.

Lemma 2.3 ([18]). *Let G be a graph of order n. Then the following statements hold.*

(i) *$G \in \mathscr{G}_n^2$ if and only if each block of G is either an edge, a cycle, or a θ_3-graph.*
(ii) *$G \in \mathscr{G}_n^3$ if and only if each block of G is either an edge, a cycle, or a θ_t-graph where $t = 3$ or $t = 4$.*

In what follows, we will provide some structural properties for the graph G with the maximum spectral radius among all graphs in $\mathscr{G}_n^2$ (or $\mathscr{G}_n^3$). For Lemmas 2.4–2.8, we prove the case for $G \in \mathscr{G}_n^2$, the case for $G \in \mathscr{G}_n^3$ is similar. Let $G \in \mathscr{G}_n^2$ (or $G \in \mathscr{G}_n^3$) such that $\rho(G)$ is maximal, and let $\boldsymbol{x}$ be the Perron vector of $A(G)$ corresponding to $\rho(G)$.

Lemma 2.4. *Let $G \in \mathscr{G}_n^2$ (or $G \in \mathscr{G}_n^3$). If $\rho(G)$ is maximal, then the length of cycles in any block of G is at most 4. In particular, for any block H $(\neq K_2)$ in G, we have*

(i) *if $G \in \mathscr{G}_n^2$, then* $H \cong \begin{cases} K_3, & H \text{ is a chordless cycle,} \\ \theta(1,2,2), & H \text{ has a cycle of length } 4; \end{cases}$

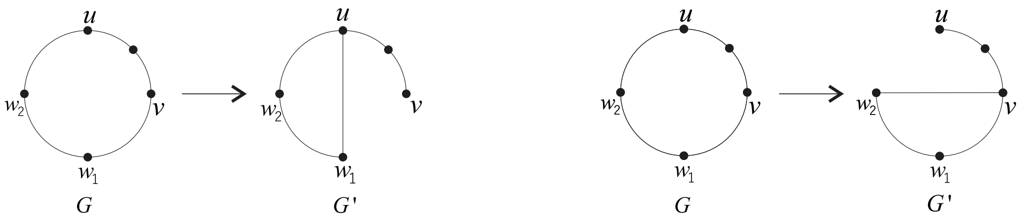


FIGURE 3. Graphs G and G' in Lemma 2.4.

FIGURE 4. Graphs G and G' in Lemma 2.5.

(ii) *if* $G \in \mathscr{G}_n^3$, *then* $H \cong \begin{cases} K_3, & H \text{ is a chordless cycle,} \\ \theta(1,2,2) \textit{ or } \theta(1,2,2,2), & H \text{ has a cycle of length } 4. \end{cases}$

Proof. Suppose to the contrary that G contains a cycle C_l of the length $l \geq 5$. By Lemma 2.3, we know that the block containing C_l is either a cycle or a θ_3-graph. Thus, C_l is either a block itself or a subgraph of a θ_3-graph. Since $l \geq 5$, there exist at least four vertices, say $u, v, w_1, w_2 \in V(C_l)$ such that $w_1 \in N(v) \setminus (N(u) \cup \{u\})$ and $w_2 \in N(u) \setminus (N(v) \cup \{v\})$. Now let $G' = \begin{cases} G - \{vw_1\} + \{uw_1\} & \text{if } x_u \geq x_v, \\ G - \{uw_2\} + \{vw_2\} & \text{if } x_u < x_v. \end{cases}$, where G and G' are shown in Figure 3. Obviously, $G' \in \mathcal{G}_n^2$. Then Lemma 2.2 implies that $\rho(G') > \rho(G)$, a contradiction. Moreover, for any block H in G, by Lemma 2.3, we have $H \cong \begin{cases} K_3, & H \text{ is a chordless cycle,} \\ \theta(1,2,2), & H \text{ has a cycle of length } 4. \end{cases}$ This completes the proof of Lemma 2.4. □

We now establish the number of K_2-blocks in G.

Lemma 2.5. *Let* $G \in \mathscr{G}_n^2$ *(or* $G \in \mathscr{G}_n^3$*). If* $\rho(G)$ *is maximal, then* G *contains at most one* K_2*-block.*

Proof. Suppose to the contrary that G has at least two K_2-blocks, say $e_1 = u_1v_1$ and $e_2 = u_2v_2$, where u_1 and u_2 are pendant vertices (*i.e.*, $d_G(u_1) = d_G(u_2) = 1$). Let $G' = \begin{cases} G - \{u_2v_2\} + \{u_1v_2\} & \text{if } x_{u_1} \geq x_{u_2}, \\ G - \{u_1v_1\} + \{u_2v_1\} & \text{if } x_{u_1} < x_{u_2}, \end{cases}$ where G and G' are shown in Figure 4. Obviously, $G' \in \mathscr{G}_n^2$. Then Lemma 2.2 implies that $\rho(G') > \rho(G)$, a contradiction. Hence, G contains at most one K_2-block. □

The following two lemmas (Lems. 2.6 and 2.7) will establish that all blocks in G are connected by a common cut-vertex.

Lemma 2.6. *Let* $G \in \mathscr{G}_n^2$ *(or* $G \in \mathscr{G}_n^3$*). If* $\rho(G)$ *is maximal, then any two blocks in* G *cannot be connected by a cut-edge.*

Proof. Assume to the contrary that there exists a cut-edge $uv \in E(G)$ connecting two blocks in G. From Lemmas 2.3, 2.4 and 2.5, we know that each block in G is K_2, K_3 or $\theta(1,2,2)$, and there is only one K_2-block in G, which is uv. Let $\mathscr{B} = \{K_3, \theta(1,2,2)\}$. Let $B_1, B_2 \in \mathscr{B}$, and let B_1 and B_2 are connected by the edge uv.

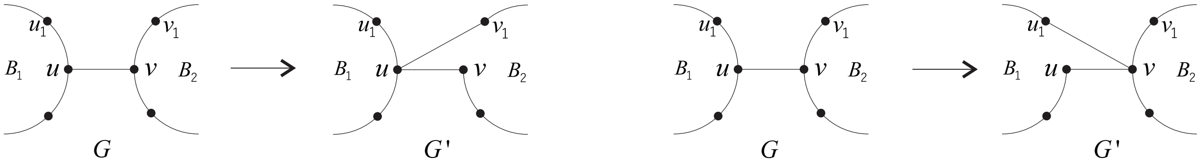


FIGURE 5. Graphs G and G' in Lemma 2.6.

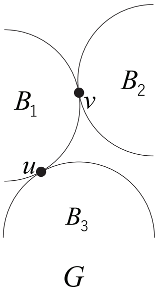


FIGURE 6. A graph G in Lemma 2.7.

Let $G' = \begin{cases} G - \{vv_1\} + \{uv_1\} & \text{if } x_u \geq x_v, \\ G - \{uu_1\} + \{u_1v\} & \text{if } x_u < x_v, \end{cases}$ where G and G' are shown in Figure 5. Obviously, $G' \in \mathscr{G}_n^2$. Then Lemma 2.2 implies that $\rho(G') > \rho(G)$, a contradiction. Thus, any two blocks in G cannot be connected by a cut-edge. □

Lemma 2.7. *Let $G \in \mathscr{G}_n^2$ (or $G \in \mathscr{G}_n^3$). If $\rho(G)$ is maximal, then all blocks in G are connected by a common cut-vertex.*

Proof. From Lemmas 2.3 and 2.4, we know that each block in G is K_2, K_3 or $\theta(1,2,2)$. Let $\mathscr{B}^* = \{K_2, K_3, \theta(1,2,2)\}$. Suppose to the contrary that G (shown in Fig. 6) contains three blocks, say B_1, B_2 and B_3, are connected by two cut-vertices u and v, where $B_1, B_2, B_3 \in \mathscr{B}^*$. Let $\{w_1, w_2, \ldots, w_p\} = N_{B_2}(v) \subset N(v) \setminus (N(u) \cup \{u\})$ and $\{z_1, z_2, \ldots, z_q\} = N_{B_3}(u) \subset N(u) \setminus (N(v) \cup \{v\})$, where $p, q \geq 1$. Let $G' = \begin{cases} G - \{vw_i : 1 \leq i \leq p\} + \{uw_i : 1 \leq i \leq p\} & \text{if } x_u \geq x_v, \\ G - \{uz_i : 1 \leq i \leq q\} + \{vz_i : 1 \leq i \leq q\} & \text{if } x_u < x_v. \end{cases}$ Clearly, $G' \in \mathscr{G}_n^2$. Then Lemma 2.2 implies that $\rho(G') > \rho(G)$, a contradiction. Thus, all blocks in G are connected by a common cut-vertex. □

We now further establish that at most one K_3-block in G.

Lemma 2.8. *Let $G \in \mathscr{G}_n^2$ (or $G \in \mathscr{G}_n^3$). If $\rho(G)$ is maximal, then G contains at most one K_3-block.*

Proof. Suppose to the contrary that there exists two K_3-blocks in G, denoted by H_1 and H_2, with vertex sets $V(H_1) = \{u_1, u_2, u_3\}$ and $V(H_2) = \{v_1, v_2, v_3\}$. From Lemma 2.7, we know that H_1 and H_2 are connected by a common cut-vertex, say u $(= u_1$ or $v_1)$. Let $G' = \begin{cases} G - \{v_2v_3\} + \{u_3v_3\} & \text{if } x_{u_3} \geq x_{v_3}, \\ G - \{u_2u_3\} + \{u_3v_3\} & \text{if } x_{u_3} < x_{v_3}, \end{cases}$ where G and G' are shown in Figure 7. Clearly, in each case, $G' \in \mathscr{G}_n^2$. Then Lemma 2.2 implies that $\rho(G') > \rho(G)$, a contradiction. Thus G contains at most one K_3-block, as desired. □

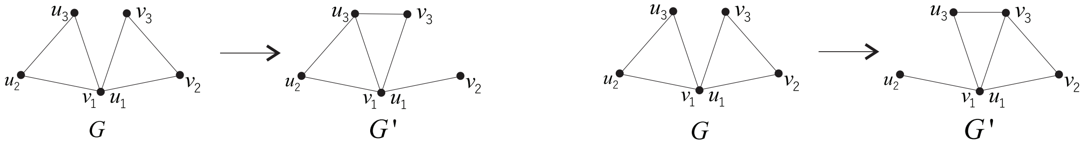


FIGURE 7. Graphs G and G' in Lemma 2.8.

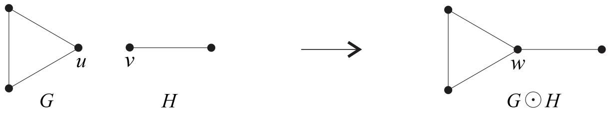


FIGURE 8. The graph $K_3 \odot K_2$.

3. PROOF OF THEOREM 1.1

For two vertex-disjoint graphs G and H, a coalescence of G and H, denoted by $G \odot H$, is obtained from $G \cup H$ by identifying an arbitrary vertex u of G with an arbitrary vertex v of H. Formally, $V(G \odot H) = (V(G) \setminus \{u\}) \cup (V(H) \setminus \{v\}) \cup \{w\}$ and $E(G \odot H) = E(G) \cup E(H) \setminus (\{uz : z \in N_G(u)\} \cup \{vy : y \in N_H(v)\}) \cup \{ws : s \in N_G(u) \cup N_H(v)\}$, where w is a new vertex which satisfies $N_{G\odot H}(w) = \{N_G(u) \cup N_H(v)\} \setminus \{u, v\}$. Figure 8 is an example for $K_3 \odot K_2$.

Specifically, let $\odot pG$ be a graph obtained by coalescing p isomorphic copies of G by identifying one arbitrary vertex from each copy. We now present a structural characterization on the graphs with the maximum spectral radius within $\mathscr{G}_n^2$.

Lemma 3.1. *For $G \in \mathscr{G}_n^2$, if $\rho(G)$ is maximal, then the structure of G is determined as follows:*

$$G \cong \begin{cases} K_3 \odot \frac{n-3}{3}\theta(1,2,2), & n \equiv 0 \pmod 3, \\ \odot \frac{n-1}{3}\theta(1,2,2), & n \equiv 1 \pmod 3, \\ K_2 \odot \frac{n-2}{3}\theta(1,2,2), & n \equiv 2 \pmod 3. \end{cases}$$

Proof. By Lemmas 2.5, 2.7 and 2.8, we conclude that G contains at most one K_2-block, one K_3-block and all blocks in G are connected by a common cut-vertex w. If G contains both K_2-block and K_3-block, then let $G' = G + \{w_1 w_2\}$, where w_1 ($\neq w$) is a vertex in K_2-block, w_2 ($\neq w$) is a vertex in K_3-block, G and G' are shown in Figure 9. Clearly, $G' \in \mathscr{G}_n^2$. Thus, Lemma 2.1 implies that $\rho(G) < \rho(G')$, a contradiction. That is G does not simultaneously contain both K_2-block and K_3-block. It follows that the structure of G is determined as follows:

$$G \cong \begin{cases} K_3 \odot \frac{n-3}{3}\theta(1,2,2), & n \equiv 0 \pmod 3, \\ \odot \frac{n-1}{3}\theta(1,2,2), & n \equiv 1 \pmod 3, \\ K_2 \odot \frac{n-2}{3}\theta(1,2,2), & n \equiv 2 \pmod 3, \end{cases}$$

as desired. □

Let $\mathscr{H} = \{K_1, K_2, K_3\}$. For any $H \in \mathscr{H}$, let $G^2_{n,i,r-i}$ be a 2-cactus graph of order n obtained from H and $r\,\theta(1,2,2)$-blocks, by coalescing the vertices of degree 3 from $i\,\theta(1,2,2)$-blocks with H and coalescing the vertices of degree 2 from $(r-i)\,\theta(1,2,2)$-blocks with H, where $0 \leq i \leq r$.

Now, we present the proof of Theorem 1.1.

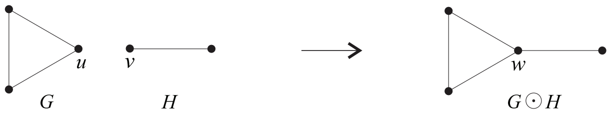


FIGURE 9. Graphs G and G' in Lemma 3.1.

Proof of Theorem 1.1

We will prove that for $G \in \mathscr{G}_n^2$, if $\rho(G)$ is maximal, then all $\theta(1,2,2)$-blocks in G are coalesced at their vertices of degree 3. That is, $\rho(G^2_{n,i,r-i}) < \rho(G^2_{n,i+1,r-i-1})$, where $0 \leq i \leq r$. For $2 \leq n \leq 6$, we check $\rho(G^2_{n,i,r-i}) < \rho(G^2_{n,i+1,r-i-1})$ holds by the Wolfram Mathematica [14]. In what follows, we assume that $n \geq 7$. Let $\boldsymbol{x}$ be the Perron vector of $A(G^2_{n,i,r-i})$, where $G^2_{n,i,r-i}$ is shown in Figure 10. By symmetry, we have

$$x_{u_1} = x_{u_2}. \tag{3}$$

For equation (1), we obtain

$$\rho(G^2_{n,i,r-i})x_{u_1} = x_u + x_{u_2} + x_{u_3}, \tag{4}$$

$$\rho(G^2_{n,i,r-i})x_{u_3} = x_{u_1} + x_{u_2}. \tag{5}$$

Combining (3), (4) and (5), we obtain

$$x_u = \frac{\rho(G^2_{n,i,r-i})^2 - \rho(G^2_{n,i,r-i}) - 2}{\rho(G^2_{n,i,r-i})} \cdot x_{u_1}. \tag{6}$$

For $n = 7$, using the Wolfram Mathematica [14], we calculate that $3 = \rho(G^2_{7,0,2}) < \rho(G^2_{7,1,1}) \approx 3.11 < \rho(G^2_{7,2,0}) = \sqrt{5} + 1$. Note that for $n \geq 8$, any graph $G^2_{n,i,r-i}$ contains one of $G^2_{7,0,2}$, $G^2_{7,1,1}$, or $G^2_{7,2,0}$ as a subgraph. Then $\rho(G^2_{n,i,r-i}) \geq \rho(G^2_{7,0,2}) \geq 3$ for $n \geq 7$, by Lemma 2.1. Thus

$$\frac{\rho(G^2_{n,i,r-i})^2 - \rho(G^2_{n,i,r-i}) - 2}{\rho(G^2_{n,i,r-i})} > 1.$$

Therefore, by (6), we have $x_u > x_{u_1}$. Note that $G^2_{n,i+1,r-i-1} \cong G^2_{n,i,r-i} - u_1u_3 + uu_3$, where $u_3 \in N(u_1) \setminus \big(N(u) \cup \{u\}\big)$. Then Lemma 2.2 implies that $\rho(G^2_{n,i,r-i}) < \rho(G^2_{n,i+1,r-i-1})$. This implies that for $G \in \mathscr{G}_n^2$, if $\rho(G)$ is maximal, then in G, all $\theta(1,2,2)$-blocks are coalesced at their vertices of degree 3. By combining Lemma 3.1, we can conclude that among all the graphs in $\mathscr{G}_n^2$ with $n \geq 2$, the maximal spectral radius is obtained at G, where

$$G \cong \begin{cases} G_1^2, \ n \equiv 0 \pmod 3, \\ G_2^2, \ n \equiv 1 \pmod 3, \\ G_3^2, \ n \equiv 2 \pmod 3, \end{cases}$$

and G_1^2, G_2^2 and G_3^2 are shown in Figure 1, respectively. This completes the proof of Theorem 1.1. □

4. PROOF OF THEOREM 1.2

Let G be a graph with the maximum spectral radius among all graphs in $\mathscr{G}_n^3$. In Section 2, we have established that G contains at most one K_2-block and at most one K_3-block, and all blocks in G are connected by a common cut-vertex. We now further demonstrate that G has at most one $\theta(1,2,2)$-block.

Lemma 4.1. *For $G \in \mathscr{G}_n^3$, if $\rho(G)$ is maximal, then G contains at most one $\theta(1,2,2)$-block.*

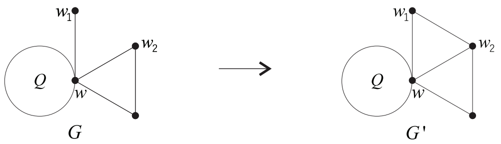


FIGURE 10. The graph $G^2_{n,i,r-i}$.

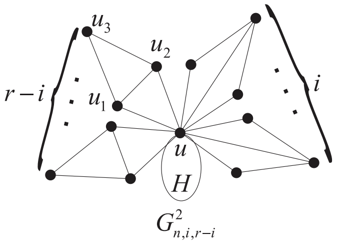


FIGURE 11. Graphs G and G' in Lemma 4.1.

Proof. Assume to the contrary that G contains at least two $\theta(1,2,2)$-blocks. Let G_1 and G_2 be two $\theta(1,2,2)$-blocks in G with vertex sets $V(G_1)=\{u_1,u_2,u_3,u_4\}$ and $V(G_2)=\{v_1,v_2,v_3,v_4\}$. From Lemma 2.7, we know that G_1 and G_2 are connected by a cut-vertex. Let $\boldsymbol{x}$ be the Perron vector of $A(G)$, $d_{G_1}(u_1)=d_{G_2}(v_1)=3$ and $d_{G_1}(u_2)=d_{G_2}(v_2)=2$. We now consider the following three cases.

Case 1. u_1 and v_1 are coalesced at one cut-vertex.

Let $G'=\begin{cases} G-\{u_3u_4\}+\{u_4v_3\} \text{ if } x_{v_3}\geq x_{u_3}, \\ G-\{v_3v_4\}+\{u_3v_4\} \text{ if } x_{v_3}< x_{u_3}. \end{cases}$ (shown in Fig. 11). Obviously, $G'\in\mathscr{G}_n^3$. By Lemma 2.2, we have $\rho(G')>\rho(G)$, a contradiction.

Case 2. u_2 and v_2 are coalesced at one cut-vertex.

From the proof of Theorem 1.1, we get $x_{v_2}>x_{v_1}$. Let $G'=G-\{v_1v_4\}+\{v_2v_4\}$, where $v_4\in N(v_1)\setminus\big(N(v_2)\cup\{v_2\}\big)$. The graph G and G' are shown in Figure 11. Clearly, $G'\in\mathscr{G}_n^3$. By Lemma 2.1, we have $\rho(G')>\rho(G)$, a contradiction.

Case 3. u_2 and v_1 are coalesced at one cut-vertex.

From the proof of Theorem 1.1, we obtain $x_{u_2}>x_{u_1}$. Let $G'=G-\{u_1u_4\}+\{u_2u_4\}$, where $u_4\in N(u_1)\setminus\big(N(u_2)\cup\{u_2\}\big)$. The graph G and G' are shown in Figure 11. Obviously, $G'\in\mathscr{G}_n^3$. By Lemma 2.1, we have $\rho(G')>\rho(G)$, a contradiction.

In view of the above arguments, we conclude that G contains at most one $\theta(1,2,2)$-block. □

Furthermore, by applying a similar argument as used for 2-cactus graphs, we can obtain the structure of the extremal graph with respect to the maximum spectral radius for 3-cactus graphs.

Lemma 4.2. *For $G\in\mathscr{G}_n^3$, if $\rho(G)$ is maximal, then the structure of G is determined as follows:*

$$G\cong\begin{cases} \theta(1,2,2)\odot\frac{n-4}{4}\theta(1,2,2,2), & \text{if } n\equiv 0 \pmod 4, \\ \odot\frac{n-1}{4}\theta(1,2,2,2), & \text{if } n\equiv 1 \pmod 4, \\ K_2\odot\frac{n-2}{4}\theta(1,2,2,2), & \text{if } n\equiv 2 \pmod 4, \\ K_3\odot\frac{n-3}{4}\theta(1,2,2,2), & \text{if } n\equiv 3 \pmod 4. \end{cases}$$

Proof. By Lemmas 2.5, 2.7, 2.8 and 4.1, we conclude that G contains at most one K_2-block, one K_3-block, one $\theta(1,2,2)$-block and all blocks are connected by a cut-vertex. From Lemma 3.1, G does not contain K_2-block

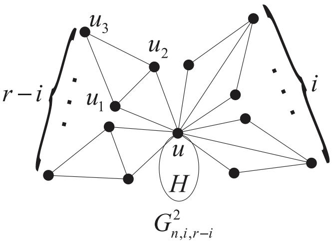


FIGURE 12. Graphs G and G' in Lemma 4.2.

and K_3-block. We will establish that G does not contain K_3-block and $\theta(1,2,2)$-block. Let $Q' \cong \odot r\theta(1,2,2,2)$ and G contains both K_3-block and $\theta(1,2,2)$-block. The G is shown in Figure 12. Let $\boldsymbol{x}$ be the Perron vector of $A(G)$. By symmetry, we have $x_{u_1} = x_{u_2}$ and $x_{u_4} = x_{u_5}$. From equation (1), we conclude that

$$\rho(G)x_{u_2} = x_{u_1} + x_{u_3}, \tag{7}$$
$$\rho(G)x_{u_4} = x_{u_3} + x_{u_6}, \tag{8}$$
$$\rho(G)x_{u_6} = x_{u_3} + x_{u_4} + x_{u_5}. \tag{9}$$

Combining equation (7), (8), and (9), we can obtain

$$\rho(G)(x_{u_4} - x_{u_2}) = x_{u_6} - x_{u_2}, \tag{10}$$
$$\rho(G)(x_{u_6} - x_{u_2}) = 2x_{u_4} - x_{u_2}. \tag{11}$$

Putting equation (10) into equation (11), we have

$$x_{u_4} = (\rho(G)^2 - 1)(x_{u_4} - x_{u_2}). \tag{12}$$

Since $G^2_{6,1,0}$ is a subgraph of G, then by Lemma 2.1, we have $\rho(G) \geq \rho(G^1_{6,1,0}) > 2$. This together with (12) implies that $x_{u_4} > x_{u_2}$. Thus, from (11), we have $x_{u_6} > x_{u_2}$. Let $G' = G - \{u_1u_2\} + \{u_2u_6\}$. The G' is shown in Figure 12. Clearly, $G' \in \mathscr{G}^3_n$. By Lemma 2.2, $\rho(G') > \rho(G)$, a contradiction. Thus, G does not contain K_3-block and $\theta(1,2,2)$-block. In summary, we have

$$G \cong \begin{cases} \theta(1,2,2) \odot \frac{n-4}{4}\theta(1,2,2,2), & \text{if } n \equiv 0 \pmod 4, \\ \odot \frac{n-1}{4}\theta(1,2,2,2), & \text{if } n \equiv 1 \pmod 4, \\ K_2 \odot \frac{n-2}{4}\theta(1,2,2,2), & \text{if } n \equiv 2 \pmod 4, \\ K_3 \odot \frac{n-3}{4}\theta(1,2,2,2), & \text{if } n \equiv 3 \pmod 4, \end{cases}$$

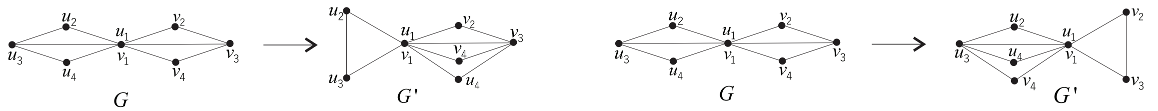
as desired. □

Let $\mathscr{F} = \{K_1, K_2, K_3, \theta(1,2,2)\}$. For any $F \in \mathscr{F}$, if $F \cong \theta(1,2,2)$-block, then from the proof of Theorem 1.1, we have that the vertex of degree 3 from F is coalesced at one cut-vertex of G. Let $R^3_{n,i,n-i}$ be a 3-cactus graph of order n obtained from F and $r\theta(1,2,2,2)$-blocks, by coalescing the vertices of degree 4 from $i\theta(1,2,2,2)$-blocks with F and coalescing the vertices of degree 2 from $(r-i)\theta(1,2,2,2)$-blocks with F, where $0 \leq i \leq r$.

We now give the proof of Theorem 1.2.

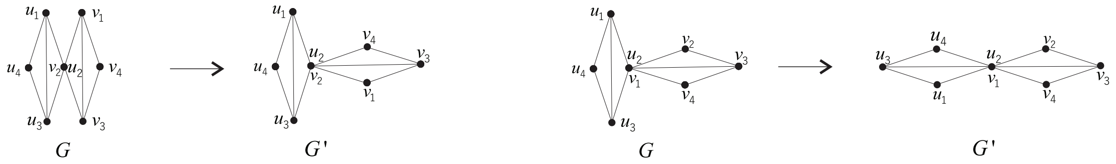
Proof of Theorem 1.2

We will prove that if G is a graph with the maximum spectral radius among all graphs $\mathscr{G}^3_n$, then all $\theta(1,2,2,2)$-blocks in G are coalesced at their vertices of degree 4. That is, we need prove that $\rho(R^3_{n,i,r-i}) < \rho(R^3_{n,i+1,r-i-1})$, where $0 \leq i \leq r$. By the Wolfram Mathematica [14], we check that $\rho(R^3_{n,i,r-i}) < \rho(R^3_{n,i+1,r-i-1})$ holds for $2 \leq n \leq 16$. In what follows, we assume that $n \geq 17$.



Graphs G and G' in Case 1

Graphs G and G' in Case 1



Graphs G and G' in Case 2

Graphs G and G' in Case 3

FIGURE 13. The graph $R^3_{n,i,r-i}$.

Let $\boldsymbol{x}$ be the Perron vector of $A(R^3_{n,i,r-i})$, where $R^3_{n,i,r-i}$ is shown in Figure 13. By symmetry, we have $x_{u_1} = x_{u_2}$ and $x_{u_3} = x_{u_4}$. From equation (1), we derive

$$\rho(R^3_{n,i,r-i})x_{u_3} = x_{u_1} + x_{u_2} = 2x_{u_1}, \tag{13}$$

$$\rho(R^3_{n,i,r-i})x_{u_1} = x_u + x_{u_2} + x_{u_3} + x_{u_4}. \tag{14}$$

From equation (13), we have

$$x_{u_3} = \frac{2x_{u_1}}{\rho(R^3_{n,i,r-i})}. \tag{15}$$

Substituting (15) into (14), we obtain

$$x_u = \frac{\rho(R^3_{n,i,r-i})^2 - \rho(R^3_{n,i,r-i}) - 4}{\rho(R^3_{n,i,r-i})} x_{u_1}. \tag{16}$$

By Rayleigh's quotient inequality, we get

$$\begin{aligned} \rho(R^3_{n,i+1,r-i-1}) - \rho(R^3_{n,i,r-i}) &> \boldsymbol{x}^T A(R^3_{n,i+1,r-i-1})\boldsymbol{x} - \boldsymbol{x}^T A(R^3_{n,i,r-i})\boldsymbol{x} \\ &= 2(x_u x_{u_4} + x_u x_{u_3} + x_{u_3}x_{u_4} - x_{u_1}x_{u_3} - x_{u_2}x_{u_3} - x_{u_1}x_{u_2}) \\ &= 2\left(\frac{3\rho(R^3_{n,i,r-i})^2 - 8\rho(R^3_{n,i,r-i}) - 12}{\rho(R^3_{n,i,r-i})^2}\right)x_{u_1}^2. \end{aligned} \tag{17}$$

Since $R^3_{17,0,4}$ is a subgraph of $R^3_{n,i,r-i}$, we have $\rho(R^3_{n,0,r}) \geq \rho(R^3_{17,0,4}) = 4 > 3.8$. It follows that $3\rho(R^3_{n,i,r-i})^2 - 8\rho(R^3_{n,i,r-i}) - 12 > 0$. Thus, from (17), we have $\rho(R^3_{n,i,r-i}) < \rho(R^3_{n,i+1,r-i-1})$, where $0 \leq i \leq r$. By combining the statements of Lemma 4.2, we conclude that among all the graphs in $\mathscr{G}^3_n$ with $n \geq 2$, the maximal spectral radius is attained at G, where

$$G \cong \begin{cases} G^3_1,\ n \equiv 0 \pmod 4, \\ G^3_2,\ n \equiv 1 \pmod 4, \\ G^3_3,\ n \equiv 2 \pmod 4, \\ G^3_4,\ n \equiv 3 \pmod 4, \end{cases}$$

and G^3_1, G^3_2, G^3_3 and G^3_4 are shown in Figure 2. This completes the proof of Theorem 1.2. $\square$

5. Concluding remarks

In this paper, we have solved the Brualdi–Solheid problem for the classes of 2-cactus and 3-cactus graphs, characterizing the extremal graphs that attain the maximum spectral radius in each family. Our structural analysis reveals that these extremal graphs are coalescences of specific blocks: K_2, K_3, $\theta(1,2,2)$, and $\theta(1,2,2,2)$, all sharing a common cut vertex.

A natural and challenging extension is to consider the general case of k-cactus graphs for $k \geq 4$. Based on the patterns observed for $k=2$ and $k=3$, we conjecture that the extremal graph for general k is also a coalescence of θ-type blocks at a common vertex, where each block is a θ-graph with $t=k+1$ internally disjoint paths, and the path lengths are chosen to maximize the spectral radius under the edge–cycle constraint. Specifically, we suspect that the optimal block is of the form $\theta(1,2,\ldots,2)$ (with $k-1$ copies of 2), to an extremal graph of the form $\odot_r \theta(1,2,\ldots,2)$ for some r depending on n.

Proving this conjecture for arbitrary k appears nontrivial, as the number of possible block structures grows rapidly with k, and spectral comparisons become increasingly complex. We suggest several directions for future research:

- Characterization of optimal θ-blocks: Determine, for each k, the θ-graph with $t=k+1$ paths that maximizes the spectral radius subject to the k-cactus condition.
- Structural lemmas for general k: Develop more general graph transformations that preserve the k-cactus property while increasing the spectral radius, extending Lemma 2.2 to broader settings.
- Computational exploration: Use symbolic or numerical computation to test conjectures for small $k \geq 4$ and moderate n, which may reveal further structural patterns.
- Connections with edge-maximization: Relate the spectral extremal problem to the edge–maximization results for k-cactus graphs obtained by Zhang and Huang [18], possibly uncovering a unified extremal structure.

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Conflicts of interest

The authors have no relevant financial or non-financial interests to disclose.

Data availability statement

Data sharing not applicable to this article as no datasets were generated or analysed during the current study.

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