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EXTREMAL OCTAGONAL CHAINS WITH RESPECT TO THE SPECTRAL RADIUS*

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Abstract. Octagonal systems are tree-like graphs comprised of octagons that represent a class of polycyclic conjugated hydrocarbons. In this paper, a roll-attaching operation for the calculation of the characteristic polynomials of octagonal chain graphs is proposed. Based on these characteristic polynomials, the extremal octagonal chains with n octagons having the maximum and minimum spectral radii are identified.

Key words. Octagonal chains, Spectral radius, Extremal graphs.

AMS subject classifications. 05C50, 15A42.

1. Introduction. In this paper, we consider only connected, simple and finite graphs. For graph theoretic notation and terminology not defined here, we refer the readers to Bondy and Murty [4].

Let $G = (V_G, E_G)$ be a graph with vertex set V_G and edge set E_G. Then $G - v$, $G - uv$ denote the graphs obtained from G by deleting vertex $v \in V_G$, or edge $uv \in E_G$, respectively. This notation is naturally extended if more than one vertex or edge are deleted. Similarly, $G + uv$ is obtained from G by inserting the edge $uv \notin E_G$. Denote by P_n and C_n the path and cycle on n vertices, respectively.

Let $V_G = \{v_1, v_2, \dots, v_n\}$ and $A(G) = (a_{ij})_{n\times n}$ be the *adjacency matrix* of order n whose entries $a_{ij} = 1$ if v_i, v_j are adjacent and 0 otherwise. Since $A(G)$ is symmetric and real, the eigenvalues of $A(G)$, also referred to as the *eigenvalues* of G, can be arranged as $\lambda_1 > \lambda_2 > \cdots > \lambda_k$ with multiplicity $n_1, n_2, \dots, n_k$, respectively. Then the *spectrum* of G is the set of eigenvalues of $A(G)$ together with their multiplicities, denoted by $\{\lambda_1^{(n_1)}, \lambda_2^{(n_2)}, \dots, \lambda_k^{(n_k)}\}$. The largest eigenvalue $\lambda_1(G)$ of $A(G)$ is called the *spectral radius* or *index* of G, denoted by $\rho(G)$. The *characteristic polynomial* of G is

$$\varphi(G, x) = \det(xI_n - A(G)),$$

where I_n is an identity matrix of order n, and can also be expressed in the coefficients forms as follows:

$$\varphi(G, x) = \det(xI - A(G)) = \sum_{i=0}^{n} a_i x^{n-i}.$$

As proposed by Brualdi and Solheid [5], an interesting problem is to determine the extremal graphs in some class with respect to the spectral radius. This problem has attracted much attention in the literature

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(see, for example, [10, 11]). However, the problem, especially the minimization version, appears hard for some graphs (see, for example, [15, 26, 29, 30, 31]). In contrast, tools for dealing with maximization version are more developed (see also [12, 14]). The minimal index problem plays an important role in modeling virus propagation in real networks (see [27] for more details). The adjacent spectral radius has been extensively studied. Primarily the study has focussed on graphs with pendent vertices. There is also some work on 2-connected graphs.

Here we will mention only a few relevant results. Some fundamental results on spectral radius of connected graphs with cyclomatic number are obtained in mathematical literature. In particular, in 1973, Lovász and Pelikán [24] found that of all trees, the star has the largest spectral radius and the path has the smallest, respectively. For trees, we refer the readers to [10, 14, 19, 23, 25]. The corresponding results for unicyclic graphs can be found in [2, 7, 22]. Those for bicyclic graphs can be found in [28, 32], whereas those for tricyclic or quasi-k-cyclic graphs can be found in [16, 17, 18]. It seems that the study on the index of graphs without pendant vertices is hard. Up to now, very few papers concerned this problem. Chen et al. [8] considered the largest eigenvalue of complete bipartite graphs, missing at most two edges. Das et al. [13] focused on a conjecture on the index of almost complete bipartite graph proposed in [8]. Zhang and Tian [33] determined the hexagonal chain graphs with n hexagons having the largest and smallest adjacency spectral radii, respectively.

In order to formulate our main results, we need to introduce some notation. An *octagonal system* is a 2-connected graph consisting of some regular octagons. It seems that the first study on octagonal systems in mathematical chemistry is [6]. The *octagonal chains* are defined recursively as follows. An octagon O_1 is an octagonal chain, with itself as the terminal octagon. If $G_{n-1} = O_1O_2\cdots O_{n-1}$ is an octagon chain consisting of $n-1 \geqslant 2$ octagons, where O_i is the i^{th} octagon for $1 \leqslant i \leqslant n-1$ and O_{n-1} is terminal octagon, then the graph obtained from G_{n-1} by identifying an edge of O_{n-1} incident to only one octagon of G_{n-1} with an edge of an octagon O_n is an octagonal chain with terminal octagon O_n, denoted by $G_n = O_1O_2\cdots O_n$.

Let $G_n = O_1O_2\cdots O_n$ be an octagonal chain with $n \geqslant 3$. Let $u_{i-2}v_{i-2}$ be the common edge of O_{i-2} and O_{i-1}, and $u_{i-1}v_{i-1}$ be the common edge of O_{i-1} and O_i for $i \geq 3$. Let k be the number of edges encountered when traversing O_{i-1} starting at $u_{i-2}v_{i-2}$ and ending at $u_{i-1}v_{i-1}$ in a clockwise direction. Then $k \in \{2,3,4,5,6\}$ and the join is $\alpha, \beta, \gamma, \delta, \varepsilon$ according to the value of k. For example, let $O_{n-1} = qpabcdefq$ with $e_{n-1} = pq$, and denote one edge of O_n by rs. Then G_n can be obtained from G_{n-1} and O_n by α (respectively β, γ, δ, ε) join (see Figure 1).

As it is irrelevant to which join the first and second octagons are, we set $k_1 = k_2 = \gamma$. Then

$$G_n = \gamma\gamma k_3 \cdots k_n. \tag{1.1}$$

If $k_i = \gamma$ for each i in (1.1), then G_n is a *linear chain*, which is denoted by L_n. If $k_i \in \{\alpha, \varepsilon\}$ (or $\{\beta, \delta\}$) and $k_i \neq k_{i+1}$ for each $i \geqslant 3$ in (1.1), then G_n is called a *zigzag chain*, we denote it by Z_n^1 (or Z_n^2). If $k_i = \alpha$ (or ε) for each $i \geqslant 3$ in (1.1), then G_n is a *helix chain* and we denote it by H_n^1. If $k_i = \beta$ (or δ) for each $i \geqslant 3$ in (1.1), then G_n is also a *helix chain*, which is denoted by H_n^2 (see Figure 2). Thus, we can see that $G_1 = L_1 = Z_1^1 = Z_1^2 = H_1^1 = H_1^2$, $G_2 = L_2 = Z_2^1 = Z_2^2 = H_2^1 = H_2^2$ and $G_3 \in \{L_3, Z_3^1 = H_3^1, Z_3^2 = H_3^2\}$.

The current work is motivated by the paper [33], in which Zhang and Tian characterized the hexagonal chain graphs with the largest and smallest adjacency indices, respectively. In this paper, we propose a roll-attaching operation for calculating the characteristic polynomials of octagonal chain graphs and consider the extremal problems on the spectral radius of octagonal chains as follows.

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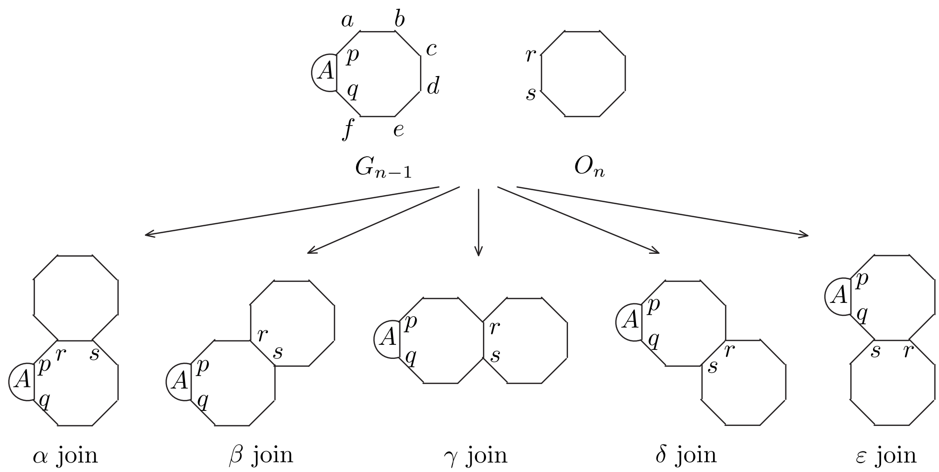

FIGURE 1. *Five cases of attaching an octagon O_n to an octagonal chain G_{n-1}.*

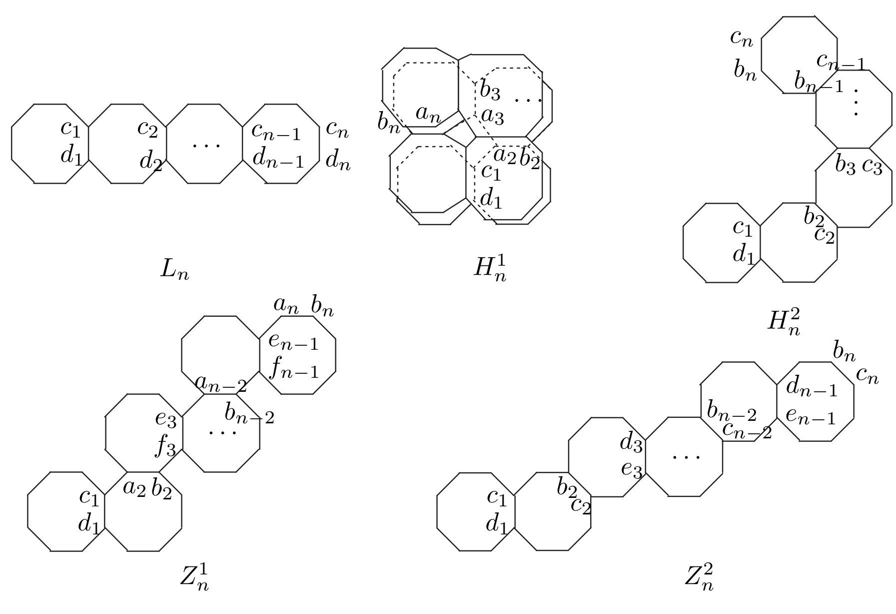

FIGURE 2. *Graphs L_n, H_n^1, H_n^2, Z_n^1 and Z_n^2.*

THEOREM 1.1. *The helix chain H_n^1 uniquely maximizes the spectral radius among all octagonal chains with n octagons.*

THEOREM 1.2. *The linear chain L_n uniquely minimizes the spectral radius among all octagonal chains with n octagons.*

The organization of this paper is as follows. In Section 2, we give some auxiliary results on the characteristic polynomials of graphs, which are used to study the spectral radius of octagonal chains. In Section 3, we introduce a roll-attaching operation on the octagonal chains. Then we establish some technical lemmas

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that help us characterize the extremal graphs. Based on the results in the previous sections, we give the proofs of our main results in Section 4.

2. Preliminaries. In this section, we introduce some preliminary results that will be used to study the spectral radius of octagonal chains. For convenience, let $\mathcal{C}_e(G)$ be the set of cycles in G containing edge e, and $\mathcal{C}_v(G)$ be the set of cycles in G containing vertex v. Denote the set of octagonal chains with n octagons by $\mathcal{G}_n$ and the symbol $\sim$ denotes that two vertices in question are adjacent. First we recall the following bounds.

Lemma 2.1. [1] *Let G be a connected graph with n vertices and m edges. Then $\rho(G) \geqslant \frac{2m}{n}$.*

Given an octagonal chain G_n in $\mathcal{G}_n$ with $n \geqslant 1$, it is straightforward to check that G_n has $6n+2$ vertices and $7n+1$ edges. Thus, Lemma 2.1 implies the following result.

Lemma 2.2. *For any octagonal chain $G_n \in \mathcal{G}_n$ with $n \geqslant 2$, $\rho(G_n) > 2$.*

Next we introduce some recursion formulas about characteristic polynomials.

Lemma 2.3. [9, 21, 3] *Let G_1 and G_2 be two vertex disjoint graphs. Then*

$$\varphi(G_1 \cup G_2, x) = \varphi(G_1, x)\varphi(G_2, x).$$

Lemma 2.4. [9, 21, 3] *Let $e = uv$ be an edge of a simple graph G. Then*

$$\varphi(G, x) = \varphi(G - uv, x) - \varphi(G - u - v, x) - 2 \sum_{C \in \mathcal{C}_e(G)} \varphi(G - V_C, x).$$

Moreover, if e does not belong to any cycles, then

$$\varphi(G, x) = \varphi(G - uv, x) - \varphi(G - u - v, x).$$

Lemma 2.5. [20] *Let H be a subgraph of G with $uv \in E_H$ and denote $\rho(G)$ by ρ. If v is not the unique neighbor of u in graph H, then*

$$\varphi(H, \rho) - \rho\varphi(H - v, \rho) + \varphi(H - u - v, \rho) < 0.$$

Lemma 2.6. [20] *Let G_1 and G_2 be graphs. If $\varphi(G_1, \rho(G_2)) < 0$, then $\rho(G_1) > \rho(G_2)$.*

Let $H_n^1 = O_1O_2 \cdots O_n = \gamma\gamma\alpha\alpha \cdots \alpha$ be a helix chain. Let c_1d_1 be the common edge of O_1 and O_2 and a_ib_i be the common edge of O_i and O_{i+1} for $i \geqslant 2$ as depicted in Figure 2.

Lemma 2.7. *Let the helix chain H_k^1 be a subgraph of a octagonal chain G_n with $1 \leqslant k \leqslant n$. Denote $\rho(G_n)$ by ρ. Then $\varphi(H_1^1 - c_1, \rho) = \varphi(H_1^1 - d_1, \rho)$ and $\varphi(H_k^1 - b_k, \rho) < \varphi(H_k^1 - a_k, \rho)$ for $2 \leqslant k \leqslant n$.*

Proof. If $k = 1$, it is obvious that $\varphi(H_1^1 - c_1, \rho) = \varphi(P_7, \rho) = \varphi(H_1^1 - d_1, \rho)$, as desired.

If $2 \leqslant k \leqslant n$, then we show our result by induction. For the case of $k = 2$, by Lemma 2.4,

$$\varphi(H_2^1 - a_2, x) = (x^5 - 4x^3 + 3x)\varphi(H_1^1, x) - (x^4 - 3x^2 + 1)\varphi(H_1^1 - d_1, x)$$

and

$$\begin{aligned}\varphi(H_2^1 - b_2, x) = (x^5 - 3x^3 + x)\varphi(H_1^1, x) - (x^4 - 3x^2 + 1)\varphi(H_1^1 - c_1, x) \\ -(x^4 - 2x^2)\varphi(H_1^1 - d_1, x) + (x^3 - 2x)\varphi(H_1^1 - c_1 - d_1, x).\end{aligned}$$

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Note that H_1^1 is a subgraph of G_n and c_1 is not the unique neighbor of d_1. Hence, by Lemma 2.5

$$\varphi(H_1^1,\rho)-\rho\varphi(H_1^1-c_1,\rho)+\varphi(H_1^2-c_1-d_1,\rho)<0.$$

According to $\varphi(H_1^1-c_1,\rho)=\varphi(H_1^1-d_1,\rho)$ and $\rho>2$ for $n\geqslant 2$, we have (based on Lemma 2.5) that

$$\begin{aligned}\varphi(H_2^1-b_2,\rho)-\varphi(H_2^1-a_2,\rho)=&(\rho^3-2\rho)[\varphi(H_1^1,\rho)-\rho\varphi(H_1^1-c_1,\rho)+\varphi(H_1^2-c_1-d_1,\rho)]\\&+(\rho^2-1)[\varphi(H_1^1-c_1,\rho)-\varphi(H_1^1-d_1,\rho)]<0.\end{aligned}$$

Then we assume the inequality $\varphi(H_t^1-b_t,\rho)<\varphi(H_t^1-a_t,\rho)$ holds for $1<t<k$ and consider the case of k. Note that

$$\begin{aligned}\varphi(H_k^1-b_k,\rho)-\varphi(H_k^1-a_k,\rho)=&(\rho^3-2\rho)\varphi(H_{k-1}^1,\rho)-(\rho^4-3\rho^2+1)\varphi(H_{k-1}^1\\&-a_{k-1},\rho)-(\rho^2-1)\varphi(H_{k-1}^1-b_{k-1},\rho)\\&+(\rho^3-2\rho)\varphi(H_{k-1}^1-a_{k-1}-b_{k-1},\rho).\end{aligned}\tag{2.2}$$

By induction, $\varphi(H_{k-1}^1-b_{k-1},\rho)<\varphi(H_{k-1}^1-a_{k-1},\rho)$. Combining $\rho>2$ we have

$$\begin{aligned}&(\rho^4-3\rho^2+1)(\varphi(H_{k-1}^1-a_{k-1},\rho)-\varphi(H_{k-1}^1-b_{k-1},\rho))\\&=[\rho^2(\rho^2-4)+\rho^2+1][\varphi(H_{k-1}^1-a_{k-1},\rho)-\varphi(H_{k-1}^1-b_{k-1},\rho)]>0;\end{aligned}$$

that is,

$$\begin{aligned}&(\rho^4-3\rho^2+1)\varphi(H_{k-1}^1-a_{k-1},\rho)+(\rho^2-1)\varphi(H_{k-1}^1-b_{k-1},\rho)\\&>(\rho^4-2\rho^2)\varphi(H_{k-1}^1-b_{k-1},\rho).\end{aligned}$$

Hence, in view of (2.2),

$$\begin{aligned}\varphi(H_k^1-b_k,\rho)-\varphi(H_k^1-a_k,\rho)<&(\rho^3-2\rho)[\varphi(H_{k-1}^1,\rho)-\rho\varphi(H_{k-1}^1-b_{k-1},\rho)\\&+\varphi(H_{k-1}^1-a_{k-1}-b_{k-1},\rho)]<0,\end{aligned}$$

where the last inequality follows by Lemmas 2.2 and 2.5. ∎

Let G_1 and G_2 be two vertex disjoint graphs such that $u_1,\ v_1\in V_{G_1}$ and $u_2,\ v_2\in V_{G_2}$. Then the graph $G_1\diamond G_2$ is constructed from G_1 and G_2 by connecting u_1 and u_2 (respectively v_1 and v_2) with an edge e_1 (respectively e_2). Graph $G_1\diamond G_2$ is depicted in Figure 3.

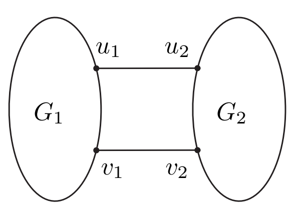

FIGURE 3. *Graph* $G_1\diamond G_2$.

LEMMA 2.8. *For the graph* $G=G_1\diamond G_2$ *through edges* $e_1=u_1u_2$ *and* $e_2=v_1v_2$, *then*

$$\begin{aligned}\varphi(G,x)=&\varphi(G_1,x)\varphi(G_2,x)-\varphi(G_1-u_1,x)\varphi(G_2-u_2,x)-\varphi(G_1-v_1,x)\varphi(G_2-v_2,x)\\&+\varphi(G_1-u_1-v_1,x)\varphi(G_2-u_2-v_2,x)-2\sum_{C\in\mathcal{C}_{e_1}(G)}\varphi(G-V_C,x).\end{aligned}$$

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Proof. By Lemma 2.4,

$$\varphi(G,x)=\varphi(G-u_1u_2,x)-\varphi(G-u_1-u_2,x)-2\sum_{C\in\mathcal{C}_{e_1}(G)}\varphi(G-V_C,x).$$

Applying Lemma 2.4 again,

$$\begin{aligned}\varphi(G-u_1u_2,x)&=\varphi(G-u_1u_2-v_1v_2,x)-\varphi(G-u_1u_2-v_1-v_2,x),\\ \varphi(G-u_1-u_2,x)&=\varphi(G-u_1-u_2-v_1v_2,x)-\varphi(G-u_1-u_2-v_1-v_2,x).\end{aligned}$$

Thus,

$$\begin{aligned}\varphi(G,x)=&\ \varphi(G-u_1u_2-v_1v_2,x)-\varphi(G-u_1u_2-v_1-v_2,x)-\varphi(G-u_1-u_2-v_1v_2,x)\\ &+\varphi(G-u_1-u_2-v_1-v_2,x)-2\sum_{C\in\mathcal{C}_{e_1}(G)}\varphi(G-V_C,x).\end{aligned}$$

Note that

$$\begin{aligned}&G-u_1u_2-v_1v_2\cong G_1\cup G_2,\\ &G-u_1-u_2-v_1-v_2\cong(G_1-u_1-u_2)\cup(G_2-v_1-v_2),\\ &G-u_1-u_2-v_1v_2\cong(G_1-u_1)\cup(G_2-u_2),\\ &G-u_1u_2-v_1-v_2\cong(G_1-v_1)\cup(G_2-v_2).\end{aligned}$$

Hence, by Lemma 2.3

$$\begin{aligned}\varphi(G,x)&=\varphi(G_1\cup G_2,x)-\varphi((G_1-v_1)\cup(G_2-v_2),x)-\varphi((G_1-u_1)\cup(G_2-u_2),x)\\ &\quad+\varphi((G_1-u_1-u_2)\cup(G_2-v_1-v_2),x)-2\sum_{C\in\mathcal{C}_{e_1}(G)}\varphi(G-V_C,x)\\ &=\varphi(G_1,x)\varphi(G_2,x)-\varphi(G_1-u_1,x)\varphi(G_2-u_2,x)-\varphi(G_1-v_1,x)\varphi(G_2-v_2,x)\\ &\quad+\varphi(G_1-u_1-v_1,x)\varphi(G_2-u_2-v_2,x)-2\sum_{C\in\mathcal{C}_{e_1}(G)}\varphi(G-V_C,x).\end{aligned}$$

∎

3. Some technical lemmas on the roll-attaching operation. In this section, we present a few technical lemmas. First we introduce a roll-attaching operation on the octagonal chains as follows. Let $k\in\{\varepsilon,\delta,\gamma,\beta,\alpha\}$, then define $\bar{k}$ as

$$\bar{k}=\begin{cases}\alpha, & \text{if } k=\varepsilon;\\ \beta, & \text{if } k=\delta;\\ \gamma, & \text{if } k=\gamma;\\ \delta, & \text{if } k=\beta;\\ \varepsilon, & \text{if } k=\alpha.\end{cases}$$

We call $\bar{k}$ the *rolling* of k. Given an octagonal chain $G_n=O_1O_2\cdots O_n=\gamma\gamma k_3\cdots k_n$, $B=O_iO_{i+1}\cdots O_n$ is an *octagonal subchain* of G_n. We also set $B=k_ik_{i+1}\cdots k_n$ (where $k_1=k_2=\gamma$ if $i=1$) and denote the *rolling* of B by $\bar{B}=\bar{k}_i\bar{k}_{i+1}\cdots\bar{k}_n$. Hence, $\bar{G}_n=\gamma\gamma\bar{k}_3\cdots\bar{k}_n$ is the rolling of G_n. Obviously, $\bar{G}_n$ is isomorphic to G_n.

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Suppose $G_n = O_1O_2\cdots O_n = \gamma\gamma k_3\cdots k_n$ is an octagonal chain. Let $A = O_1O_2\cdots O_{i-2} = \gamma\gamma k_3\cdots k_{i-2}$ and $B = O_iO_{i+1}\cdots O_n = k_ik_{i+1}\cdots k_n$. Let $e_{i-2} = pq$ (respectively $e_{i-1} = rs$) be the common edge of O_{i-2} and O_{i-1} (respectively O_{i-1} and O_i). Then

- G_n can be regarded as an octagonal chain obtained from A by attaching O_{i-1} through a k_{i-1} join and then from $O_1O_2\cdots O_{i-1}$ by attaching B through a k_i join. Label the vertices of $V_{O_{i-1}}\setminus V_{O_{i-2}}$ by a, b, c, d, e, f in a clockwise direction. One can see that if $k_i = \alpha$, then denote the resulting graph by G_n^α. If $k_i = \beta$, then denote the resulting graph by G_n^β. If $k_i = \gamma$, then denote the resulting graph by G_n^γ. If $k_i = \delta$, then denote the resulting graph by G_n^δ. If $k_i = \varepsilon$, then denote the resulting graph by G_n^ε. Graphs G_n^α, G_n^β, G_n^γ, G_n^δ and G_n^ε are depicted in Figure 4;
- define the *roll-attaching operation* on G_n with respect to B as follows: attach the rolling $\bar{B}$ of B to $AO_{i-1} = \gamma\gamma k_3\cdots k_{i-1}$ by k_i' join. It is easy to see that the resulting octagonal chain obtained by this roll-attaching operation can be written as $\gamma\gamma k_3\cdots k_{i-1}k_i'\bar{k}_{i+1}\cdots\bar{k}_n$, where $k_i' \in \{\alpha,\beta,\gamma,\delta,\varepsilon\}$. If $k_i' = \alpha$, then denote the resulting graph by $G_n^{\alpha'}$. If $k_i' = \beta$, then denote the resulting graph by $G_n^{\beta'}$. If $k_i' = \gamma$, then denote the resulting graph as $G_n^{\gamma'}$. If $k_i' = \delta$, then denote the resulting graph by $G_n^{\delta'}$. If $k_i' = \varepsilon$, then denote the resulting graph by $G_n^{\varepsilon'}$. Graphs $G_n^{\alpha'}$, $G_n^{\beta'}$, $G_n^{\gamma'}$, $G_n^{\delta'}$ and $G_n^{\varepsilon'}$ are depicted in Figure 4.

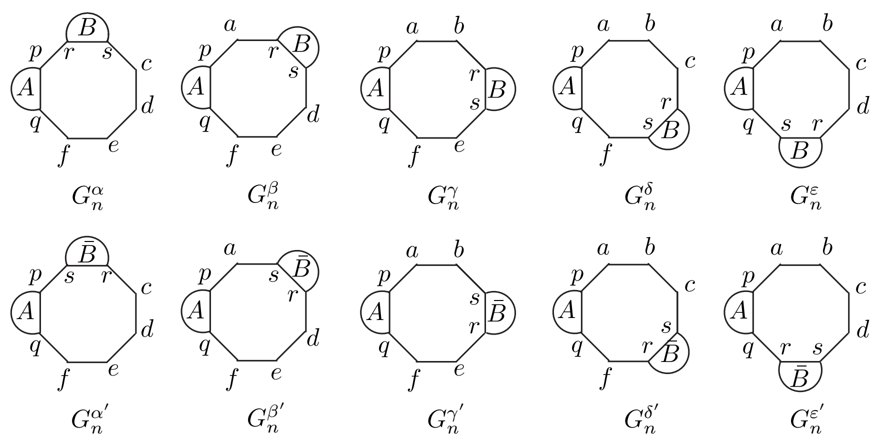

FIGURE 4. *Graphs* G_n^α, G_n^β, G_n^γ, G_n^δ, G_n^ε *and* $G_n^{\alpha'}$, $G_n^{\beta'}$, $G_n^{\gamma'}$, $G_n^{\delta'}$, $G_n^{\varepsilon'}$.

In what follows, we consider the octagonal chains in $\mathcal{G}_n$ with $n \geqslant 3$. Our first lemma gives conditions under which we can replace an α join by a β join and decrease the spectral radius.

LEMMA 3.1. *Let* $G_n^{\alpha'} = Ak_{i-1}\alpha\bar{k}_{i+1}\cdots\bar{k}_n$ *and* $G_n^\beta = Ak_{i-1}\beta k_{i+1}\cdots k_n$ *as depicted in Figure 4. If* $\varphi(A-q,\rho(G_n^\beta)) \leqslant \varphi(A-p,\rho(G_n^\beta))$, *then* $\rho(G_n^{\alpha'}) > \rho(G_n^\beta)$.

Proof. By Lemmas 2.4 and 2.8,

$$\begin{aligned}\varphi(G_n^{\alpha'},x) = {} & \varphi(A,x)[(x^4-3x^2+1)\varphi(B,x)-(x^3-2x)\varphi(B-r,x)]\\ & +\varphi(A-p-q,x)[(x^3-2x)\varphi(B-s,x)-(x^2-1)\varphi(B-r-s,x)]\\ & -\varphi(A-p,x)[(x^4-3x^2+1)\varphi(B-s,x)-(x^3-2x)\varphi(B-r-s,x)]\\ & -\varphi(A-q,x)[(x^3-2x)\varphi(B,x)-(x^2-1)\varphi(B-r,x)]\\ & -2\sum_{C\in\mathcal{C}_{ps}(G_n^{\alpha'})}\varphi(G_n^{\alpha'}-V_C,x)\end{aligned}\tag{3.3}$$

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and

$$\begin{aligned}\varphi(G_n^{\beta},x) = {} & \varphi(A,x)[(x^4-2x^2)\varphi(B,x) \\ & -(x^3-2x)\varphi(B-r,x)-(x^3-x)\varphi(B-s,x)+(x^2-1)\varphi(B-r-s,x)] \\ & +\varphi(A-p-q,x)[(x^2-1)\varphi(B,x)-x\varphi(B-s,x)] \\ & -\varphi(A-p,x)[(x^3-2x)\varphi(B,x)-(x^2-1)\varphi(B-s,x)] \\ & -\varphi(A-q,x)[(x^3-x)\varphi(B,x)-(x^2-1)\varphi(B-r,x) \\ & -x^2\varphi(B-s,x)+x\varphi(B-r-s,x)]-2\sum_{C\in\mathcal{C}_{pa}(G_n^{\beta})}\varphi(G_n^{\beta}-V_C,x). \end{aligned} \tag{3.4}$$

Comparing equations (3.3) and (3.4), using $\mathcal{C}_{ps}(G_n^{\alpha'})=\mathcal{C}_{pa}(G_n^{\beta})$, yields

$$\sum_{C\in\mathcal{C}_{ps}(G_n^{\alpha'})}\varphi(G_n^{\alpha'}-V_C,x)=\sum_{C\in\mathcal{C}_{pa}(G_n^{\beta})}\varphi(G_n^{\beta}-V_C,x).$$

Hence,

$$\begin{aligned}\varphi(G_n^{\alpha'},x)-\varphi(G_n^{\beta},x) = {} & -[(x^2-1)\varphi(A,x)-(x^3-2x)\varphi(A-p,x) \\ & +(x^2-1)\varphi(A-p-q,x)-x\varphi(A-q,x)] \\ & \times[\varphi(B,x)-x\varphi(B-r,x)+\varphi(B-r-s,x)].\end{aligned}$$

For convenience, let $\rho(G_n^{\beta})=\rho$. Since $\varphi(A-q,\rho)\leqslant\varphi(A-p,\rho)$ and $\rho>2$, then $(\rho^3-2\rho)(\varphi(A-p,\rho)-\varphi(A-q,\rho))\geqslant 0$. Hence, $(\rho^3-2\rho)\varphi(A-p,\rho)+\rho\varphi(A-q,\rho)\geqslant(\rho^3-\rho)\varphi(A-q,\rho)$. Note that

$$\varphi(A,\rho)-\rho\varphi(A-q,\rho)+\varphi(A-p-q,\rho)<0,\quad \varphi(B,\rho)-\rho\varphi(B-r,\rho)+\varphi(B-r-s,\rho)<0.$$

Hence,

$$\begin{aligned}\varphi(G_n^{\alpha'},\rho)-\varphi(G_n^{\beta},\rho) = {} & -[(\rho^2-1)\varphi(A,\rho)-(\rho^3-2\rho)\varphi(A-p,\rho) \\ & +(\rho^2-1)\varphi(A-p-q,\rho)-\rho\varphi(A-q,\rho)] \\ & \times[\varphi(B,\rho)-\rho\varphi(B-r,\rho)+\varphi(B-r-s,\rho)] \\ \leqslant {} & -(\rho^2-1)[\varphi(A,\rho)-\rho\varphi(A-q,\rho)+\varphi(A-p-q,\rho)] \\ & \times[\varphi(B,\rho)-\rho\varphi(B-r,\rho)+\varphi(B-r-s,\rho)]<0.\end{aligned}$$

Thus, $\varphi(G_n^{\alpha'},\rho)<\varphi(G_n^{\beta},\rho)$ and by Lemma 2.6, $\rho(G_n^{\alpha'})>\rho(G_n^{\beta})$. ∎

Lemma 3.2 gives conditions under which we can replace an α join by a γ join and decrease the spectral radius.

LEMMA 3.2. *Let* $G_n^{\alpha}=Ak_{i-1}\alpha k_{i+1}\cdots k_n, G_n^{\alpha'}=Ak_{i-1}\alpha\bar{k}_{i+1}\cdots\bar{k}_n$ *and* $G_n^{\gamma}=Ak_{i-1}\gamma k_{i+1}\cdots k_n$ *as depicted in Figure 4.*

(i) *If* $\varphi(A-q,\rho(G_n^{\gamma}))\leqslant\varphi(A-p,\rho(G_n^{\gamma}))$ *and* $\varphi(B-r,\rho(G_n^{\gamma}))\leqslant\varphi(B-s,\rho(G_n^{\gamma}))$, *then* $\rho(G_n^{\alpha})>\rho(G_n^{\gamma})$.
(ii) *If* $\varphi(A-q,\rho(G_n^{\gamma}))\leqslant\varphi(A-p,\rho(G_n^{\gamma}))$ *and* $\varphi(B-r,\rho(G_n^{\gamma}))>\varphi(B-s,\rho(G_n^{\gamma}))$, *then* $\rho(G_n^{\alpha'})>\rho(G_n^{\gamma})$.

Proof. For convenience, denote $\rho(G_n^{\gamma})$ by ρ.

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(i) By Lemmas 2.4 and 2.8,

$$\begin{aligned}\varphi(G_n^\alpha,x)=\ &\varphi(A,x)[(x^4-3x^2+1)\varphi(B,x)-(x^3-2x)\varphi(B-s,x)]\\ &+\varphi(A-p-q,x)[(x^3-2x)\varphi(B-r,x)-(x^2-1)\varphi(B-r-s,x)]\\ &-\varphi(A-p,x)[(x^4-3x^2+1)\varphi(B-r,x)-(x^3-2x)\varphi(B-r-s,x)]\\ &-\varphi(A-q,x)[(x^3-2x)\varphi(B,x)-(x^2-1)\varphi(B-s,x)]\\ &-2\sum_{C\in\mathcal{C}_{pr}(G_n^\alpha)}\varphi(G_n^\alpha-V_C,x)\end{aligned}\tag{3.5}$$

and

$$\begin{aligned}\varphi(G_n^\gamma,x)=\ &\varphi(A,x)[(x^4-2x^2+1)\varphi(B,x)-(x^3-x)\varphi(B-r,x)\\ &-(x^3-x)\varphi(B-s,x)+x^2\varphi(B-r-s,x)]\\ &+\varphi(A-p-q,x)[x^2\varphi(B,x)-x\varphi(B-s,x)-x\varphi(B-r,x)+\varphi(B-r-s,x)]\\ &-\varphi(A-p,x)[(x^3-x)\varphi(B,x)-(x^2-1)\varphi(B-r,x)\\ &-x^2\varphi(B-s,x)+x\varphi(B-r-s,x)]\\ &-\varphi(A-q,x)[(x^3-x)\varphi(B,x)-(x^2-1)\varphi(B-s,x)\\ &-Fx^2\varphi(B-r,x)\varphi(B-r-s,x)]-2\sum_{C\in\mathcal{C}_{pa}(G_n^\gamma)}\varphi(G_n^\gamma-V_C,x).\end{aligned}\tag{3.6}$$

Note that $\mathcal{C}_{pr}(G_n^\alpha)=\mathcal{C}_{pa}(G_n^\gamma)$. Then compare (3.5) with (3.6),

$$\sum_{C\in\mathcal{C}_{pr}(G_n^\alpha)}\varphi(G_n^\alpha-V_C,x)=\sum_{C\in\mathcal{C}_{pa}(G_n^\gamma)}\varphi(G_n^\gamma-V_C,x).$$

Hence,

$$\begin{aligned}\varphi(G_n^\alpha,x)-\varphi(G_n^\gamma,x)=\ &-[x^2\varphi(A,x)-(x^3-x)\varphi(A-p,x)\\ &+x^2\varphi(A-p-q,x)-x\varphi(A-q,x)]\\ &\times[\varphi(B,x)-x\varphi(B-r,x)+\varphi(B-r-s,x)]\\ &-x[\varphi(A,x)-x\varphi(A-p,x)+\varphi(A-p-q,x)]\\ &\times[\varphi(B-r,x)-\varphi(B-s,x)].\end{aligned}\tag{3.7}$$

Bearing mind that $\varphi(A-q,\rho)\leqslant\varphi(A-p,\rho)$ and by Lemma 2.5,

$$(\rho^3-\rho)\varphi(A-p,\rho)+\rho\varphi(A-q,\rho)\geqslant\rho^3\varphi(A-q,\rho),$$

$$\varphi(B,\rho)-\rho\varphi(B-r,\rho)+\varphi(B-r-s,\rho)<0.$$

Thus,

$$\begin{aligned}\varphi(G_n^\alpha,\rho)-\varphi(G_n^\gamma,\rho)\leqslant&-\rho^2[\varphi(A,\rho)-\rho\varphi(A-q,\rho)+\varphi(A-p-q,\rho)]\\ &\times[\varphi(B,\rho)-\rho\varphi(B-r,\rho)+\varphi(B-r-s,\rho)]\\ &-\rho[\varphi(A,\rho)-\rho\varphi(A-p,\rho)+\varphi(A-p-q,\rho)]\\ &\times[\varphi(B-r,\rho)-\varphi(B-s,\rho)].\end{aligned}$$

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Combining Lemma 2.5,

$$\varphi(A,\rho)-\rho\varphi(A-p,\rho)+\varphi(A-p-q,\rho)<0,\quad \varphi(A,\rho)-\rho\varphi(A-q,\rho)+\varphi(A-p-q,\rho)<0.$$

Note that $\varphi(B-r,\rho)\leqslant\varphi(B-s,\rho)$. Hence, we get $\varphi(G_n^\alpha,\rho)<\varphi(G_n^\gamma,\rho)$. By Lemma 2.6, $\rho(G_n^\alpha)>\rho(G_n^\gamma)$.

(ii) Note that $\mathcal{C}_{ps}(G_n^{\alpha'})=\mathcal{C}_{pa}(G_n^\gamma)$. Then combining (3.3) and (3.6) yields

$$\begin{aligned}\varphi(G_n^{\alpha'},x)-\varphi(G_n^\gamma,x)=&-x[x\varphi(A,x)-(x^2-1)\varphi(A-p,x)+x\varphi(A-p-q,x)\\&-\varphi(A-q,x)]\times[\varphi(B,x)-x\varphi(B-s,x)-\varphi(B-r-s,x)]\\&-[x\varphi(A,x)-(x^2-1)\varphi(A-p,x)+x\varphi(A-p-q,x)\\&-\varphi(A-q,x)]\times[\varphi(B-s,x)-\varphi(B-r,x)].\end{aligned}$$

Note that $\varphi(A-q,\rho)\leqslant\varphi(A-p,\rho)$ and $\rho>2$. Hence, $(\rho^2-1)(\varphi(A-p,\rho)-\varphi(A-q,\rho))\geqslant0$, that is,

$$(\rho^2-1)\varphi(A-p,\rho)+\varphi(A-q,\rho)\geqslant\rho^2\varphi(A-q,\rho).$$

Together with Lemma 2.5,

$$\varphi(A,\rho)-\rho\varphi(A-q,\rho)+\varphi(A-p-q,\rho)<0,\quad \varphi(B,\rho)-\rho\varphi(B-s,\rho)-\varphi(B-r-s,\rho)<0.$$

Hence, by $\varphi(B-r,\rho)>\varphi(B-s,\rho)$,

$$\begin{aligned}\varphi(G_n^{\alpha'},\rho)-\varphi(G_n^\gamma,\rho)\leqslant&-\rho^2[\varphi(A,\rho)-\rho\varphi(A-q,\rho)+\varphi(A-p-q,\rho)]\\&\times[\varphi(B,\rho)-\rho\varphi(B-s,\rho)+\varphi(B-r-s,\rho)]\\&-\rho[\varphi(A,\rho)-\rho\varphi(A-q,\rho)+\varphi(A-p-q,\rho)]\\&\times[\varphi(B-s,\rho)-\varphi(B-r,\rho)]<0.\end{aligned}$$

According to Lemma 2.6, $\rho(G_n^{\alpha'})>\rho(G_n^\gamma)$. ∎

Lemma 3.3 gives conditions under which we can replace an α join by a δ join and decrease the spectral radius.

LEMMA 3.3. *Let* $G_n^\alpha=Ak_{i-1}\alpha k_{i+1}\cdots k_n$, $G_n^{\alpha'}=Ak_{i-1}\alpha\bar{k}_{i+1}\cdots\bar{k}_n$ *and* $G_n^\delta=Ak_{i-1}\delta k_{i+1}\cdots k_n$ *as depicted in Figure 4.*

(i) *If* $\varphi(A-q,\rho(G_n^\delta))\leqslant\varphi(A-p,\rho(G_n^\delta))$ *and* $\varphi(B-r,\rho(G_n^\delta))\leqslant\varphi(B-s,\rho(G_n^\delta))$, *then* $\rho(G_n^\alpha)>\rho(G_n^\delta)$.
(ii) *If* $\varphi(B-r,\rho(G_n^\delta))>\varphi(B-s,\rho(G_n^\delta))$, *then* $\rho(G_n^{\alpha'})>\rho(G_n^\delta)$.

Proof. For convenience, denote $\rho(G_n^\delta)$ by ρ.

(i) By Lemmas 2.4 and 2.8,

$$\begin{aligned}\varphi(G_n^\delta,x)=&\,\varphi(A,x)[(x^4-2x^2)\varphi(B,x)-(x^3-2x)\varphi(B-s,x)-(x^3-x)\varphi(B-r,x)\\&+(x^2-1)\varphi(B-r-s,x)]+\varphi(A-p-q,x)[(x^2-1)\varphi(B,x)-x\varphi(B-r,x)]\\&-\varphi(A-p,x)[(x^3-x)\varphi(B,x)-(x^2-1)\varphi(B-s,x)-x^2\varphi(B-r,x)\\&+x\varphi(B-r-s,x)]-\varphi(A-q,x)[(x^3-2x)\varphi(B,x)-(x^2-1)\varphi(B-r,x)]\\&-2\sum_{C\in\mathcal{C}_{pa}(G_n^\delta)}\varphi(G_n^\delta-V_C,x).\end{aligned}\tag{3.8}$$

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Note that $\mathcal{C}_{pr}(G_n^{\alpha}) = \mathcal{C}_{pa}(G_n^{\delta})$. Hence, in view of (3.5) and (3.8),

$$\begin{aligned}\varphi(G_n^{\alpha},x)-\varphi(G_n^{\delta},x)= &-(x^2-1)[\varphi(A,x)-x\varphi(A-p,x)+\varphi(A-p-q,x)]\\ &\times[\varphi(B,x)-x\varphi(B-r,x)\\ &+\varphi(B-r-s,x)]-(x^2-1)[\varphi(A-q,x)-\varphi(A-p,x)]\\ &\times[\varphi(B-r,x)-\varphi(B-s,x)].\end{aligned}$$

Combining Lemma 2.5 yields

$$\varphi(A,\rho)-\rho\varphi(A-p,\rho)+\varphi(A-p-q,\rho)<0,\quad \varphi(B,\rho)-\rho\varphi(B-r,\rho)+\varphi(B-r-s,\rho)<0.$$

Notice that $\varphi(A-q,\rho)\leqslant\varphi(A-p,\rho), \varphi(B-r,\rho)\leqslant\varphi(B-s,\rho)$ and $\rho>2$. Hence, $\varphi(G_n^{\alpha},\rho)<\varphi(G_n^{\delta},\rho)$. By Lemma 2.6, $\rho(G_n^{\alpha})>\rho(G_n^{\delta})$.

(ii) Put $\triangle := \varphi(G_n^{\alpha'},x)-\varphi(G_n^{\delta},x)$. Note that $\mathcal{C}_{ps}(G_n^{\alpha'}) = \mathcal{C}_{pa}(G_n^{\delta})$. Hence, in view of (3.3) and (3.8), we get

$$\begin{aligned}\triangle =&(1-x^2)[\varphi(A,x)-x\varphi(A-p,x)+\varphi(A-p-q,x)]\\ &\times[\varphi(B,x)-x\varphi(B-s,x)+\varphi(B-r-s,x)]\\ &-x[\varphi(A,x)-x\varphi(A-p,x)+\varphi(A-p-q,x)][\varphi(B-s,x)-\varphi(B-r,x)].\end{aligned}$$

By Lemma 2.5,

$$\varphi(A,\rho)-\rho\varphi(A-p,\rho)+\varphi(A-p-q,\rho)<0,\quad \varphi(B,\rho)-\rho\varphi(B-s,\rho)+\varphi(B-r-s,\rho)<0.$$

According to $\varphi(B-r,\rho)>\varphi(B-s,\rho)$ and $\rho>2$, $\varphi(G_n^{\alpha'},\rho)<\varphi(G_n^{\delta},\rho)$. By Lemma 2.6, $\rho(G_n^{\alpha'})>\rho(G_n^{\delta})$. ☐

Lemma 3.4 gives conditions under which we can replace an α join by an ε join and decrease the spectral radius.

LEMMA 3.4. *Let $G_n^{\alpha} = Ak_{i-1}\alpha k_{i+1}\cdots k_n, G_n^{\alpha'} = Ak_{i-1}\alpha\bar{k}_{i+1}\cdots\bar{k}_n$ and $G_n^{\varepsilon} = Ak_{i-1}\varepsilon k_{i+1}\cdots k_n$ as depicted in Figure 4.*

(i) *If $\varphi(A-q,\rho(G_n^{\varepsilon}))<\varphi(A-p,\rho(G_n^{\varepsilon}))$ and $\varphi(B-r,\rho(G_n^{\varepsilon}))\geqslant\varphi(B-s,\rho(G_n^{\varepsilon}))$, then $\rho(G_n^{\alpha})>\rho(G_n^{\varepsilon})$.*
(ii) *If $\varphi(A-q,\rho(G_n^{\varepsilon}))<\varphi(A-p,\rho(G_n^{\varepsilon}))$ and $\varphi(B-r,\rho(G_n^{\varepsilon}))<\varphi(B-s,\rho(G_n^{\varepsilon}))$, then $\rho(G_n^{\alpha'})>\rho(G_n^{\varepsilon})$.*

Proof. For convenience, denote $\rho(G_n^{\varepsilon})$ by ρ.

(i) By Lemmas 2.4 and 2.8,

$$\begin{aligned}\varphi(G_n^{\varepsilon},x)=&\varphi(A,x)[(x^4-3x^2+1)\varphi(B,x)-(x^3-2x)\varphi(B-r,x)]\\ &+\varphi(A-p-q,x)[(x^3-2x)\varphi(B-s,x)-(x^2-1)\varphi(B-r-s,x)]\\ &-\varphi(A-p,x)[(x^3-2x)\varphi(B,x)-(x^2-1)\varphi(B-r,x)]\\ &-\varphi(A-q,x)[(x^4-3x^2+1)\varphi(B-s,x)-(x^3-2x)\varphi(B-r-s,x)]\\ &-2\sum_{C\in\mathcal{C}_{pa}(G_n^{\varepsilon})}\varphi(G_n^{\varepsilon}-V_C,x).\end{aligned}\tag{3.9}$$

Note that $\mathcal{C}_{pr}(G_n^{\alpha}) = \mathcal{C}_{pa}(G_n^{\varepsilon})$. In view of (3.5) and (3.9),

$$\begin{aligned}\varphi(G_n^{\alpha},x)-\varphi(G_n^{\varepsilon},x)=&-(x^3-2x)[\varphi(A,x)+\varphi(A-p-q,x)][\varphi(B-s,x)-\varphi(B-r,x)]\\ &+(x^3-2x)\varphi(A-p,x)[\varphi(B,x)-x\varphi(B-r,x)+\varphi(B-r-s,x)]\\ &-(x^3-2x)\varphi(A-q,x)[\varphi(B,x)-x\varphi(B-s,x)+\varphi(B-r-s,x)].\end{aligned}$$

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By Lemma 2.5, $\varphi(B,\rho)-\rho\varphi(B-s,\rho)+\varphi(B-r-s,\rho)<0$. Together with $\varphi(A-q,\rho)<\varphi(A-p,\rho)$ and $\rho>2$,

$$\begin{aligned}\varphi(G_n^{\alpha},\rho)-\varphi(G_n^{\varepsilon},\rho)&<-(\rho^3-2\rho)[\varphi(A,\rho)+\varphi(A-p-q,\rho)][\varphi(B-s,\rho)-\varphi(B-r,\rho)]\\&\quad+(\rho^3-2\rho)\varphi(A-q,\rho)[\varphi(B,\rho)-\rho\varphi(B-r,\rho)+\varphi(B-r-s,\rho)]\\&\quad-(\rho^3-2\rho)\varphi(A-q,\rho)[\varphi(B,\rho)-\rho\varphi(B-s,\rho)+\varphi(B-r-s,\rho)]\\&=-(\rho^3-2\rho)[\varphi(A,\rho)+\varphi(A-p-q,\rho)][\varphi(B-s,\rho)-\varphi(B-r,\rho)]\\&\quad+(\rho^4-2\rho^2)\varphi(A-q,\rho)[\varphi(B-s,\rho)-\varphi(B-r,\rho)]\\&=-(\rho^3-2\rho)[\varphi(A,\rho)-\rho\varphi(A-q,\rho)+\varphi(A-p-q,\rho)]\\&\quad\times[\varphi(B-s,\rho)-\varphi(B-r,\rho)].\end{aligned}$$

Combining Lemma 2.5 yields $\varphi(A,\rho)-\rho\varphi(A-q,\rho)+\varphi(A-p-q,\rho)<0$. Note that $\varphi(B-r,\rho)\geqslant\varphi(B-s,\rho)$ and $\rho>2$. Hence, we get $\varphi(G_n^{\alpha},\rho)<\varphi(G_n^{\varepsilon},\rho)$. By Lemma 2.6, $\rho(G_n^{\alpha})>\rho(G_n^{\varepsilon})$.

(ii) Note that $\mathcal{C}_{ps}(G_n^{\alpha'})=\mathcal{C}_{pa}(G_n^{\varepsilon})$. In view of (3.3) and (3.9), we get

$$\begin{aligned}\varphi(G_n^{\alpha'},x)-\varphi(G_n^{\varepsilon},x)&=-[\varphi(A-q,x)-\varphi(A-p,x)]\\&\quad\times[(x^3-2x)\varphi(B,x)-(x^4-3x^2+1)\varphi(B-s,x)\\&\quad+(x^3-2x)\varphi(B-r-s,x)-(x^2-1)\varphi(B-r,x)].\end{aligned}$$

Note that $\varphi(B-r,\rho)<\varphi(B-s,\rho)$ and $\rho>2$. Hence,

$$\begin{aligned}&(\rho^4-3\rho^2+1)(\varphi(B-s,\rho)-\varphi(B-r,\rho))\\&=[\rho^2(\rho^2-1)+\rho^2+1](\varphi(B-s,\rho)-\varphi(B-r,\rho))\\&>0,\end{aligned}$$

that is,

$$(\rho^4-3\rho^2+1)\varphi(B-s,\rho)+(\rho^2-1)\varphi(B-r,\rho)>(\rho^4-2\rho^2)\varphi(B-r,\rho).$$

As $\varphi(A-q,\rho)<\varphi(A-p,\rho)$ and $\rho>2$,

$$\varphi(G_n^{\alpha'},\rho)-\varphi(G_n^{\varepsilon},\rho)<-(\rho^3-2\rho)[\varphi(A-q,\rho)-\varphi(A-p,\rho)][\varphi(B,\rho)-\rho\varphi(B-r,\rho)+\varphi(B-r-s,\rho)].$$

Note that $\varphi(B,\rho)-\rho\varphi(B-r,\rho)+\varphi(B-r-s,\rho)<0$. Then $\varphi(G_n^{\alpha'},\rho)<\varphi(G_n^{\varepsilon},\rho)$. By Lemma 2.6, $\rho(G_n^{\alpha'})>\rho(G_n^{\varepsilon})$. ∎

Lemma 3.5 gives conditions under which we can replace a γ join by an α join and increase the spectral radius.

Lemma 3.5. *Let* $G_n^{\gamma}=Ak_{i-1}\gamma k_{i+1}\cdots k_n$, $G_n^{\gamma'}=Ak_{i-1}\gamma\bar{k}_{i+1}\cdots\bar{k}_n$ *and* $G_n^{\alpha}=Ak_{i-1}\alpha k_{i+1}\cdots k_n$ *as depicted in Figure 4 with* $A\cong\bar{A}$. *Then* $\rho(G_n^{\gamma})<\rho(G_n^{\alpha})$ *if* $\varphi(B-r,\rho(G_n^{\gamma}))\leqslant\varphi(B-s,\rho(G_n^{\gamma}))$ *and* $\rho(G_n^{\gamma'})<\rho(G_n^{\alpha})$ *otherwise.*

Proof. As $A\cong\bar{A}$, it is obvious that $\varphi(A-q,x)=\varphi(A-p,x)$. Let $\rho(G_n^{\gamma})=\rho$. By Eq. (3.7)

$$\begin{aligned}\varphi(G_n^{\alpha},x)-\varphi(G_n^{\gamma},x)&=-x^2[\varphi(A,x)-(x-1)\varphi(A-p,x)+\varphi(A-p-q,x)\\&\quad-\varphi(A-q,x)]\times[\varphi(B,x)-x\varphi(B-r,x)+\varphi(B-r-s,x)]\\&\quad-x[\varphi(A,x)-x\varphi(A-p,x)+\varphi(A-p-q,x)]\\&\quad\times[\varphi(B-r,x)-\varphi(B-s,x)].\end{aligned}$$

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Note that $\varphi(A-q,x)=\varphi(A-p,x)$. Hence,

$$\begin{aligned}\varphi(G_n^{\alpha},\rho)-\varphi(G_n^{\gamma},\rho)=&-\rho^2[\varphi(A,\rho)-\rho\varphi(A-p,\rho)+\varphi(A-p-q,\rho)]\\&\times[\varphi(B,\rho)-\rho\varphi(B-r,\rho)+\varphi(B-r-s,\rho)]\\&-\rho[\varphi(A,\rho)-\rho\varphi(A-p,\rho)+\varphi(A-p-q,\rho)]\\&\times[\varphi(B-r,\rho)-\varphi(B-s,\rho)].\end{aligned}$$

According to Lemma 2.5,

$$\varphi(A,\rho)-\rho\varphi(A-p,\rho)+\varphi(A-p-q,\rho)<0,\quad \varphi(B,\rho)-\rho\varphi(B-r,\rho)+\varphi(B-r-s,\rho)<0.$$

If $\varphi(B-r,\rho)\leqslant\varphi(B-s,\rho)$, then together with $\rho>2$, $\varphi(G_n^{\alpha},\rho)<\varphi(G_n^{\gamma},\rho)$. By Lemma 2.6, the result $\rho(G_n^{\alpha})>\rho(G_n^{\gamma})$ holds.

Next we consider $\varphi(B-r,\rho)>\varphi(B-s,\rho)$. By Lemmas 2.4 and 2.8,

$$\begin{aligned}\varphi(G_n^{\gamma'},x)=&\varphi(A,x)[(x^4-2x^2+1)\varphi(B,x)-(x^3-x)\varphi(B-r,x)\\&-(x^3-x)\varphi(B-s,x)+x^2\varphi(B-r-s,x)]\\&+\varphi(A-p-q,x)[x^2\varphi(B,x)-x\varphi(B-s,x)-x\varphi(B-r,x)\\&+\varphi(B-r-s,x)]-\varphi(A-p,x)[(x^3-x)\varphi(B,x)-(x^2-1)\varphi(B-s,x)\\&-x^2\varphi(B-r,x)+x\varphi(B-r-s,x)]\\&-\varphi(A-q,x)[(x^3-x)\varphi(B,x)-(x^2-1)\varphi(B-r,x)\\&-x^2\varphi(B-s,x)+x\varphi(B-r-s,x)]-2\sum_{C\in\mathcal{C}_{pa}(G_n^{\gamma'})}\varphi(G_n^{\gamma'}-V_C,x).\end{aligned}\tag{3.10}$$

Note that $\mathcal{C}_{pr}(G_n^{\alpha})=\mathcal{C}_{pa}(G_n^{\gamma'})$. Hence, in view of (3.5) and (3.10),

$$\begin{aligned}\varphi(G_n^{\alpha},x)-\varphi(G_n^{\gamma'},x)=&-x\varphi(A,x)[x\varphi(B,x)-(x^2-1)\varphi(B-r,x)\\&+x\varphi(B-r-s,x)-\varphi(B-s,x)]\\&-x\varphi(A-p-q,x)[x\varphi(B,x)-(x^2-1)\varphi(B-r,x)\\&+x\varphi(B-r-s,x)-\varphi(B-s,x)]\\&+(x^2-1)\varphi(A-p,x)[x\varphi(B,x)-(x^2-1)\varphi(B-r,x)\\&+x\varphi(B-r-s,x)-\varphi(B-s,x)]\\&+\varphi(A-q,x)[x\varphi(B,x)-(x^2-1)\varphi(B-r,x)\\&+x\varphi(B-r-s,x)-\varphi(B-s,x)].\end{aligned}$$

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Since $\varphi(A-q,x)=\varphi(A-p,x)$,

$$\begin{aligned}\varphi(G_n^{\alpha},x)-\varphi(G_n^{\gamma'},x)=&-x\varphi(A,x)[x\varphi(B,x)-(x^2-1)\varphi(B-r,x)\\&+x\varphi(B-r-s,x)-\varphi(B-s,x)]\\&-x\varphi(A-p-q,x)[x\varphi(B,x)-(x^2-1)\varphi(B-r,x)\\&+x\varphi(B-r-s,x)-\varphi(B-s,x)]\\&+x^2\varphi(A-p,x)[x\varphi(B,x)-(x^2-1)\varphi(B-r,x)\\&+x\varphi(B-r-s,x)-\varphi(B-s,x)]\\=&-x[\varphi(A,x)-x\varphi(A-p,x)+\varphi(A-p-q,x)]\\&\times[x\varphi(B,x)-(x^2-1)\varphi(B-r,x)\\&+x\varphi(B-r-s,x)-\varphi(B-s,x)].\end{aligned}$$

Note that $\varphi(B-r,\rho)>\varphi(B-s,\rho)$. Hence,

$$(\rho^2-1)\varphi(B-r,\rho)+\varphi(B-s,\rho)>\rho^2\varphi(B-s,\rho).$$

By the condition $A\cong\bar{A}$, $\rho(G_n^{\gamma'})=\rho(\bar{G}_n^{\gamma'})=\rho(G_n^{\gamma})=\rho$. According to Lemma 2.5,

$$\begin{aligned}&\varphi(A,\rho)-\rho\varphi(A-p,\rho)+\varphi(A-p-q,\rho)<0,\\&\varphi(B,\rho)-\rho\varphi(B-s,\rho)+\varphi(B-r-s,\rho)<0.\end{aligned}$$

As $\rho>2$,

$$\begin{aligned}\varphi(G_n^{\alpha},\rho)-\varphi(G_n^{\gamma'},\rho)<&-\rho^2[\varphi(A,\rho)-\rho\varphi(A-p,\rho)+\varphi(A-p-q,\rho)]\\&\times[\varphi(B,\rho)-\rho\varphi(B-s,\rho)+\varphi(B-r-s,\rho)]<0,\end{aligned}$$

Hence, $\varphi(G_n^{\alpha},\rho)<\varphi(G_n^{\gamma'},\rho)$, i.e., $\varphi(G_n^{\alpha},\rho(G_n^{\gamma'}))<\varphi(G_n^{\gamma'},\rho(G_n^{\gamma'}))$ and then $\rho(G_n^{\gamma'})<\rho(G_n^{\alpha})$. ☐

Lemma 3.6 gives conditions under which we can replace a γ join by a β join and increase the spectral radius.

LEMMA 3.6. *Let $G_n^{\gamma}=Ak_{i-1}\gamma k_{i+1}\cdots k_n$ and $G_n^{\beta}=Ak_{i-1}\beta k_{i+1}\cdots k_n$ as depicted in Figure 4. If $A\cong\bar{A}$, then $\rho(G_n^{\gamma})<\rho(G_n^{\beta})$.*

Proof. Note that $\mathcal{C}_{pa}(G_n^{\beta})=\mathcal{C}_{pa}(G_n^{\gamma})$ and $\varphi(A-p,x)=\varphi(A-q,x)$. Hence, in view of (3.4) and (3.6),

$$\varphi(G_n^{\beta},x)-\varphi(G_n^{\gamma},x)=-[\varphi(A,x)-x\varphi(A-p,x)+\varphi(A-p-q,x)][\varphi(B,x)-x\varphi(B-r,x)+\varphi(B-r-s,x)].$$

Denote $\rho(G_n^{\gamma})$ by ρ. By Lemma 2.5,

$$\varphi(A,\rho)-\rho\varphi(A-p,\rho)+\varphi(A-p-q,\rho)<0,\quad \varphi(B,\rho)-\rho\varphi(B-r,\rho)+\varphi(B-r-s,\rho)<0.$$

Then $\varphi(G_n^{\beta},\rho)<\varphi(G_n^{\gamma},\rho)$. And by Lemma 2.6, the result $\rho(G_n^{\gamma})<\rho(G_n^{\beta})$ holds. ☐

Lemma 3.7 gives conditions under which we can replace a γ join by a δ join and increase the spectral radius.

LEMMA 3.7. *Let $G_n^{\gamma}=Ak_{i-1}\gamma k_{i+1}\cdots k_n$ and $G_n^{\delta}=Ak_{i-1}\delta k_{i+1}\cdots k_n$ as depicted in Figure 4. If $A\cong\bar{A}$, then $\rho(G_n^{\gamma})<\rho(G_n^{\delta})$.*

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Proof. Note that $G_n^\delta \cong \bar{G}_n^\delta$ and $G_n^{\gamma'} \cong \bar{G}_n^{\gamma'}$. Together with $A \cong \bar{A}$, $\bar{G}_n^\delta \cong G_n^{\beta'}$ and $\bar{G}_n^{\gamma'} = G_n^\gamma$. By Lemma 3.6, we get $\rho(G_n^\beta) > \rho(G_n^\gamma)$ and $\rho(G_n^{\beta'}) > \rho(G_n^{\gamma'})$. Thus, $\rho(G_n^\delta) = \rho(\bar{G}_n^\delta) = \rho(G_n^{\beta'}) > \rho(G_n^{\gamma'}) = \rho(\bar{G}_n^{\gamma'}) = \rho(G_n^\gamma)$, as desired. ∎

Lemma 3.8 gives conditions under which we can replace a γ join by an ε join and increase the spectral radius.

Lemma 3.8. *Let $G_n^\gamma = Ak_{i-1}\gamma k_{i+1}\cdots k_n, G_n^{\gamma'} = Ak_{i-1}\gamma\bar{k}_{i+1}\cdots\bar{k}_n$ and $G_n^\varepsilon = Ak_{i-1}\varepsilon k_{i+1}\cdots k_n$ as depicted in Figure 4. Suppose $A \cong \bar{A}$, then $\rho(G_n^{\gamma'}) < \rho(G_n^\varepsilon)$ if $\varphi(B-r,\rho(G_n^\gamma)) \leqslant \varphi(B-s,\rho(G_n^\gamma))$ and $\rho(G_n^\gamma) < \rho(G_n^\varepsilon)$ otherwise.*

Proof. Note that $G_n^\varepsilon \cong \bar{G}_n^\varepsilon$. Hence, together with $A \cong \bar{A}$ one has $\bar{G}_n^\varepsilon \cong G_n^{\alpha'}$. Assume, without loss of generality, that $\varphi(B-r,\rho(G_n^\gamma)) \leqslant \varphi(B-s,\rho(G_n^\gamma))$. Then by Lemma 3.5, $\rho(G_n^\alpha) > \rho(G_n^\gamma)$. According to the structure of G_n^α and $G_n^{\alpha'}$ (respectively G_n^γ and $G_n^{\gamma'}$), under the condition $\varphi(B-s,\rho(G_n^\gamma)) \leqslant \varphi(B-r,\rho(G_n^\gamma))$, the result $\rho(G_n^\alpha) > \rho(G_n^\gamma)$ is equivalent to $\rho(G_n^{\alpha'}) > \rho(G_n^{\gamma'})$. Hence, $\rho(G_n^\varepsilon) = \rho(\bar{G}_n^\varepsilon) = \rho(G_n^{\alpha'}) > \rho(G_n^{\gamma'})$, as desired. ∎

4. Proofs of our main results. In this section, we determine the graph with the maximum (respectively minimum) spectral radius among all octagonal chains in $\mathcal{G}_n$.

Proof of Theorem 1.1. We know $G_1 = L_1 = Z_1^1 = Z_1^2 = H_1^1 = H_1^2$ and $G_2 = L_2 = Z_2^1 = Z_2^2 = H_2^1 = H_2^2$. Then in order to complete the proof, it suffices to consider the case $n \geqslant 3$.

Let $G_n = \gamma\gamma k_3\cdots k_n$ be an octagonal chain with the maximum spectral radius in $\mathcal{G}_n$. We show $G_n \cong H_n^1 = \gamma\gamma\alpha\cdots\alpha$ or $G_n \cong H_n^1 = \gamma\gamma\varepsilon\cdots\varepsilon$. Note that $\gamma\gamma\alpha\cdots\alpha \cong \gamma\gamma\varepsilon\cdots\varepsilon$. Here, we only show $G_n \cong H_n^1 = \gamma\gamma\alpha\cdots\alpha$. Suppose to the contrary that $G_n \ncong H_n^1$. Denote by k_i the first element of $k_3, k_4, \ldots, k_n$ such that $k_i \in \{\beta,\gamma,\delta,\varepsilon\}$. Let $A = k_1\cdots k_{i-2}$ and $B = k_i\cdots k_n$. Note that $A \cong H_{i-2}^1$. Denote by pq the common edge of O_{i-2} and O_{i-1} and rs the common edge of O_{i-1} and O_i. Then by Lemma 2.7, $\varphi(A-q,\rho(G_n)) \leqslant \varphi(A-p,\rho(G_n))$.

If $k_i = \beta$, then $G_n = \gamma\gamma\alpha\cdots\alpha\beta k_{i+1}\cdots k_n$. Let $G_n' = \gamma\gamma\alpha\cdots\alpha\alpha\bar{k}_{i+1}\cdots\bar{k}_n$. By Lemma 3.1, $\rho(G_n) < \rho(G_n')$, which contradicts the choice of G_n.

If $k_i = \gamma$, then $G_n = \gamma\gamma\alpha\cdots\alpha\gamma k_{i+1}\cdots k_n$. Let

$$G_n' = \gamma\gamma\alpha\cdots\alpha\alpha k_{i+1}\cdots k_n \quad \text{and} \quad G_n'' = \gamma\gamma\alpha\cdots\alpha\alpha\bar{k}_{i+1}\cdots\bar{k}_n.$$

By Lemma 3.2, we know that if $\varphi(B-r,\rho(G_n)) \leqslant \varphi(B-s,\rho(G_n))$, then $\rho(G_n) < \rho(G_n')$; if $\varphi(B-r,\rho(G_n)) > \varphi(B-s,\rho(G_n))$, then $\rho(G_n) < \rho(G_n'')$, a contradiction.

If $k_i = \delta$, then $G_n = \gamma\gamma\alpha\cdots\alpha\delta k_{i+1}\cdots k_n$. Let

$$G_n' = \gamma\gamma\alpha\cdots\alpha\alpha k_{i+1}\cdots k_n \quad \text{and} \quad G_n'' = \gamma\gamma\alpha\cdots\alpha\alpha\bar{k}_{i+1}\cdots\bar{k}_n.$$

By Lemma 3.3, we know that if $\varphi(B-r,\rho(G_n)) \leqslant \varphi(B-s,\rho(G_n))$, then $\rho(G_n) < \rho(G_n')$; if $\varphi(B-r,\rho(G_n)) > \varphi(B-s,\rho(G_n))$, then $\rho(G_n) < \rho(G_n'')$, a contradiction.

If $k_i = \varepsilon$ with $i = 3$, then $G_n = \gamma\gamma\varepsilon k_4\cdots k_n$ and $A = \gamma$. Note that $A \cong \bar{A} = \gamma$. Then we consider the graph $\bar{G}_n = \gamma\gamma\alpha\bar{k}_4\cdots\bar{k}_n$. Denote by $\bar{k}_j$ the first element of $\bar{k}_4,\ldots,\bar{k}_n$ such that $\bar{k}_j \in \{\beta,\gamma,\delta,\varepsilon\}$. Let $A' = \gamma\gamma\alpha\bar{k}_4\cdots\bar{k}_{j-2}$ and $B' = \bar{k}_j\cdots\bar{k}_n$. Note that $A' \cong H_{j-2}^1$. Denote by $p'q'$ the common edge of O_{j-2} and O_{j-1} and $r's'$ the common edge of O_{j-1} and O_j. Then by Lemma 2.7, $\varphi(A'-q',\rho(\bar{G}_n)) < \varphi(A'-p',\rho(\bar{G}_n))$.

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Note that $\bar{k}_j \in \{\beta, \gamma, \delta, \varepsilon\}$. Hence, by Lemmas 3.1–3.4, there exists another graph G'_n in $\mathcal{G}_n$ such that $\rho(G_n) = \rho(\bar{G}_n) < \rho(G'_n)$, a contradiction.

If $k_i = \varepsilon$ with $i \geqslant 4$, then $G_n = \gamma\gamma\alpha \cdots \alpha\varepsilon k_{i+1} \cdots k_n$ and $A \cong H^1_{i-2}$ contains at least two octagons. Then by Lemma 2.7, $\varphi(A - q, \rho(G_n)) < \varphi(A - p, \rho(G_n))$. Let $G'_n = \gamma\gamma\alpha \cdots \alpha\alpha k_{i+1} \cdots k_n$ and $G''_n = \gamma\gamma\alpha \cdots \alpha\alpha\bar{k}_{i+1} \cdots \bar{k}_n$. By Lemma 3.4, we know that if $\varphi(B - r, \rho(G_n)) \leqslant \varphi(B - s, \rho(G_n))$, then $\rho(G_n) < \rho(G''_n)$; if $\varphi(B - r, \rho(G_n)) > \varphi(B - s, \rho(G_n))$, then $\rho(G_n) < \rho(G'_n)$, which contradicts the choice of G_n.

Hence, $G_n = \gamma\gamma\alpha\alpha \cdots \alpha$, that is, the helix chain H^1_n maximizes the spectral radius among $\mathcal{G}_n$. □

Proof of Theorem 1.2. We know that $G_1 = L_1 = Z^1_1 = Z^2_1 = H^1_1 = H^2_1$ and $G_2 = L_2 = Z^1_2 = Z^2_2 = H^1_2 = H^2_2$. Thus, it suffices to consider the case $n \geqslant 3$. Let $G_n = \gamma\gamma k_3 \cdots k_n$ be an octagonal chain with the minimum spectral radius in $\mathcal{G}_n$. We show $G_n \cong L_n = \gamma\gamma \cdots \gamma$.

Suppose to the contrary that $G_n \ncong L_n$. Denote by k_i the first element of $k_3, k_4, \ldots, k_n$ such that $k_i \neq \gamma$, i.e. $G_n = \gamma\gamma \cdots \gamma k_i k_{i+1} \cdots k_n$, where $k_i \in \{\alpha, \beta, \delta, \varepsilon\}$. Let $A = k_1 \cdots k_{i-2}$ and $B = k_i \cdots k_n$. Note that $A \cong \bar{A}$. Denote by pq the common edge of O_{i-2} and O_{i-1} and rs the common edge of O_{i-1} and O_i.

If $k_i = \alpha$, then $G_n = \gamma\gamma \cdots \gamma\alpha k_{i+1} \cdots k_n$. Let $G'_n = \gamma\gamma \cdots \gamma\gamma k_{i+1} \cdots k_n$ and $G''_n = \gamma\gamma \cdots \gamma\gamma\bar{k}_{i+1} \cdots \bar{k}_n$. By Lemma 3.5, we know that if $\varphi(B-r, \rho(G'_n)) \leqslant \varphi(B-s, \rho(G'_n))$, then $\rho(G_n) > \rho(G'_n)$; if $\varphi(B-r, \rho(G'_n)) > \varphi(B - s, \rho(G'_n))$, then $\rho(G_n) > \rho(G''_n)$, which contradicts the choice of G_n.

If $k_i = \beta$, then $G_n = \gamma\gamma \cdots \gamma\beta k_{i+1} \cdots k_n$. Let $G'_n = \gamma\gamma \cdots \gamma\gamma k_{i+1} \cdots k_n$. By Lemma 3.6, we know that $\rho(G_n) > \rho(G'_n)$, a contradiction.

If $k_i = \delta$, then $G_n = \gamma\gamma \cdots \gamma\delta k_{i+1} \cdots k_n$. Let $G'_n = \gamma\gamma \cdots \gamma\gamma k_{i+1} \cdots k_n$. By Lemma 3.7, we know that $\rho(G_n) > \rho(G'_n)$, a contradiction.

If $k_i = \varepsilon$, then $G_n = \gamma\gamma \cdots \gamma\varepsilon k_{i+1} \cdots k_n$. Let $G'_n = \gamma\gamma \cdots \gamma\gamma k_{i+1} \cdots k_n$ and $G''_n = \gamma\gamma \cdots \gamma\gamma\bar{k}_{i+1} \cdots \bar{k}_n$. By Lemma 3.8, we know that if $\varphi(B-r, \rho(G'_n)) \leqslant \varphi(B-s, \rho(G'_n))$, then $\rho(G_n) > \rho(G''_n)$; if $\varphi(B-r, \rho(G'_n)) > \varphi(B - s, \rho(G'_n))$, then $\rho(G_n) > \rho(G'_n)$, contradiction.

Hence, $G_n = \gamma\gamma \cdots \gamma$, that is, the line chain L_n attains the minimum spectral radius among $\mathcal{G}_n$. □

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