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Research article

Extremal unicyclic graphs for the eccentricity spectral radius

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Abstract: Let $U_{n,d}$ denote the set of n-vertex unicyclic graphs with at least one pendant vertex and odd diameter $d \geq 3$. In this paper, we first prove the irreducibility of the eccentricity matrix $\varepsilon(G)$ of the unicyclic graph $G \in U_{n,d}$ when $| V(P_{d+1}) \cap V(C_r) | \leq 2$, and we determine the maximum ε-spectral radius $\varepsilon_1(G)$ of all unicyclic graphs with $d = 3$. Furthermore, we identify the extremal graphs of the following two types unicyclic graphs $G \in U_{n,d}$ with fixed odd $d \geq 5$, having the maximum eccentricity spectral radius: $| V(P_{d+1}) \cap V(C_r) | \leq 1$ or $| V(P_{d+1}) \cap V(C_r) | = 2$ with even $r \geq 4$, where P_{d+1} is one of diametral paths of G, C_r is the unique cycle of G, $V(P_{d+1})$ and $V(C_r)$ represent, respectively, the vertex sets of P_{d+1} and C_r.

Keywords: unicyclic graph; eccentricity matrix; eccentricity spectral radius; diameter
Mathematics Subject Classification: 05C50, 15A18

1. Introduction

All graphs considered in this paper are simple and connected. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. Two vertices u and v are adjacent (or neighbors) if they are joined by an edge e; we write $u \sim v$, and then, $u \nsim v$ denotes that they are nonadjacent. An induced subgraph of G obtained by deleting a set of edges $E' \subset E(G)$ is denoted by $G - E'$. If there is only a single edge e in E', we write $G - e$. If $e \notin E(G)$, we denote by $G + e$ a graph obtained from G by inserting the edge e.

We now define some distance-related concepts for a graph G. The distance $d_G(u, v)$ between two vertices u and v is the minimum length of the paths joining them. Let $D(G) = (d_{uv})$ be the distance

matrix of G, where $d_{uv} = d_G(u, v)$. The eccentricity $e_G(u)$ of a vertex $u \in V(G)$ is defined as $e_G(u) = \max\{d_G(u, v) \mid v \in V(G)\}$. The diameter of graph G, denoted by $diam(G)$ (or simply d) , is defined as the maximum eccentricity of all the vertices of G.

Randić, Orel, and Balaban [1,2] defined the so-called $\mathbf{D}_{\mathrm{MAX}}$ matrix and pointed out that this matrix appears very sensitive to the branching pattern of molecular graphs studied in theoretical chemistry. It was renamed as the eccentricity matrix of G by Wang, Lu, Belardo, and Randić [3], denoted by $\varepsilon(G)$. The elements of the eccentricity matrix $\varepsilon(G)$ are defined as follows:

$$(\varepsilon(G))_{uv} = \begin{cases} d_G(u, v) & \text{if } d_G(u, v) = \min\{e(u), e(v)\}; \\ 0 & \text{otherwise.} \end{cases} \tag{1.1}$$

The collection of eigenvalues of $\varepsilon(G)$ together with multiplicities is called the ε-spectrum of graph G, denoted by $\mathrm{Spec}_\varepsilon(G)$. Two graphs are said to be eccentricity cospectral if they have the same ε-spectrum. Because $\varepsilon(G)$ is symmetric, all ε-eigenvalues of G are real. Let $\varepsilon_1 > \varepsilon_2 > \cdots > \varepsilon_s$ be all the distinct ε-eigenvalues. Therefore, the ε-spectrum of G can be written as

$$\mathrm{Spec}_\varepsilon(G) = \begin{Bmatrix} \varepsilon_1 & \varepsilon_2 & \dots & \varepsilon_s \\ m_1 & m_2 & \dots & m_s \end{Bmatrix},$$

where m_i is the algebraic multiplicity of the eigenvalue ε_i $(1 \le i \le s)$. We denote by $\rho := \varepsilon_1(G)$ the largest eigenvalue of $\varepsilon(G)$, which is called the ε-spectral radius of G. It is well–known that the adjacency matrix $A(G)$ and distance matrix $D(G)$ of a connected graph G are irreducible. However, it is unfortunate that this property does not necessarily hold for the eccentricity matrix $\varepsilon(G)$. In [3], the authors raised a thought-provoking question: For which connected graphs is the eccentricity matrix either reducible or irreducible?

In the subsequent study, sufficient conditions were established for the reducibility of the eccentricity matrix of connected graphs [4]. The eccentricity spectrum of certain graphs including threshold graphs [5], paths, complete graphs [6, 7], complete multipartite graphs [8], cycles [9], has been depicted. In order to comprehensively understand the characteristics of this matrix, a significant body of research has been conducted on the spectral properties and graph energy of a large number of graphs [10, 11], which has been applied in the field of chemistry [3, 12]. More recently, eccentricity-based operators have been widely applied to the analysis of chemical networks. For instance, Asif, Atif, Akhtar, Hanif, and Siddiqui [13] studied the cubic zirconia network through eccentricity operators. This further demonstrates the relevance of eccentricity-based invariants in chemistry and motivates our study of the eccentricity spectral radius.

The problem of maximizing and minimizing the spectral radius for a given graph class is an active area of research in spectral graph theory. It has been extensively studied in the context of the eccentricity matrix (see [14–16]). Moreover, extremal problems for other graph-associated spectra have also attracted considerable attention, Lin, Chen, and Liu [17] determined the maximum ABC spectral radius of connected graphs with a given maximum degree, which reflects sustained interest in extremal spectral problems for graphs. In particular, Lei, Wang, and Li [18] explored the problem of the second least ε-eigenvalue. In their pioneering work, Wei, Li, and Zhang [19] determined n-vertex trees having the second minimum ε-spectral radius.

In view of the more novel properties of eccentricity matrix, further investigation is warranted. In particular, Wang, Lu, Brunetti, Lu, and Huang [20] proposed an investigation into the issue of the

ε-spectral radius of graphs under graft transformations. In parallel, spectral techniques have become powerful tools in the analysis of complex networks. Liu, Tang, Cai, and Cao [21] performed spectrum and coherence analysis of networks under noise disturbance, further illustrating the broad applicability of graph spectra in network science. Inspired by the seminal works of [16, 20], it is natural and interesting to study the relationship between eccentricity spectrum and diameter, order, and matching number.

The ε-eigenvalues of the unicyclic graph C_n, which has no pendant vertex, were determined by Wang [3]. However, the eccentricity spectrum of unicyclic graphs with pendant vertices has not been considered. Let $U_{n,d}$ denote the set of n-vertex unicyclic graphs with odd diameter d and at least one pendant vertex. A natural question arises: Does the eccentricity matrix of unicyclic graphs in $U_{n,d}$ belong to the class of matrices which are irreducible? Our answer is affirmative when $\mid V(P_{d+1}) \cap V(C_r) \mid \leq 2$. Based on this, we determine the extremal graphs of two types of unicyclic graphs $G \in U_{n,d}$ with fixed odd $d \geq 5$ having the maximum ε-spectral radius:

$$(i) \mid V(P_{d+1}) \cap V(C_r) \mid \leq 1;\ (ii) \mid V(P_{d+1}) \cap V(C_r) \mid = 2 \text{ with even } r \geq 4.$$

Here, P_{d+1} is one of the diametral paths of G, C_r is the unique cycle of G, and $V(P_{d+1})$ and $V(C_r)$ represent the vertex sets of P_{d+1} and C_r, respectively. To facilitate subsequent study, $\mathcal{U}^r_{n,d}$ represents the set of all unicyclic graphs that satisfy either of the above two conditions.

Our main results are given and proven in Section 2. Concretely, we first determine the maximum ε-spectral radius $\varepsilon_1(G)$ of the unicyclic graph G with $d = 3$, which is elaborated in Lemmas 2.4–2.7 and Theorem 2.2. In Section 2.2, the extremal graphs having the maximum ε-spectral radius among all unicyclic graphs in $\mathcal{U}^r_{n,d}$ with fixed odd $d \geq 5$ are characterized, and the main result is presented in Theorem 2.4. Finally, some concluding remarks are presented in Section 3.

2. Main results

In this section, our aim is to characterize the extremal unicyclic graphs for the ε-spectral radius. First, we implement edge-shift transformations on unicyclic graphs and repeatedly utilize several fundamental properties of non-negative irreducible matrices throughout the proof procedure.

It is well-known that the eccentricity matrix of an even-cycle C_{2k} is reducible, whereas the eccentricity matrix of an odd-cycle C_{2k+1} is irreducible. Consequently, we first verify the irreducibility of the eccentricity matrix for some unicyclic graphs in the set $U_{n,d}$. This essential prerequisite guarantees the validity of subsequent spectral comparisons and plays a crucial role in proving Lemmas 2.8–2.15.

Lemma 2.1. *([22]) Let M and N be the non-negative irreducible matrices with same order. If $(N)_{ij} \leq (M)_{ij}$ for each i, j, then $\rho(N) \leq \rho(M)$ with equality if and only if $M = N$, where $\rho(N)$ and $\rho(M)$ denote the spectral radius of N and M, respectively.*

The following lemma presents a classical conclusion from the Perron–Frobenius theory of non-negative matrices.

Lemma 2.2. *([23], Theorem 8.4.4) Suppose $A = (a_{ij}) \in \mathbb{R}^{n\times n}$ is irreducible such that $a_{ij} \geq 0$ for $i, j \in \{1, 2, \ldots, n\}$. Then,*

(1) ρ is the largest eigenvalue of A, and $\rho > 0$;
(2) there exists a unique positive unit vector $\mathbf{x} = (x_1, \ldots, x_n)^T \in \mathbb{R}^n$, called the Perron eigenvector, such that $A\mathbf{x} = \rho\mathbf{x}$.

A matrix M is said to be irreducible if it is not permutationally similar to an upper triangular block matrix. In other words, M is reducible if there exists a permutation matrix P such that $P^T MP = \begin{pmatrix} A & B \\ O & C \end{pmatrix}$, where A and C are square blocks.

To determine whether an $n \times n$ non-negative symmetric matrix M is irreducible, it is useful to consider its corresponding *matrix graph* G^M, which is defined as follows. Let $V(G^M) = \{1, 2, \ldots, n\}$; then, $ij \in E(G^M)$ if and only if $M_{ij} \neq 0$. It is well-known that M is irreducible if and only if G^M is connected (see [23]). Using this statement, we prove the following result.

Theorem 2.1. *Let G be a unicyclic graph in $U_{n,d}$ defined above such that $|V(C_r) \cap V(P_{d+1})| \leq 2$. Then, $\varepsilon(G)$ is irreducible. Here, C_r represents the unique cycle and P_{d+1} denotes one of diametral paths of G.*

Proof. Let A' be the matrix obtained from the eccentricity matrix $\varepsilon(G)$ of G by replacing every nonzero entry by 1, and regard A' as the adjacency matrix of a graph T, that is, $A' = A(T)$. Then, A' is irreducible if and only if T is connected graph. Consequently, if T is connected, then $\varepsilon(G)$ is also irreducible.

Let $C_r = v_0v_1 \cdots v_{r-1}v_0$ be the unique cycle of G, and let $P_{d+1} = uu_1u_2 \cdots u_{d-1}v$ denote one of diametral paths of G. Clearly, $e_G(u) = e_G(v) = d$, and hence, u and v are adjacent in T. Suppose that P_{d+1} passes through $l + 1$ ($l \geq 1$) vertices of C_r, without loss of generality, and assume that it passes precisely through $v_0, v_1, \ldots, v_l$, so that

$$uu_1 \cdots u_{k-1}v_0(= u_k)v_1(= u_{k+1}) \cdots v_l(= u_{k+l})u_{k+l+1} \cdots u_{d-1}v$$

is a shortest u–v path in G. For $0 \leq i \leq r-1$, let T_i be the component of $G - E(C_r)$ containing v_i. G_i denotes the component of $G - E(C_r) - E(P_{d+1})$ containing u_j for $1 \leq j \leq d-1$.

Case 1. $|V(C_r) \cap V(P_{d+1})| \leq 1$.

In this case, the diametral path P_{d+1} meets C_r in at most one vertex, and the girth of C_r is at most d. For $1 \leq i \leq d-1$, let Q_i be the component of $G - E(P_{d+1})$ containing u_i.

For any vertex $x \in \bigcup_{1 \leq i \leq \frac{d-1}{2}} V(Q_i)$, one has $d_G(u_i, u) < d_G(u_i, v)$, and therefore,

$$d_G(x, u) = d_G(x, u_i) + d_G(u_i, u) < d_G(x, u_i) + d_G(u_i, v) = d_G(x, v) = e_G(x) \leq d.$$

Hence, $(\varepsilon(G))_{xv} = e_G(x) \neq 0$, so $x \sim v$ in T.

Analogously, for any vertex $y \in \bigcup_{\frac{d+1}{2} \leq i \leq d-1} V(Q_i)$, one has $d_G(u_i, v) < d_G(u_i, u)$, and

$$d_G(y, v) = d_G(y, u_i) + d_G(u_i, v) < d_G(y, u_i) + d_G(u_i, u) = d_G(y, u) = e_G(y) \leq d.$$

Thus, $(\varepsilon(G))_{yu} = e_G(y) \neq 0$, and $y \sim u$ in T. It follows that every vertex of $V(T) \setminus \{u, v\}$ is adjacent in T to either u or v. Hence, T is connected, and therefore, $\varepsilon(G)$ is irreducible.

Case 2. $|V(C_r) \cap V(P_{d+1})| = 2$.

In this case, P_{d+1} meets C_r in exactly two vertices, which are $v_0(= u_k)$ and $v_1(= u_{k+1})$ by the above assumption, and the girth of C_r is at most $d + 2$.

Subcase 2.1. Suppose $d_G(u, v_0) < \frac{d-1}{2}$; that is, $k \leq \frac{d-3}{2}$.

For any vertex $x \in \bigcup_{0\le j\le r-1,\ j\neq 1} V(T_j)$, one has

$$d_G(x,u) \le d_G\Big(x, u_{\frac{d-1}{2}}\Big) + d_G\Big(u_{\frac{d-1}{2}}, u\Big) < d_G\Big(x, u_{\frac{d-1}{2}}\Big) + d_G\Big(u_{\frac{d-1}{2}}, v\Big) = d_G(x,v) = e_G(x) \le d.$$

Hence, $(\varepsilon(G))_{xv} = e_G(x) \neq 0$, and $x \sim v$ in the graph T.

Now, consider the vertices in $V(T_1)$, noting that $V(T_1) = \Big(\bigcup_{k+1\le j\le d-1} V(G_j)\Big)\bigcup\{v\}$. For any $y \in \bigcup_{k+1\le j\le \frac{d-1}{2}} V(G_j)$, one has

$$d_G(y,u) \le d_G\Big(y, u_{\frac{d-1}{2}}\Big) + d_G\Big(u_{\frac{d-1}{2}}, u\Big) < d_G\Big(y, u_{\frac{d-1}{2}}\Big) + d_G\Big(u_{\frac{d-1}{2}}, v\Big) = d_G(y,v) = e_G(y) \le d,$$

so $(\varepsilon(G))_{yv} = e_G(y) \neq 0$, and $y \sim v$ in T.

For any $z \in \bigcup_{\frac{d+1}{2}\le j\le d-1} V(G_j)$, one has

$$d_G(z,v) \le d_G\Big(z, u_{\frac{d+1}{2}}\Big) + d_G\Big(u_{\frac{d+1}{2}}, v\Big) < d_G\Big(z, u_{\frac{d+1}{2}}\Big) + d_G\Big(u_{\frac{d+1}{2}}, u\Big) = d_G(z,u) = e_G(z) \le d,$$

so $(\varepsilon(G))_{zu} = e_G(z) \neq 0$, and $z \sim u$ in T.

Thus, T is connected under this condition, and $\varepsilon(G)$ is irreducible.

Subcase 2.2. Suppose $d_G(u,v_0) = d_G(v,v_1) = \frac{d-1}{2}$, i.e., $k = \frac{d-1}{2}$.

If r is odd, then for every vertex $x \in V\Big(T_{\frac{r+1}{2}}\Big)$, one has $d_G(x,u) = d_G(x,v) = e_G(x) \le d$, so x is adjacent in T to both u and v. For every $y \in \bigcup_{2\le j\le r-1,\ j\neq \frac{r+1}{2}} V(T_j)$, one has either

$$d_G(y,v) < d_G(y,u) = e_G(y) \le d \quad \text{or} \quad d_G(y,u) < d_G(y,v) = e_G(y) \le d,$$

so y is adjacent in T to either u or v. Moreover, every vertex $w \in \bigcup_{1\le i\le \frac{d-1}{2}} V(G_i)$ satisfies $d_G(w,u) < d_G(w,v) \le d$, and every vertex $t \in \bigcup_{\frac{d+1}{2}\le i\le d-1} V(G_i)$ satisfies $d_G(t,v) < d_G(t,u) \le d$. Consequently, $w \sim v$ and $t \sim u$. Hence, T is connected when C_r is an odd cycle.

If r is even, then for every $y \in \bigcup_{2\le j\le r-1} V(T_j)$, one has either

$$d_G(y,v) < d_G(y,u) = e_G(y) \le d \quad \text{or} \quad d_G(y,u) < d_G(y,v) = e_G(y) \le d,$$

so y is adjacent in T to either u or v. For $w \in \bigcup_{1\le i\le \frac{d-1}{2}} V(G_i)$, one has $d_G(w,u) < d_G(w,v) \le d$, and for $t \in \bigcup_{\frac{d+1}{2}\le i\le d-1} V(G_i)$, one has $d_G(t,v) < d_G(t,u) \le d$; hence $w \sim v$, and $t \sim u$. Thus, T is also connected when C_r is an even cycle.

Therefore, T is also connected when $d_G(u,v_0) = d_G(v,v_1) = \frac{d-1}{2}$, and $\varepsilon(G)$ is irreducible.

Combining Subcases 2.1 and 2.2, we conclude that $\varepsilon(G)$ is irreducible when $|V(C_r) \cap V(P_{d+1})| = 2$.

This completes the proof. □

Next, we introduce a special class of unicyclic graphs for subsequent discussion.

Let $U(n,r;n_1,n_2,\ldots,n_r)$ denote the unicyclic graph constructed from an r-cycle $C_r = u_1u_2\cdots u_ru_1$, where n_i pendant vertices are attached to the cycle vertex u_i for each $1 \le i \le r$. The order is $n = \sum_{i=1}^{r}(n_i+1)$.

Remark 2.1. *It is worth noting that the situation will be more complicated if the diameter d is even. For instance, the eccentricity matrix of $U(8,4;1,1,1,1)$ is reducible, whereas those of $U(7,4;1,1,1,0)$ and $U(6,4;1,0,1,0)$ are irreducible; see Figure 1.*

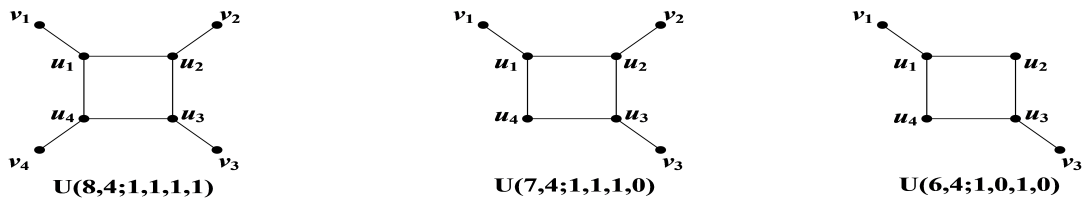


Figure 1. The three unicyclic graphs with diameter $d = 4$.

2.1. Unicyclic graphs with $d = 3$

Let $U_{n,d}^{a,b}$ denote the unicyclic graph constructed from the path $P_{d+1} = u_0u_1 \dots u_d$ by attaching $a-2$ pendant vertices $\{x_3, x_4, \dots, x_a\}$ to the vertex u_1 and b pendant vertices $\{y_1, y_2, \dots, y_b\}$ to the vertex u_{d-1}, and containing the unique 3-cycle $C_3 = u_1x_1x_2u_1$. This construction satisfies the conditions $a + b = n - d - 1$ and $b \geq 0$, $a \geq 2$, as illustrated in Figure 2.

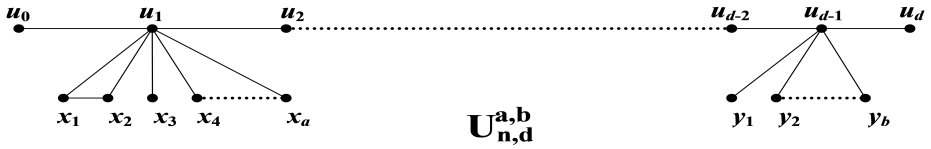


Figure 2. The unicyclic graph $U_{n,d}^{a,b}$.

If the unicyclic graph $G \in U_{n,3}$ contains the unique cycle C_r, then the girth of C_r is at most 5. We divide unicyclic graphs with $d = 3$ into four types for definition.

Let $U_{n,3}^{a,b,c}$ (where $a + b + c = n - 3$, $a, b \geq 1$, and $c \geq 0$) denote the unicyclic graph obtained from the 3-cycle $C_3 = v_1v_2v_3v_1$ by attaching a, b, and c pendant vertices to the vertices v_1, v_2, and v_3, respectively.

Let $C_{n,3}^{a,b}$ (where $a + b = n - 4$, $a \geq 1$, and $b \geq 0$) be the unicyclic graph obtained from the 4-cycle $C_4 = u_0u_1u_2u_3$ by attaching a, b pendant vertices to the vertices u_1, u_2, respectively. If $a \geq 2$, and $b \geq 1$, then $\varepsilon_1(C_{n,3}^{a,b}) < \varepsilon_1(U_{n,3}^{a,b})$. Clearly, $C_{n,3}^{a,b} = U_{n,3}^{a,b} - x_1x_2 + u_0u_3$, based on $\varepsilon(C_{n,3}^{a,b}) \leq \varepsilon(U_{n,3}^{a,b})$ and $\varepsilon(C_{n,3}^{a,b}) \neq \varepsilon(U_{n,3}^{a,b})$ by the elements $\left(\varepsilon(C_{n,3}^{a,b})\right)_{u_0u_3} = 0 < 3 = \left(\varepsilon(U_{n,3}^{a,b})\right)_{u_0u_3}$, and $\left(\varepsilon(C_{n,3}^{a,b})\right)_{uv} = \left(\varepsilon(U_{n,3}^{a,b})\right)_{uv}$ for all vertices $u, v \in V(C_{n,3}^{a,b})\backslash\{u_0, u_3\}$, and $\varepsilon_1(C_{n,3}^{a,b}) < \varepsilon_1(U_{n,3}^{a,b})$ holds true by Lemma 2.1.

Let $Q_{n,3}^{a,b}$ (where $a + b = n - 5$, $b \geq 1$, and $a \geq 0$) denote the unicyclic graph obtained from the 5-cycle $C_5 = u_1u_2u_3u_4u_5u_1$ by attaching a and b pendant vertices to the vertices u_1 and u_5, respectively (see Figure 3).

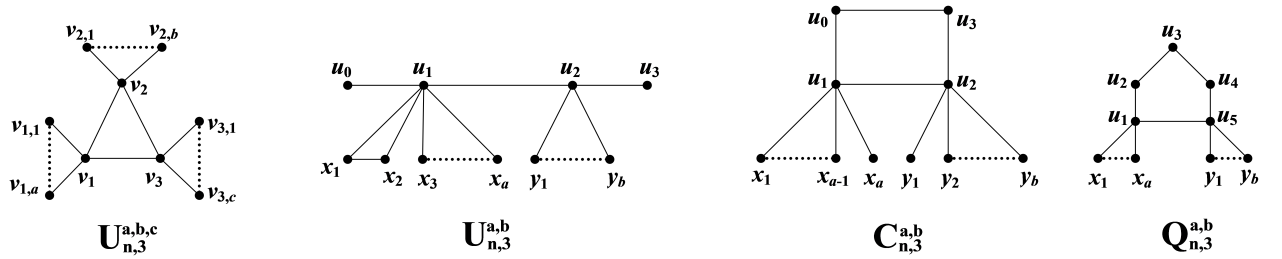


Figure 3. The unicyclic graphs $U^{a,b,c}_{n,3}$, $U^{a,b}_{n,3}$, $C^{a,b}_{n,3}$, and $Q^{a,b}_{n,3}$.

We first calculate the ε-spectral radius of unicyclic graphs $U^{a,b,c}_{n,3}$, $U^{a,b}_{n,3}$, $C^{a,b}_{n,3}$ and $Q^{a,b}_{n,3}$ for diameter $d = 3$. Subsequently, we perform an edge transformation on unicyclic graphs with odd diameter $d \geq 5$ to characterize the extremal graph with the maximum ε-spectral radius in Section 2.2.

Lemma 2.3. *([16], Lemma 1.6) Let G be an n-vertex connected graph with diameter d. Then, $\varepsilon_1(G) \geq d$, and $\varepsilon_n(G) \leq -d$.*

Lemma 2.4. *Let $U^{a,b,c}_{n,3} \in U_{n,3}(n \geq 7)$ be a unicyclic graph with the unique cycle $C_3 = v_1v_2v_3v_1$. Then, the eccentricity spectral radius of $U^{a,b,c}_{n,3}$ is maximized if and only if the pairwise differences among a, b, and c are at most* 1.

Proof. Let T_i denote the component of $U^{a,b,c}_{n,3} - E(C_3)$ that contains v_i, $V_i = V(T_i)\backslash\{v_i\}$ $(i = 1, 2, 3)$ and $|V_1| = a$, $|V_2| = b$ and $|V_3| = c$, where $a + b + c = n - 3$, $a, b \geq 1$, and $c \geq 0$. Let $\mathbf{x}$ be a Perron eigenvector corresponding to $\rho = \varepsilon_1(U^{a,b,c}_{n,3})$, whose coordinate with respect to vertex $v \in V(U^{a,b,c}_{n,3})$ is x_v. For all $u_i, u_i' \in V_i$ $(1 \leq i \leq 3)$, we obtain $x_{u_i} = x_{u_i'}$, and

$$\rho x_{v_1} = 2bx_{u_2} + 2cx_{u_3}, \quad \rho x_{v_2} = 2ax_{u_1} + 2cx_{u_3}, \quad \rho x_{u_1} = 2x_{v_2} + 2x_{v_3} + 3bx_{u_2} + 3cx_{u_3};$$
$$\rho x_{v_3} = 2ax_{u_1} + 2bx_{u_2}, \quad \rho x_{u_2} = 2x_{v_1} + 2x_{v_3} + 3ax_{u_1} + 3cx_{u_3}, \quad \rho x_{u_3} = 2x_{v_1} + 2x_{v_2} + 3ax_{u_1} + 3bx_{u_2}.$$

Then, ρ is the largest eigenvalue of the matrix $\begin{pmatrix} 0 & 0 & 0 & 0 & 2b & 2c \\ 0 & 0 & 0 & 2a & 0 & 2c \\ 0 & 0 & 0 & 2a & 2b & 0 \\ 0 & 2 & 2 & 0 & 3b & 3c \\ 2 & 0 & 2 & 3a & 0 & 3c \\ 2 & 2 & 0 & 3a & 3b & 0 \end{pmatrix}$.

Let

$$f_{a,b,c}(\lambda) = \begin{vmatrix} \lambda & 0 & 0 & 0 & -2b & -2c \\ 0 & \lambda & 0 & -2a & 0 & -2c \\ 0 & 0 & \lambda & -2a & -2b & 0 \\ 0 & -2 & -2 & \lambda & -3b & -3c \\ -2 & 0 & -2 & -3a & \lambda & -3c \\ -2 & -2 & 0 & -3a & -3b & \lambda \end{vmatrix}$$
$$= \lambda^6 - [8(a + b + c) + 9(ab + ac + bc)]\lambda^4 - [24(ab + ac + bc) + 54abc]\lambda^3$$
$$+ 48(ab + ac + bc)\lambda^2 + 288abc\lambda - 256abc.$$

Therefore, ρ is the largest root of $f_{a,b,c}(\lambda) = 0$.

Let $\rho' = \varepsilon_1(U_{n,3}^{a+1,b,c-1})$ be the largest root of the equation $f_{a+1,b,c-1}(\lambda) = 0$, and suppose $a \geq c \geq 1$. By Lemma 2.3, we get $\rho' \geq diam(U_{n,3}^{a+1,b,c-1}) = 3$. Then,

$$\begin{aligned} f_{a,b,c}(\rho') &= f_{a,b,c}(\rho') - f_{a+1,b,c-1}(\rho') \\ &= (c-a-1)\left[9\rho'^4 + (24+54b)\rho'^3 - 48\rho'^2 - 288b\rho' + 256b\right] \\ &= (c-a-1)\left[3(3\rho'-4)(\rho'+4)\rho'^2 + 18b\left(\rho'^2 - \frac{4}{3}\right)^2(3\rho'+8)\right] < 0. \end{aligned}$$

It follows that $f_{a,b,c}(\rho') < 0$, so we have $\rho' < \rho = \varepsilon_1(U_{n,3}^{a,b,c})$ by $f_{a,b,c}(\rho) = 0$ and $\lim f_{a,b,c}(\rho) \to +\infty$ as $\rho \to +\infty$. Similarly, we have $\varepsilon_1\left(U_{n,3}^{a,b+1,c-1}\right) < \varepsilon_1(U_{n,3}^{a,b,c})$ when $b \geq c \geq 1$, and $\varepsilon_1\left(U_{n,3}^{a+1,b-1,c}\right) < \varepsilon_1(U_{n,3}^{a,b,c})$ when $a \geq b \geq 1$. Obviously, the eccentricity spectral radius of $U_{n,3}^{a,b,c}$ achieves the maximum value when the differences between a, b, and c are all less than or equal to 1. □

The set of neighbors of a vertex v in graph G is denoted $N_G(v)$, and let $deg_G(v) = |N_G(v)|$ denote the degree of v.

Lemma 2.5. *Let $U_{n,3}^{a,b} \in U_{n,3}$ ($n \geq 7$) be a unicyclic graph as shown in Figure 3, where $a + b = n - 4$. Then, the eccentricity spectral radius of $U_{n,3}^{a,b}$ reaches its maximum value if and only if $| b - a | \leq 1$.*

Proof. Let $\mathbf{x}$ be a Perron eigenvector corresponding to $\rho = \varepsilon_1(U_{n,3}^{a,b})$, whose coordinate with respect to vertex $v \in V(U_{n,3}^{a,b})$ is x_v. Let $W = N(u_1)\backslash\{u_2\}$ and $U = N(u_2)\backslash\{u_1\}$ with $|W| = a + 1$ and $|U| = b + 1$. For each $w \in W$ and $u \in U$, according to the structure of graph $U_{n,3}^{a,b}$, we obtain

$$\rho x_{u_1} = 2(b+1)x_u; \qquad \rho x_{u_2} = 2(a+1)x_w; \qquad \rho x_w = 2x_{u_2} + 3(b+1)x_u; \qquad \rho x_u = 2x_{u_1} + 3(a+1)x_w.$$

Then, ρ is the largest eigenvalue of the matrix $\begin{pmatrix} 0 & 0 & 0 & 2(b+1) \\ 0 & 0 & 2(a+1) & 0 \\ 0 & 2 & 0 & 3(b+1) \\ 2 & 0 & 3(a+1) & 0 \end{pmatrix}$.

Let

$$g_{a,b}(\lambda) = \begin{vmatrix} \lambda & 0 & 0 & -2(b+1) \\ 0 & \lambda & -2(a+1) & 0 \\ 0 & -2 & \lambda & -3(b+1) \\ -2 & 0 & -3(a+1) & \lambda \end{vmatrix} = \lambda^4 - (9ab + 13a + 13b + 17)\lambda^2 + 16(a+1)(b+1).$$

Note that $a + b = n - 4$, and hence, $\varepsilon_1(U_{n,3}^{a,b})$ is the largest root of the equation $\lambda^4 - (9ab + 13n - 35)\lambda^2 + 16(ab + n - 3) = 0$.

Let $\rho' = \varepsilon_1\left(U_{n,3}^{a+1,b-1}\right)$ be the largest root of $g_{a+1,b-1}(\lambda) = 0$ with $a \geq b \geq 1$. By Lemma 2.3, we have $\rho' \geq diam\left(U_{n,3}^{a+1,b-1}\right) = 3$. Then,

$$g_{a,b}(\rho') = g_{a,b}(\rho') - g_{a+1,b-1}(\rho') = (9\rho'^2 - 16)(b - a - 1) < 0.$$

Thus, $g_{a,b}(\rho') < 0$, and we obtain $\rho' < \rho = \varepsilon_1(U_{n,3}^{a,b})$ by $g_{a,b}(\rho) = 0$ and $\lim g_{a,b}(\rho) \to +\infty$ as $\rho \to +\infty$. Obviously, the eccentricity spectral radius of $U_{n,3}^{a,b}$ attains its maximum value when $| b - a | \leq 1$. □

Lemma 2.6. *Let $C_{n,3}^{a,b} \in U_{n,3}$ ($n \geq 7$) be a unicyclic graph as shown in Figure 3, where $a + b = n - 4$. Then, the eccentricity spectral radius of $C_{n,3}^{a,b}$ reaches its maximum value if and only if $| b - a | \leq 1$.*

Proof. Let $\mathbf{x}$ be a Perron eigenvector corresponding to $\rho = \varepsilon_1(C_{n,3}^{a,b})$, whose coordinate with respect to vertex $v \in V(C_{n,3}^{a,b})$ is x_v. Let $X = N(u_1)\backslash\{u_0, u_2\}$ and $Y = N(u_2)\backslash\{u_1, u_3\}$ with $|X| = a$ and $|Y| = b$. For each $x \in X$ and $y \in Y$, according to the structure of graph $C_{n,3}^{a,b}$, we obtain

$$\begin{aligned}
&\rho x_{u_0} = 2x_{u_2} + 3bx_y, \qquad \rho x_{u_1} = 2x_{u_3} + 2bx_y, \qquad \rho x_{u_2} = 2x_{u_0} + 2ax_x;\\
&\rho x_{u_3} = 2x_{u_1} + 3ax_x, \qquad \rho x_x = 2x_{u_2} + 3x_{u_3} + 3bx_y, \qquad \rho x_y = 2x_{u_1} + 3x_{u_0} + 3ax_x.
\end{aligned}$$

Thus, ρ is the largest eigenvalue of the matrix $M = \begin{pmatrix} 0 & 0 & 2 & 0 & 0 & 3b \\ 0 & 0 & 0 & 2 & 0 & 2b \\ 2 & 0 & 0 & 0 & 2a & 0 \\ 0 & 2 & 0 & 0 & 3a & 0 \\ 0 & 0 & 2 & 3 & 0 & 3b \\ 3 & 2 & 0 & 0 & 3a & 0 \end{pmatrix}$.

Let the function

$$t_{a,b}(\lambda) = \det(\lambda I - M) = \lambda^6 - (9ab + 13a + 13b + 8)\lambda^4 + (97ab + 52a + 52b + 16)\lambda^2 - 144ab.$$

Hence, $\varepsilon_1(C_{n,3}^{a,b})$ is the largest root of $t_{a,b}(\lambda) = 0$.

Let $\eta = \varepsilon_1\left(C_{n,3}^{a+1,b-1}\right)$ be the largest root of $t_{a+1,b-1}(\lambda) = 0$ with $a \geq b \geq 1$. We have $\eta > 3$ by $t_{a+1,b-1}(3) = 225 - 585(a + b) < 0$ and $t_{a+1,b-1}(\lambda) \to +\infty$ as $\lambda \to +\infty$. Thus, we obtain

$$t_{a,b}(\eta) = t_{a,b}(\eta) - t_{a+1,b-1}(\eta) = (b - a - 1)(\eta^2 - 9)(9\eta^2 - 16) < 0.$$

It follows that $t_{a,b}(\eta) < 0$, so we get $\varepsilon_1\left(C_{n,3}^{a+1,b-1}\right) = \eta < \rho = \varepsilon_1(C_{n,3}^{a,b})$ by $t_{a,b}(\rho) = 0$ and $\lim t_{a,b}(\rho) \to +\infty$ as $\rho \to +\infty$. Therefore, the ε-spectral radius of $C_{n,3}^{a,b}$ attains the maximum when $| b - a | \leq 1$. □

Lemma 2.7. *Let $Q_{n,3}^{a,b} \in U_{n,3}$ ($n \geq 8$) be a unicyclic graph as shown in Figure 3. Then, the eccentricity spectral radius of $Q_{n,3}^{a,b}$ reaches its maximum value if and only if $| b - a | \leq 1$.*

Proof. Let $V_1 = N_{Q_{n,3}^{a,b}}(u_1)\backslash\{u_2, u_5\}$, $V_2 = N_{Q_{n,3}^{a,b}}(u_5)\backslash\{u_1, u_4\}$, $|V_1| = a$ and $|V_2| = b$. Let $\mathbf{x}$ be a Perron eigenvector corresponding to $\rho := \varepsilon_1(Q_{n,3}^{a,b})$, whose coordinate with respect to the vertex $v \in V(Q_{n,3}^{a,b})$ is x_v. For each $x \in V_1,\ y \in V_2$, we obtain

$$\begin{aligned}
&\rho x_{u_1} = 2x_{u_3} + 2x_{u_4} + 2bx_y, \qquad \rho x_{u_2} = 2x_{u_5} + 3bx_y, \qquad \rho x_{u_3} = 2x_{u_1} + 2x_{u_5} + 3ax_x + 3bx_y,\\
&\rho x_{u_4} = 2x_{u_1} + 3ax_x, \qquad \rho x_{u_5} = 2x_{u_2} + 2x_{u_3} + 2ax_x, \qquad \rho x_x = 3x_{u_3} + 3x_{u_4} + 2x_{u_5} + 3bx_y,\\
&\rho x_y = 2x_{u_1} + 3x_{u_2} + 3x_{u_3} + 3ax_x.
\end{aligned}$$

Then, ρ is the largest eigenvalue of $\begin{pmatrix} 0 & 0 & 2 & 2 & 0 & 0 & 2b \\ 0 & 0 & 0 & 0 & 2 & 0 & 3b \\ 2 & 0 & 0 & 0 & 2 & 3a & 3b \\ 2 & 0 & 0 & 0 & 0 & 3a & 0 \\ 0 & 2 & 2 & 0 & 0 & 2a & 0 \\ 0 & 0 & 3 & 3 & 2 & 0 & 3b \\ 2 & 3 & 3 & 0 & 0 & 3a & 0 \end{pmatrix}$.

Furthermore, we have

$$\begin{vmatrix} \lambda & 0 & -2 & -2 & 0 & 0 & -2b \\ 0 & \lambda & 0 & 0 & -2 & 0 & -3b \\ -2 & 0 & \lambda & 0 & -2 & -3a & -3b \\ -2 & 0 & 0 & \lambda & 0 & -3a & 0 \\ 0 & -2 & -2 & 0 & \lambda & -2a & 0 \\ 0 & 0 & -3 & -3 & -2 & \lambda & -3b \\ -2 & -3 & -3 & 0 & 0 & -3a & \lambda \end{vmatrix}$$
$$= \lambda\Big[\lambda^6 - (9ab + 22a + 22b + 16)\lambda^4 - (54ab + 24a + 24b)\lambda^3$$
$$+ (259ab + 140a + 140b + 48)\lambda^2 + 96ab\lambda - 432ab\Big].$$

Because $a + b = n - 5$, we denote

$$\begin{aligned} h_{a,b}(\lambda) &= \lambda^6 - (9ab + 22a + 22b + 16)\lambda^4 - (54ab + 24a + 24b)\lambda^3 \\ &\quad + (259ab + 140a + 140b + 48)\lambda^2 + 96ab\lambda - 432ab \\ &= \lambda^6 - (9ab + 22n - 94)\lambda^4 - (54ab + 24n - 120)\lambda^3 \\ &\quad + (259ab + 140n - 652)\lambda^2 + 96ab\lambda - 432ab. \end{aligned}$$

Therefore, ρ is the largest root of $h_{a,b}(\lambda) = 0$. Let $\rho' = \varepsilon_1\left(Q_{n,3}^{a-1,b+1}\right)$ denote the largest root of $h_{a-1,b+1}(\lambda) = 0$, and $b \geq a \geq 1$. We have $\rho' > 3$ by $h_{a-1,b+1}(3) = -1170(a + b) - 135 < 0$ and $h_{a-1,b+1}(\lambda) \to +\infty$ as $\lambda \to +\infty$. If $\rho' > 3$, then $f(\rho') = 9\rho'^4 + 54\rho'^3 - 259\rho'^2 - 96\rho' + 432$ is a monotone increasing function because of $f'(\rho') = 36\rho'^3 + 162\rho'^2 - 518\rho' - 96 > 0$ and $f''(\rho') = 108\rho'^2 + 324\rho' - 518 > 0$, $f(\rho') > f'(3) = 0$. Then,

$$h_{a,b}(\rho') = h_{a,b}(\rho') - h_{a-1,b+1}(\rho') = (a - b - 1)(9\rho'^4 + 54\rho'^3 - 259\rho'^2 - 96\rho' + 432) < 0.$$

Thus, $h_{a,b}(\rho') < 0$, so we obtain $\rho' < \rho = \varepsilon_1(Q_{n,3}^{a,b})$ by $h_{a,b}(\rho) = 0$ and $\lim h_{a,b}(\rho) \to +\infty$ as $\rho \to +\infty$. Obviously, the eccentricity spectral radius of $Q_{n,3}^{a,b}$ achieves the maximum value when $| b - a | \leq 1$. □

Theorem 2.2. *Let the unicyclic graph $U \in U_{n,3}$ and $n \geq 8$.*

(*i*) If $n \equiv 0(\mathrm{mod}\, 3)$, then $\varepsilon_1(U) \leq \lambda_0$ with equality if and only if $U \cong U_{n,3}^{\frac{n-3}{3},\frac{n-3}{3},\frac{n-3}{3}}$, and λ_0 is the largest root of

$$\lambda^6 - (3n - 1)(n - 3)\lambda^4 - 2(n + 1)(n - 3)^2\lambda^3 + 16(n - 3)^2\lambda^2 + \frac{32}{3}(n - 3)^3\lambda - \frac{256}{27}(n - 3)^3 = 0.$$

(*ii*) If $n \equiv 1(\mathrm{mod}\, 3)$, then $\varepsilon_1(U) \leq \lambda_0$ with equality if and only if $U \cong U_{n,3}^{\frac{n-1}{3},\frac{n-4}{3},\frac{n-4}{3}}$, and λ_0 is the largest root of

$$\lambda^6 - \left(3n^2 - 10n\right)\lambda^4 - 2(n - 4)\left(n^2 - n - 4\right)\lambda^3$$
$$+ 16(n - 4)(n - 2)\lambda^2 + \frac{32(n - 1)(n - 4)^2}{3}\lambda - \frac{256(n - 1)(n - 4)^2}{27} = 0.$$

(*iii*) If $n \equiv 2(\mathrm{mod}\,3)$, then $\varepsilon_1(U) \leq \lambda_0$ with equality if and only if $U \cong U_{n,3}^{\frac{n-2}{3},\frac{n-2}{3},\frac{n-5}{3}}$, and λ_0 is the largest root of

$$\lambda^6 - \left(3n^2 - 10n\right)\lambda^4 - \left(2n^3 - 10n^2 + 24\right)\lambda^3 + 16\left(n^2 - 6n + 8\right)\lambda^2 + \frac{32(n-5)(n-2)^2}{3}\lambda - \frac{256(n-5)(n-2)^2}{27} = 0.$$

Proof. Because $U \in U_{n,3}$, we obtain that U may be isomorphic to $U_{n,3}^{a,b,c}$, $U_{n,3}^{a,b}$, $Q_{n,3}^{a,b}$, $C_{n,3}^{a,b}$ as in Figure 3. Further, $\varepsilon_1(C_{n,3}^{a,b}) < \varepsilon_1(U_{n,3}^{a,b})$ when $n \geq 8$, and $a, b \geq 2$. We therefore only study the relationship of the eccentricity spectral radius among the first three.

Case 1. $n - 3 = 6k$, *where* $k \geq 1$ *is an integer.*

By Lemmas 2.4–2.7, we only compare $\varepsilon_1(U_{n,3}^{2k,2k,2k})$, $\varepsilon_1(U_{n,3}^{3k-1,3k})$, and $\varepsilon_1(Q_{n,3}^{3k-1,3k-1})$.

Let $\rho = \varepsilon_1(U_{n,3}^{3k-1,3k})$ be the largest root of $g_{3k-1,3k}(\lambda) = 0$ and $\rho' = \varepsilon_1(Q_{n,3}^{3k-1,3k-1})$ be the largest root of $h_{3k-1,3k-1}(\lambda) = 0$. Then, we have that

$$\begin{aligned} f_{2k,2k,2k}(\rho) &= f_{2k,2k,2k}(\rho) - \rho^2 \cdot g_{3k-1,3k}(\rho) \\ &= -(27k^2 - 3k - 4)\rho^4 - \left[(432k^3 + 288k^2)\rho - (432k^2 - 48k)\right]\rho^2 - 8(256 - 288\rho)k^3 < 0, \end{aligned}$$

and

$$\begin{aligned} f_{2k,2k,2k}(\rho') &= f_{2k,2k,2k}(\rho') - h_{3k-1,3k-1}(\rho') \\ &= -(27k^2 - 30k + 19)\rho'^4 - (432k^3 - 198k^2 + 180k - 6)\rho'^3 - (1755k^2 - 714k + 27)\rho'^2 \\ &\quad + (2304k^3 - 864k^2 + 576k - 96)\rho' - (2048k^3 - 3888k^2 + 2592k - 432) < 0. \end{aligned}$$

Thus, $f_{2k,2k,2k}(\rho) < 0$, and $f_{2k,2k,2k}(\rho') < 0$, so we obtain $\varepsilon_1\left(U_{n,3}^{3k-1,3k}\right) = \rho < \varepsilon_1\left(U_{n,3}^{2k,2k,2k}\right)$ and $\varepsilon_1\left(Q_{n,3}^{3k-1,3k-1}\right) = \rho' < \varepsilon_1\left(U_{n,3}^{2k,2k,2k}\right)$ by $f_{2k,2k,2k}\left(\varepsilon_1\left(U_{n,3}^{2k,2k,2k}\right)\right) = 0$ and $\lim f_{2k,2k,2k}(\lambda) \to +\infty$ as $\lambda \to +\infty$.

Case 2. $n - 3 = 6k + 1$, *where* $k \geq 1$ *is an integer.*

By Lemmas 2.4–2.7, we compare $\varepsilon_1(U_{n,3}^{2k+1,2k,2k})$, $\varepsilon_1(U_{n,3}^{3k,3k})$, and $\varepsilon_1(Q_{n,3}^{3k-1,3k})$. Let $\rho = \varepsilon_1(U_{n,3}^{3k,3k})$ be the largest root of $g_{3k,3k}(\lambda) = 0$ and $\rho' = \varepsilon_1(Q_{n,3}^{3k-1,3k})$ be the largest root of $h_{3k-1,3k}(\lambda) = 0$. Then,

$$\begin{aligned} f_{2k+1,2k,2k}(\rho) &= f_{2k+1,2k,2k}(\rho) - \rho^2 \cdot g_{3k,3k}(\rho) \\ &= -(27k^2 + 6k - 9)\rho^4 - (256 - 288\rho)(8k^3 + 4k^2) \\ &\quad - \left[(432k^3 + 504k^2 + 96k)\rho - (432k^2 + 96k - 16)\right]\rho^2 < 0, \end{aligned}$$

and

$$\begin{aligned} f_{2k+1,2k,2k}(\rho') &= f_{2k+1,2k,2k}(\rho') - h_{3k-1,3k}(\rho') \\ &= -(27k^2 - 21k + 14)\rho'^4 - (432k^3 + 18k^2 + 114k + 24)\rho'^3 - (1755k^2 - 129k - 92)\rho'^2 \\ &\quad + (2304k^3 + 288k^2 + 288k)\rho' - (2048k^3 - 2864k^2 + 1296k) < 0. \end{aligned}$$

Hence, $f_{2k+1,2k,2k}(\rho) < 0$, and $f_{2k+1,2k,2k}(\rho') < 0$, so we get $\varepsilon_1\left(U_{n,3}^{3k,3k}\right) = \rho < \varepsilon_1\left(U_{n,3}^{2k+1,2k,2k}\right)$ and $\varepsilon_1\left(Q_{n,3}^{3k-1,3k}\right) = \rho' < \varepsilon_1\left(U_{n,3}^{2k+1,2k,2k}\right)$ by $f_{2k+1,2k,2k}\left(\varepsilon_1\left(U_{n,3}^{2k+1,2k,2k}\right)\right) = 0$ and $\lim f_{2k+1,2k,2k}(\lambda) \to +\infty$ as $\lambda \to +\infty$.

Case 3. $n-3=6k+2$, *where* $k\geq 1$ *is an integer.*

By Lemmas 2.4–2.7, we compare $\varepsilon_1(U_{n,3}^{2k+1,2k+1,2k})$, $\varepsilon_1(U_{n,3}^{3k,3k+1})$, $\varepsilon_1(Q_{n,3}^{3k,3k})$. Let $\rho=\varepsilon_1(U_{n,3}^{3k,3k+1})$ be the largest root of $g_{3k,3k+1}(\lambda)=0$, and $\rho'=\varepsilon_1(Q_{n,3}^{3k,3k})$ be the largest root of $h_{3k,3k}(\lambda)=0$. Then,

$$\begin{aligned}f_{2k+1,2k+1,2k}(\rho)&=f_{2k+1,2k+1,2k}(\rho)-\rho^2\cdot g_{3k,3k+1}(\rho)\\&=-(27k^2+15k-5)\rho^4-\Big[(432k^3+720k^2+300k+24)\rho-(432k^2+240k+16)\Big]\rho^2\\&\quad-(256-288\rho)(8k^3+8k^2+2k)<0,\end{aligned}$$

and

$$\begin{aligned}f_{2k+1,2k+1,2k}(\rho')&=f_{2k+1,2k+1,2k}(\rho')-h_{3k,3k}(\rho')\\&=-(27k^2-12k+9)\rho'^4-(432k^3+234k^2+156k+24)\rho'^3-(1755k^2+456k)\rho'^2\\&\quad+(2304k^3+1440k^2+576)\rho'-(2048k^3-1840k^2+512k)<0.\end{aligned}$$

Therefore, $f_{2k+1,2k+1,2k}(\rho)<0$, and $f_{2k+1,2k+1,2k}(\rho')<0$. Combining $f_{2k+1,2k+1,2k}\left(\varepsilon_1\left(U_{n,3}^{2k+1,2k+1,2k}\right)\right)=0$ and $\lim f_{2k+1,2k+1,2k}(\lambda)\to+\infty$ as $\lambda\to+\infty$, one has $\varepsilon_1\left(U_{n,3}^{3k,3k+1}\right)=\rho<\varepsilon_1\left(U_{n,3}^{2k+1,2k+1,2k}\right)$ and $\varepsilon_1\left(Q_{n,3}^{3k,3k}\right)=\rho'<\varepsilon_1\left(U_{n,3}^{2k+1,2k+1,2k}\right)$.

Case 4. $n-3=6k+3$, *where* $k\geq 1$ *is an integer.*

Let $\rho=\varepsilon_1(U_{n,3}^{3k+1,3k+1})$ be the largest root of $g_{3k+1,3k+1}(\lambda)=0$ and $\rho'=\varepsilon_1(Q_{n,3}^{3k,3k+1})$ be the largest root of $h_{3k,3k+1}(\lambda)=0$. Then, we obtain that

$$\begin{aligned}f_{2k+1,2k+1,2k+1}(\rho)&=f_{2k+1,2k+1,2k+1}(\rho)-\rho^2\cdot g_{3k+1,3k+1}(\rho)\\&=-(27k^2+24k-1)\rho^4-\Big[(432k^3+936k^2+612k+126)\rho-(432k^2+384k+80)\Big]\rho^2\\&\quad-(256-288\rho)(8k^3+12k^2+6k+1)<0,\end{aligned}$$

and

$$\begin{aligned}f_{2k+1,2k+1,2k+1}(\rho')&=f_{2k+1,2k+1,2k+1}(\rho')-h_{3k,3k+1}(\rho')\\&=-(27k^2-3k+13)\rho'^4-(432k^3+450k^2+306k+102)\rho'^3-(1755k^2+1041k+44)\rho'^2\\&\quad+(2304k^3+2592k^2+1440k+288)\rho'-(2048k^3-816k^2+240k+256)<0.\end{aligned}$$

Then, $f_{2k+1,2k+1,2k+1}(\rho)<0$, and $f_{2k+1,2k+1,2k+1}(\rho')<0$. By $f_{2k+1,2k+1,2k+1}\left(\varepsilon_1\left(U_{n,3}^{2k+1,2k+1,2k+1}\right)\right)=0$ and $f_{2k+1,2k+1,2k+1}(\lambda)\to+\infty$ as $\lambda\to+\infty$, we obtain $\varepsilon_1\left(U_{n,3}^{3k+1,3k+1}\right)<\varepsilon_1\left(U_{n,3}^{2k+1,2k+1,2k+1}\right)$ and $\varepsilon_1\left(Q_{n,3}^{3k,3k+1}\right)<\varepsilon_1\left(U_{n,3}^{2k+1,2k+1,2k+1}\right)$.

Case 5. $n-3=6k+4$, *where* $k\geq 1$ *is an integer.*

Let $\rho=\varepsilon_1(U_{n,3}^{3k+1,3k+2})$ be the largest root of $g_{3k+1,3k+2}(\lambda)=0$ and $\rho'=\varepsilon_1(Q_{n,3}^{3k+1,3k+1})$ be the largest root of $h_{3k+1,3k+1}(\lambda)=0$. Then, we have

$$f_{2k+2,2k+1,2k+1}(\rho)=f_{2k+2,2k+1,2k+1}(\rho)-\rho^2\cdot g_{3k+1,3k+2}(\rho)$$

$$= -(27k^2 + 33k + 3)\rho^4 - \Big[(432k^3 + 1152k^2 + 924k + 228)\rho - (432k^2 + 528k + 144)\Big]\rho^2$$
$$- (256 - 288\rho)(8k^3 + 16k^2 + 10k + 2) < 0,$$

and

$$f_{2k+2,2k+1,2k+1}(\rho') = f_{2k+2,2k+1,2k+1}(\rho') - h_{3k+1,3k+1}(\rho')$$
$$= -(27k^2 + 6k + 8)\rho'^4 - (432k^3 + 666k^2 + 456k + 126)\rho'^3 - (1755k^2 + 1626k + 347)\rho'^2$$
$$+ (2304k^3 + 3744k^2 + 2304k + 480)\rho' - (2048k^3 + 208k^2 - 30k + 80) < 0.$$

Therefore, $f_{2k+2,2k+1,2k+1}(\rho) < 0$, and $f_{2k+2,2k+1,2k+1}(\rho') < 0$, so we get $\varepsilon_1\Big(U_{n,3}^{3k+1,3k+2}\Big) < \varepsilon_1\Big(U_{n,3}^{2k+2,2k+1,2k+1}\Big)$ and $\varepsilon_1\Big(Q_{n,3}^{3k+1,3k+1}\Big) < \varepsilon_1\Big(U_{n,3}^{2k+2,2k+1,2k+1}\Big)$ by $f_{2k+2,2k+1,2k+1}\left(\varepsilon_1\Big(U_{n,3}^{2k+2,2k+1,2k+1}\Big)\right) = 0$.

Case 6. *$n - 3 = 6k + 5$, where $k \geq 0$ is an integer.*

Let $\rho = \varepsilon_1\Big(U_{n,3}^{3k+2,3k+2}\Big)$ be the largest root of $g_{3k+2,3k+2}(\lambda) = 0$ and $\rho' = \varepsilon_1\Big(Q_{n,3}^{3k+1,3k+2}\Big)$ be the largest root of $h_{3k+1,3k+2}(\lambda) = 0$. Then,

$$f_{2k+2,2k+2,2k+1}(\rho) = f_{2k+2,2k+2,2k+1}(\rho) - \rho^2 \cdot g_{3k+2,3k+2}(\rho)$$
$$= -(27k^2 + 42k + 7)\rho^4 - \Big[(432k^3 + 1368k^2 + 1344k + 408)\rho - (432k^2 + 672k + 240)\Big]\rho^2$$
$$- (256 - 288\rho)(8k^3 + 20k^2 + 16k + 4) < 0,$$

and

$$f_{2k+2,2k+2,2k+1}(\rho') = f_{2k+2,2k+2,2k+1}(\rho') - h_{3k+1,3k+2}(\rho')$$
$$= -(27k^2 + 15k + 12)\rho'^4 - (432k^3 + 882k^2 + 714k + 228)\rho'^3 - (1755k^2 + 2211k + 602)\rho'^2$$
$$+ (2304k^3 + 4896k^2 + 3744k + 960)\rho' - (2048k^3 + 1232k^2 + 208k + 160) < 0.$$

Thus, $\varepsilon_1\Big(U_{n,3}^{3k+2,3k+2}\Big) < \varepsilon_1\Big(U_{n,3}^{2k+2,2k+2,2k+1}\Big)$, and $\varepsilon_1\Big(Q_{n,3}^{3k+1,3k+2}\Big) < \varepsilon_1\Big(U_{n,3}^{2k+2,2k+2,2k+1}\Big)$.

Based on the above six cases, we obtain

$$\varepsilon_1\left(C_{n,3}^{\lfloor\frac{n-4}{2}\rfloor,\lceil\frac{n-4}{2}\rceil}\right) < \varepsilon_1\left(U_{n,3}^{\lfloor\frac{n-4}{2}\rfloor,\lceil\frac{n-4}{2}\rceil}\right) < \varepsilon_1\left(U_{n,3}^{\lfloor\frac{n-1}{3}\rfloor,\lfloor\frac{n-2}{3}\rfloor,\lfloor\frac{n-3}{3}\rfloor}\right) \quad \text{and} \quad \varepsilon_1\Big(Q_{n,3}^{\lfloor\frac{n-5}{2}\rfloor,\lceil\frac{n-5}{2}\rceil}\Big) < \varepsilon_1\left(U_{n,3}^{\lfloor\frac{n-1}{3}\rfloor,\lfloor\frac{n-2}{3}\rfloor,\lfloor\frac{n-3}{3}\rfloor}\right).$$

This completes the proof. □

Remark 2.2. *For the unicyclic graphs $G \in U_{n,3}$ with order $n = 5, 6, 7$, we calculate their eccentricity spectral radius. Surprisingly, we found that* $\max \varepsilon_1(G) \approx 5.3752$ *when $n = 5$, but not the graph $U_{5,3}^{1,1,0}$. When n equals 6 or 7, the ε-spectral radius of $U_{6,3}^{1,1,1}$ and $U_{7,3}^{2,1,1}$ are indeed the largest; see Figure 4.*

In the following section, the focus will be on the characterization of extremal unicyclic graphs with order n and odd-diameter $d \geq 5$ having maximum ε-spectral radius. Let G be a unicyclic graph of order n with the unique cycle $C_r = v_1v_2 \cdots v_rv_1$, where one of the diametral paths of G is $P_{d+1} = u_0u_1 \ldots u_d$. The ensuing discourse is to be divided into two distinct categories: (*i*) $|V(C_r) \cap V(P_{d+1})| \leq 1$; (*ii*) $|V(C_r) \cap V(P_{d+1})| = 2$, and C_r is an even cycle.

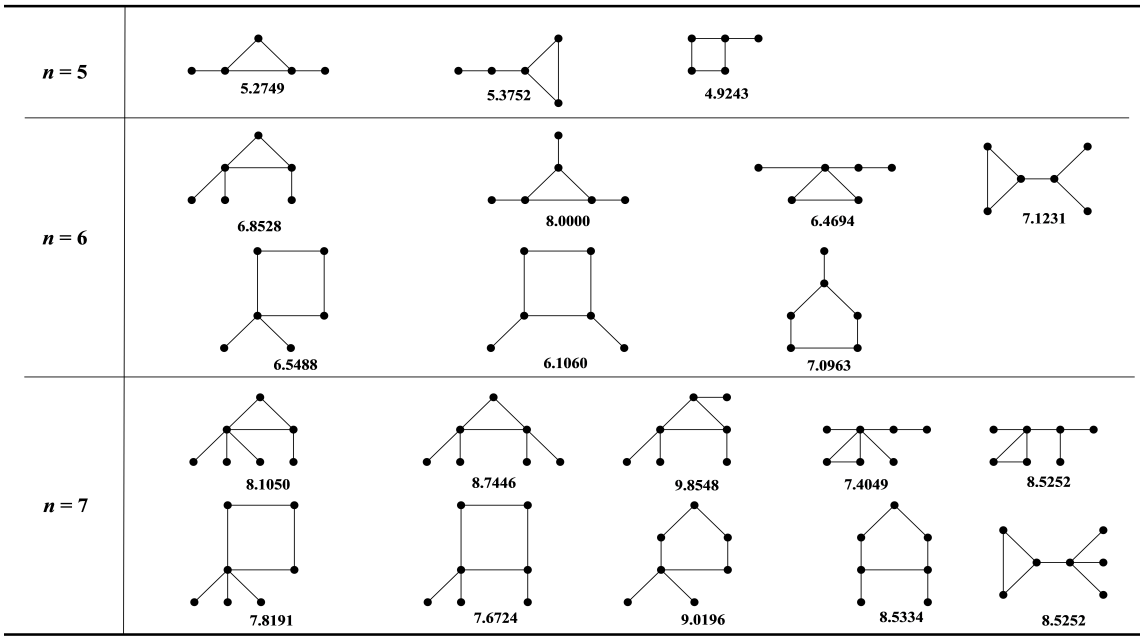


Figure 4. The ε-spectral radius of unicyclic graphs when $d = 3$ and $n = 5, 6$, or 7.

2.2. Two types of unicyclic graphs with odd-diameter $d \geq 5$.

Let $A = (a_{ij}), B = (b_{ij}) \in \mathbb{R}^{n\times n}$ be two matrices such that $a_{ij} \geq b_{ij}$ for all $i, j \in \{1, 2, \ldots, n\}$, and that there exists at least one pair (i_0, j_0) such that $a_{i_0 j_0} > b_{i_0 j_0}$. Then, we denote $A \geq B$ with equality if and only if $a_{ij} = b_{ij}$ for all $i, j \in \{1, 2, \ldots, n\}$. Further on, we need the following lemmas.

Lemma 2.8. *Let $U_1 \in U_{n,d}$ (odd $d \geq 5$) be a unicyclic graph with its unique cycle $C_r = v_1v_2 \cdots v_rv_1$ ($r \geq 3$), and there is a diametral path $P_{d+1} = u_0u_1 \ldots u_d$ such that $|V(C_r) \cap V(P_{d+1})| \leq 1$. Further, let G_j be the connected component of $U_1 - E(P_{d+1})$ containing u_j ($0 \leq j \leq d$). Assume there exists a vertex $w_1 \in V(G_i)\left(2 \leq i \leq \frac{d-1}{2}\right)$ such that $d_{G_i}(u_i, w_1) = e_{G_i}(u_i) \geq 2$, and $deg_{U_1}(w_1) = 1$. Denote the unique neighbor of w_1 by w. Let*

$$U_1' = U_1 - w_1w + w_1u_1.$$

Then, $\varepsilon_1(U_1) \leq \varepsilon_1(U_1')$, with equality if and only if $d_{G_i}(u_i, w_1) = e_{G_i}(u_i) = i$.

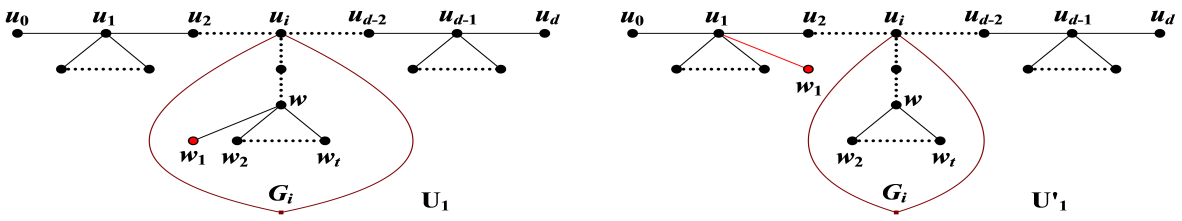


Figure 5. The unicyclic graphs of Lemma 2.8.

Proof. From graphs U_1 to U_1', see Figure 5, we consider only two situations for eccentricity $e_{G_i}(u_i)$ of the vertex u_i in G_i.

Case 1. If $e_{G_i}(u_i) = i$, we have $\varepsilon(U_1') = \varepsilon(U_1)$ by $e_{U_1}(w_1) = e_{U_1'}(w_1) = d$, $\left(\varepsilon(U_1')\right)_{w_1 y} = (\varepsilon(U_1))_{w_1 y}$ for all vertices $y \in V(U_1)\backslash\{w_1\}$ and $\left(\varepsilon(U_1')\right)_{uv} = (\varepsilon(U_1))_{uv}$ for $u, v \in V(U_1)\backslash\{w_1\}$.
Case 2. If $e_{G_i}(u_i) < i$, for any two vertices $x, y \in V(U_1)$, the element at the xth row and yth column of the matrix $\varepsilon(U_1') - \varepsilon(U_1)$ is

$$(\varepsilon(U_1'))_{xy} - (\varepsilon(U_1))_{xy} = \begin{cases} i - e_{G_i}(u_i)\,, & \text{if } x = w_1\,, \text{ and } y \in N_{U_1}(u_{d-1})\backslash\{u_{d-2}\}\,; \\ e_{U_1}(y)\,, & \text{if } x = w_1\,, \text{ and } y \in \bigcup_{j=\frac{d+1}{2}}^{d-1} V(G_j)\,; \\ 0\,, & \text{otherwise.} \end{cases}$$

Therefore, $\varepsilon(U_1) \le \varepsilon(U_1')$ with equality if and only if $d_{G_i}(u_i, w_1) = e_{G_i}(u_i) = i$. By Lemma 2.1 and Theorem 2.1, we have $\varepsilon_1(U_1) \le \varepsilon_1(U_1')$. □

After the transformation by Lemma 2.8, all the pendant vertices of the graph U_1 can be moved to be adjacent to u_1 or u_{d-1}, whereas the ε-spectral radius of the new unicyclic graph U_2 increases or remains unchanged. Subsequently, the contraction transformation is applied to the unique cycle C_r ($r \ge 3$) of the graph $U_2 \in U_{n,d}$.

Lemma 2.9. *Let $U_2 \in U_{n,d}$ (odd $d \ge 5$) be a unicyclic graph with its unique cycle $C_r = v_1 v_2 \cdots v_r v_1$ ($r \ge 4$), and there is a diametral path $P_{d+1} = u_0 u_1 \ldots u_d$ such that $|V(C_r) \cap V(P_{d+1})| \le 1$. Further, let G_j be the connected component of $U_2 - E(P_{d+1})$ containing u_j ($0 \le j \le d$). Assume there exists a vertex $v_k \in V(G_i) \cap V(C_r)\left(2 \le i \le \frac{d-1}{2}\right)$ such that $2 \le e_{G_i}(u_i) = d_{G_i}(u_i, v_k) \le i$, and $deg_{U_2}(v_k) = 2$. Let*

$$U_2' = U_2 - v_k v_{k-1} - v_k v_{k+1} + v_{k-1} v_{k+1} + v_k u_1.$$

Then, $\varepsilon_1(U_2) \le \varepsilon_1(U_2')$, with equality if and only if $d_{G_i}(u_i, v_k) = e_{G_i}(u_i) = i$.

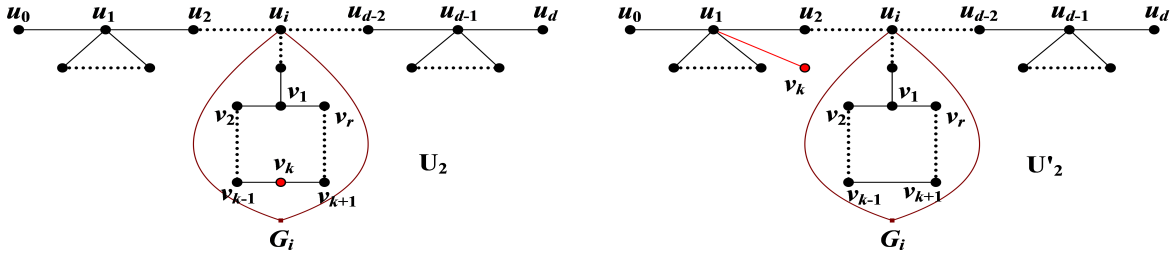


Figure 6. The unicyclic graphs of Lemma 2.9.

Proof. From graphs U_2 to U_2', see Figure 6, we obviously obtain $\varepsilon(U_2') = \varepsilon(U_2)$ if $d_{G_i}(u_i, v_k) = e_{G_i}(u_i) = i$. Otherwise, $d_{G_i}(u_i, v_k) = e_{G_i}(u_i) < i$, for any two vertices $x, y \in V(U_2)$, and then, the element at the xth row and yth column of the matrix $\varepsilon(U_2') - \varepsilon(U_2)$ is

$$(\varepsilon(U_2'))_{xy} - (\varepsilon(U_2))_{xy} = \begin{cases} i - e_{G_i}(v_k)\,, & \text{if } x = v_k\,, \text{ and } y \in N_{U_2}(u_{d-1})\backslash\{u_{d-2}\}\,; \\ e_{U_2}(y)\,, & \text{if } x = v_k\,, \text{ and } y \in \bigcup_{j=\frac{d+1}{2}}^{d-1} V(G_j)\,; \\ 0\,, & \text{otherwise.} \end{cases}$$

Therefore, $\varepsilon(U_2) \le \varepsilon(U_2')$ with equality if and only if $d_{G_i}(u_i, v_k) = e_{G_i}(u_i) = i$. We have $\varepsilon_1(U_2) \le \varepsilon_1(U_2')$ by Lemma 2.1 and Theorem 2.1. □

After multiple iterations of contraction as described in Lemma 2.9, the graph U_2 transforms into the unicyclic graph $U_3 \in U_{n,d}$, where graph U_3 contains only a unique cycle of length 3. On the other hand, the eccentricity spectral radius of the unicyclic graphs still increases or remains unchanged.

Lemma 2.10. *Let $U_3 \in U_{n,d}$ (odd $d \geq 5$) be a unicyclic graph with its unique cycle $C_3 = v_1v_2v_3v_1$, and there is a diametral path $P_{d+1} = u_0u_1 \ldots u_d$ such that $|V(C_r) \cap V(P_{d+1})| \leq 1$. Further, let G_j be the connected component of $U_3 - E(P_{d+1})$ containing u_j $(0 \leq j \leq d)$. Assume $v_3 \in V(G_i)\left(2 \leq i \leq \frac{d-1}{2}\right)$ such that $d_{G_i}(u_i, v_3) = e_{G_i}(u_i) \geq 2$, $deg_{U_3}(v_2) = deg_{U_3}(v_3) = 2$, and $deg_{U_3}(v_1) = 3$. Let*

$$U_3' = U_3 - v_1v_2 - v_1v_3 + v_2u_1 + v_3u_1.$$

Then, $\varepsilon_1(U_3) \leq \varepsilon_1(U_3')$, with equality if and only if $d_{G_i}(u_i, v_3) = e_{G_i}(u_i) = i$.

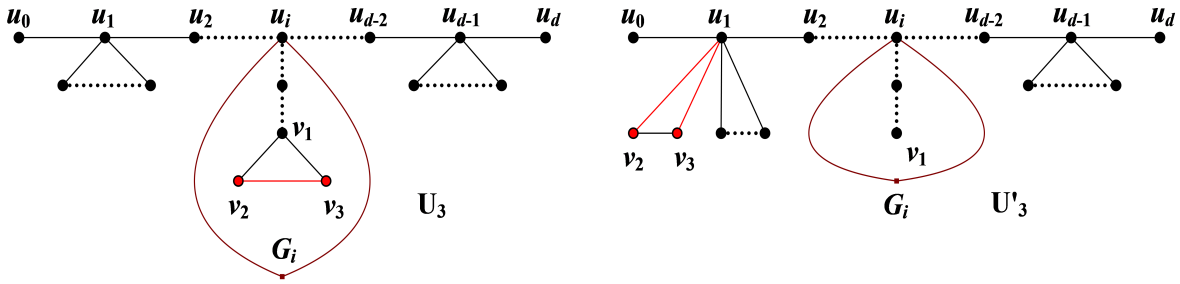


Figure 7. The unicyclic graphs of Lemma 2.10.

Proof. From graphs U_3 to U_3', see Figure 7, it is easy to obtain $\varepsilon(U_3') = \varepsilon(U_3)$ if $d_{G_i}(u_i, v_3) = e_{G_i}(u_i) = i$. Otherwise, $d_{G_i}(u_i, v_3) = e_{G_i}(u_i) < i$, for any two vertices $x, y \in V(U_3)$. The element at the xth row and yth column of the matrix $\varepsilon(U_3') - \varepsilon(U_3)$ is

$$(\varepsilon(U_3'))_{xy} - (\varepsilon(U_3))_{xy} = \begin{cases} i - e_{G_i}(v_3)\,, & \text{if } x \in \{v_2, v_3\}\,, \text{ and } y \in N_{U_3}(u_{d-1})\backslash\{u_{d-2}\}\,; \\ e_{U_3}(y)\,, & \text{if } x \in \{v_2, v_3\}\,, \text{ and } y \in \bigcup_{j=\frac{d+1}{2}}^{d-1} V(G_j)\,; \\ 0\,, & \text{otherwise.} \end{cases}$$

Therefore, $\left(\varepsilon(U_3')\right)_{xy} - (\varepsilon(U_3))_{xy} \geq 0$, so we have $\varepsilon(U_3) \leq \varepsilon(U_3')$ with equality if and only if $d_{G_i}(u_i, v_3) = e_{G_i}(u_i) = i$. We have $\varepsilon_1(U_3) \leq \varepsilon_1(U_3')$ by Lemma 2.1 and Theorem 2.1. □

Finally, the ith branch $G_i\left(2 \leq i \leq \frac{d-1}{2}\right)$ of U_3' is a pendant path with length not exceeding i, which ensures that U_3' still belongs to $U_{n,d}$. Applying repeatedly the transformation of Lemma 2.8 to graph U_3' again, a new unicyclic graph having the same structure with $U_{n,d}^{a,b}$ can be obtained.

After frequent use of Lemmas 2.8–2.10, we obtain the extremal unicyclic graph $U_{n,d}^{a,b}$ (see Figure 2), which may have the maximum ε-spectral radius under the condition $|V(C_r) \cap V(P_{d+1})| \leq 1$. Now, we study unicyclic graphs with $|V(C_r) \cap V(P_{d+1})| = 2$ and where C_r is an even cycle. The following lemmas are interesting and useful for the remainder of the paper.

Lemma 2.11. *Let $U \in U_{n,d}$ (odd $d \geq 5$) be a unicyclic graph with its unique cycle $C_r = v_1v_2 \cdots v_rv_1$, and there is a diametral path $P_{d+1} = u_0u_1 \ldots u_d$ such that $|V(C_r) \cap V(P_{d+1})| = 2$. Further, let G_j be the*

connected component of $U - E(P_{d+1}) - E(C_r)$ *containing* u_j $(0 \le j \le d)$. *Assume there exists a vertex* $w_1 \in V(G_i)\left(2 \le i \le \frac{d-1}{2}\right)$ *such that* $d_{G_i}(u_i, w_1) = e_{G_i}(u_i) \ge 2$, *and* $deg_U(w_1) = 1$. *Denote the unique neighbor of* w_1 *by* w. *Let*

$$U' = U - ww_1 + w_1u_1.$$

Then, $\varepsilon_1(U) \le \varepsilon_1(U')$, with equality if and only if $d_{G_i}(u_i, w_1) = e_{G_i}(u_i) = i$.

Proof. For two graphs U, U', we consider only the eccentricity $e_{G_i}(u_i) = d_{G_i}(u_i, w_1)$ of u_i in G_i.
Case 1. If $e_{G_i}(u_i) = i$, we obtain $\varepsilon(U') = \varepsilon(U)$ by $e_U(w_1) = e_{U'}(w_1) = d$, $(\varepsilon(U'))_{w_1y} = (\varepsilon(U))_{w_1y}$ for all vertices $y \in V(U)\backslash\{w_1\}$ and $(\varepsilon(U'))_{uv} = (\varepsilon(U))_{uv}$ for $u, v \in V(U)\backslash\{w_1\}$.
Case 2. If $e_{G_i}(u_i) < i$, for arbitrary $x, y \in V(U)$, the element at the xth row and yth column of the matrix $\varepsilon(U') - \varepsilon(U)$ is

$$(\varepsilon(U'))_{xy} - (\varepsilon(U))_{xy} = \begin{cases} i - e_{G_i}(u_i)\,, & \text{if } x = w_1\,, \text{ and } y \in \{v \in V(U) \mid d_U(v, u_0) = e_U(v) = d\}\,; \\ e_U(y)\,, & \text{if } x = w_1\,, \text{ and } y \in \{v \in V(U) \mid d_U(v, u_0) = e_U(v) < d\}\,; \\ 0\,, & \text{otherwise.} \end{cases}$$

Thus, $\varepsilon(U) \le \varepsilon(U')$ with equality if and only if $d_{G_i}(u_i, w_1) = e_{G_i}(u_i) = i$. Combining Lemma 2.1 with Theorem 2.1, we obtain $\varepsilon_1(U) \le \varepsilon_1(U')$. □

After the above edge-movement, all the pendant vertices in the connected branch tree G_j of the unicyclic graph U can be moved to be adjacent to u_1 or u_{d-1}, and the ε-spectral radius of the new unicyclic graph U' increases or remains unchanged. After multiple edge-movement changes, the resulting graph is similar to U_4 in Figure 8.

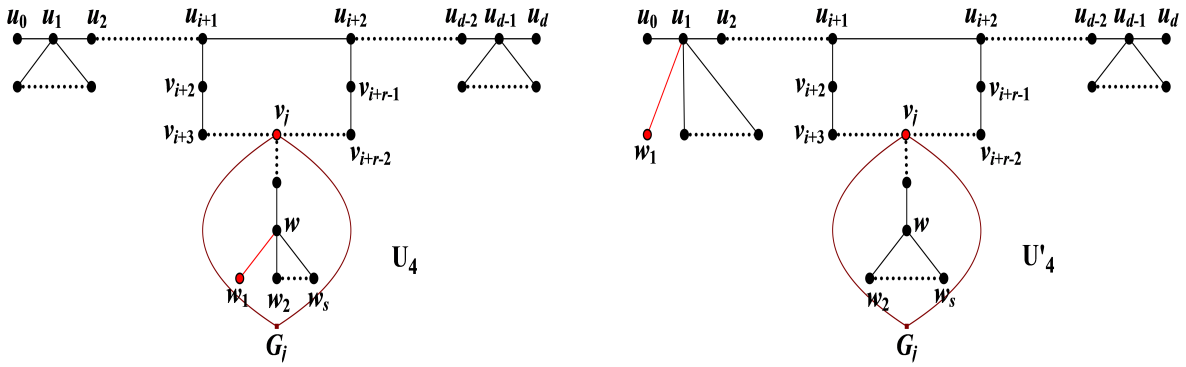


Figure 8. The unicyclic graphs of Lemma 2.12.

Lemma 2.12. *Let* $U_4 \in U_{n,d}$ *(odd* $d \ge 5$*) be a unicyclic graph with its unique even-cycle* $C_r = u_{i+1}u_{i+2}v_{i+r-1}v_{i+r-2}\ldots v_{i+2}u_{i+1}$, *and there is a diametral path* $P_{d+1} = u_0u_1\ldots u_d$ *such that* $V(C_r) \cap V(P_{d+1}) = \{u_{i+1}, u_{i+2}\}$, *and* $2 \le i + 2 \le \frac{d-1}{2}$. *Further, let* G_j *be the connected component of* $U_4 - E(P_{d+1}) - E(C_r)$ *containing* v_j $(j = i + 2,\ i + 3,\ \ldots,\ i + r - 1)$. *Assume there exists a vertex* $w_1 \in V(G_j)$ $(i + 2 \le j \le i + r - 1)$ *such that* $d_{G_j}(v_j, w_1) = e_{G_j}(v_j) \ge 1$, *and* $deg_{U_4}(w_1) = 1$. *Denote the unique neighbor of* w_1 *by* w. *Let*

$$U_4' = U_4 - ww_1 + w_1u_1.$$

Then, $\varepsilon_1(U_4) \le \varepsilon_1(U_4')$, with equality if and only if $d_{U_4}(w_1, u_d) = d$.

Proof. Discuss two cases for the distance between vertices w_1 and u_d.
Case 1. If $d_{U_4}(w_1, u_d) = d$, combining

$$(\varepsilon(U_4))_{w_1u} = (\varepsilon(U_4'))_{w_1u} = e_{U_4}(u) \text{ for } u \in \{v \in V(U_4) \mid d_{U_4}(v, u_0) = e_{U_4}(v)\};$$
$$(\varepsilon(U_4))_{w_1u} = (\varepsilon(U_4'))_{w_1u} = 0 \text{ for } u \in \{v \in V(U_4) \mid d_{U_4}(v, u_d) = e_{U_4}(v)\};$$
$$(\varepsilon(U_4))_{uv} = (\varepsilon(U_4'))_{uv} \text{ for } u, v \in V(U_4)\backslash\{w_1\},$$

we obtain $\varepsilon(U_4) = \varepsilon(U_4')$, and then, $\varepsilon_1(U_4) = \varepsilon_1(U_4')$.
Case 2. If $d_{U_4}(w_1, u_d) < d$, from graphs U_4 to U_4', for any two vertices $x, y \in V(U_4)$, the element at the xth row and yth column of the matrix $\varepsilon(U_4') - \varepsilon(U_4)$ is

$$(\varepsilon(U_4'))_{xy} - (\varepsilon(U_4))_{xy} = \begin{cases} d - e_{U_4}(w_1), & \text{if } x = w_1 \text{ ,and } y \in \{v \in V(U_4) \mid d_{U_4}(v, u_0) = d\}; \\ e_{U_4}(y), & \text{if } x = w_1 \text{ , and } y \in \{v \in V(U_4) \mid d_{U_4}(v, u_0) = e_{U_4}(v) < d\}; \\ 0, & \text{otherwise.} \end{cases}$$

Therefore, $\varepsilon(U_4) \le \varepsilon(U_4')$ when $d_{U_4}(w_1, u_d) < d$.

Combining the above two cases, we obtain $\varepsilon(U_4) \le \varepsilon(U_4')$ with equality if and only if $d_{U_4}(w_1, u_d) = d$. Hence, $\varepsilon_1(U_4) \le \varepsilon_1(U_4')$ by Lemma 2.1 and Theorem 2.1. □

Lemma 2.13. *Let $U \in U_{n,d}$ (odd $d \ge 5$) be a unicyclic graph with its unique even-cycle $C_r = u_{\frac{d-1}{2}}u_{\frac{d+1}{2}}v_{\frac{d-5}{2}+r}v_{\frac{d-7}{2}+r}\ldots v_{\frac{d+1}{2}}u_{\frac{d-1}{2}}$, and there is a diametral path $P_{d+1} = u_0u_1\ldots u_d$ such that $V(C_r) \cap V(P_{d+1}) = \{u_{\frac{d-1}{2}}, u_{\frac{d+1}{2}}\}$. Further, let G_j be the connected component of $U - E(P_{d+1}) - E(C_r)$ containing $v_j\left(j = \frac{d+1}{2}, \frac{d+3}{2}, \ldots, \frac{d-5}{2} + r\right)$. Assume there exists a vertex $w_1 \in V(G_j)\left(\frac{d+1}{2} \le j \le \frac{d+r-3}{2}\right)$ such that $d_{G_j}(v_j, w_1) = e_{G_j}(v_j) \ge 1$, and $deg_U(w_1) = 1$. Denote the unique neighbor of w_1 by w. Let*

$$U' = U - ww_1 + w_1u_1.$$

Then, $\varepsilon_1(U) < \varepsilon_1(U')$.

Proof. Discuss two cases for the distance between vertices w_1 and u_d.
Case 1. If $d_U(w_1, u_d) = d$, from graphs U to U', for any two vertices $x, y \in V(U)$, one has

$$(\varepsilon(U'))_{xy} - (\varepsilon(U))_{xy} = \begin{cases} 0, & \text{if } x = w_1 \text{ , and } y \in \{v \in V(U) \mid d_U(v, u_0) = d = d_U(w_1, v)\}; \\ d, & \text{if } x = w_1 \text{ , and } y \in \{v \in V(U) \mid d_U(v, u_0) = d > d_U(w_1, v)\}; \\ e_{U'}(y), & \text{if } x = w_1 \text{ , and } y \in \{v \in V(U) \mid d_U(v, u_0) = e_U(v) < d\}; \\ 0, & \text{otherwise.} \end{cases}$$

Case 2. If $d_U(w_1, u_d) < d$, from graph U to U', for any two vertices $x, y \in V(U)$, the element at the xth row and yth column $(\varepsilon(U'))_{xy} - (\varepsilon(U))_{xy}$ of the matrix $\varepsilon(U') - \varepsilon(U)$ is

$$\begin{cases} d - e_U(w_1), & \text{if } x = w_1 \text{ , and } y \in \{v \in V(U) \mid d_U(v, u_0) = d \text{ , and } d_U(w_1, v) = e_U(w_1)\}; \\ d, & \text{if } x = w_1 \text{ , and } y \in \{v \in V(U) \mid d_U(v, u_0) = d \text{ , and } d_U(w_1, v) < e_U(w_1)\}; \\ e_{U'}(y), & \text{if } x = w_1 \text{ , and } y \in \{v \in V(U) \mid d_U(v, u_0) = e_U(v) < d; \\ 0, & \text{otherwise.} \end{cases}$$

Combining the above two cases, we get $\varepsilon(U) \le \varepsilon(U')$ and $\varepsilon(U) \ne \varepsilon(U')$, and then, $\varepsilon_1(U) < \varepsilon_1(U')$ by Lemma 2.1 and Theorem 2.1. □

All the pendant vertices of unicyclic graphs $U \in U_{n,d}$ such that $|V(C_r) \cap V(P_{d+1})| = 2$ are adjacent to the quasi-pendant vertices u_1 and u_{d-1} of P_{d+1} by edge-moving in Lemmas 2.11–2.13. This causes the eccentricity spectral radius of U to increase or remain unchanged. Here, C_r and $P_{d+1} = u_0u_1 \dots u_d$ are the unique even cycle and one of diametral paths of U, respectively.

Subsequently, we considered implementing two types of contraction changes, which would cause ε-spectral radius of unicyclic graphs U_5, U_6 in Figures 9 and 10 to increase.

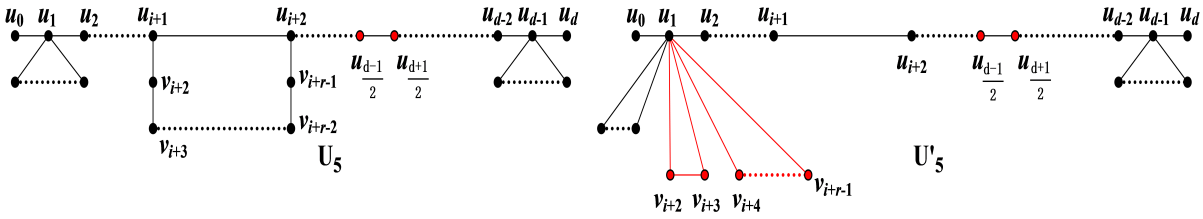


Figure 9. The two graphs of Lemma 2.14.

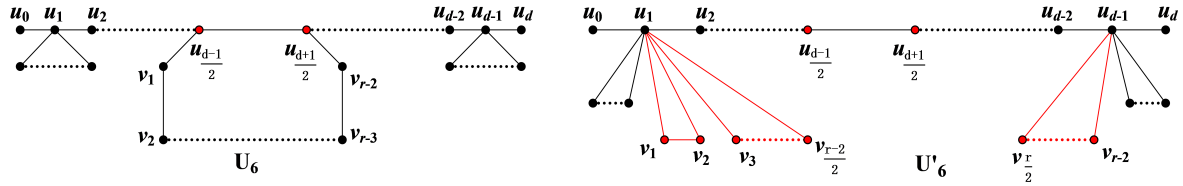


Figure 10. The two graphs of Lemma 2.15.

Lemma 2.14. *Let $U_5 \in U_{n,d}$ (odd $d \geq 5$) be a unicyclic graph with its unique even-cycle $C_r = u_{i+1}u_{i+2}v_{i+r-1}v_{i+r-2} \dots v_{i+2}u_{i+1}$, and there is a diametral path $P_{d+1} = u_0u_1 \dots u_d$ such that $V(C_r) \cap V(P_{d+1}) = \{u_{i+1}, u_{i+2}\}$, where $2 \leq i+2 \leq \frac{d-1}{2}$. Obviously, $4 \leq r \leq 2(i+2)$, and $e_{U_5}(v_j) \leq d$ for $j = i+2, i+3, \dots, i+r-1$. Let*

$$U_5' = U_5 - \bigcup_{j=i+3}^{i+r-2} v_jv_{j+1} - u_{i+1}v_{i+2} - u_{i+2}v_{i+r-1} + \bigcup_{j=i+2}^{i+r-1} v_ju_1.$$

Then, $\varepsilon_1(U_5) < \varepsilon_1(U_5')$.

Proof. When transforming from U_5 to U_5', let $W = \{v_{i+2}, v_{i+3}, \dots, v_{i+r-1}\}$. To ensure that the diameter of U_5 is d, the girth of C_r should not exceed $2(i+2)$, that is, $r \leq 2i+4$.

Case 1. If $r = 2i+4$, then $e_{U_5}(v_{2i+2}) = d$, and $e_{U_5}(w) < d$ for all vertices $w \in W\backslash\{v_{2i+2}\}$. For any two vertices $x, y \in V(U_5)$, the element at the xth row and yth column of the matrix $\varepsilon(U_5') - \varepsilon(U_5)$ is

$$(\varepsilon(U_5'))_{xy} - (\varepsilon(U_5))_{xy} = \begin{cases} d - e_{U_5}(x), & \text{if } x \in W\backslash\{v_{2i+2}\}, \text{ and } y \in N_{U_5}(u_{d-1})\backslash\{u_{d-2}\}; \\ e_{U_5}(y), & \text{if } x \in W\backslash\{v_{2i+2}\}, \text{ and } y \in \{u_{\frac{d+1}{2}}, \dots, u_{d-1}\}; \\ 0, & \text{otherwise.} \end{cases}$$

Therefore, $\varepsilon(U_5) \leq \varepsilon(U_5')$, and $\varepsilon(U_5) \neq \varepsilon(U_5')$ when $r = 2i + 4$.

Case 2. If $r < 2i + 4$, then $e_{U_5}(w) < d$ for all vertices $w \in W$. For any two vertices $x, y \in V(U_5)$, the element at the xth row and yth column of the matrix $\varepsilon(U_5') - \varepsilon(U_5)$ is

$$(\varepsilon(U_5'))_{xy} - (\varepsilon(U_5))_{xy} = \begin{cases} d - e_{U_5}(x)\,, & \text{if } x \in W\,, \text{ and } y \in N_{U_5}(u_{d-1})\backslash\{u_{d-2}\}\,; \\ e_{U_5}(y)\,, & \text{if } x \in W\,, \text{ and } y \in \{u_{\frac{d+1}{2}}, \ldots, u_{d-1}\}\,; \\ 0\,, & \text{otherwise.} \end{cases}$$

Therefore, $\varepsilon(U_5) \leq \varepsilon(U_5')$, and $\varepsilon(U_5) \neq \varepsilon(U_5')$ when $r < 2i + 4$.

Combining the two cases above, Lemma 2.1 and Theorem 2.1, we obtain $\varepsilon_1(U_5) < \varepsilon_1(U_5')$. □

Lemma 2.15. *Let $U_6 \in U_{n,d}$ (odd $d \geq 5$) be a unicyclic graph with its unique even-cycle $C_r = u_{\frac{d-1}{2}} u_{\frac{d+1}{2}} v_{r-2} \ldots v_1 u_{\frac{d-1}{2}}$ $(4 \leq r \leq d + 1)$, and there is a diametral path $P_{d+1} = u_0 u_1 \ldots u_{d-1} u_d$ such that $V(C_r) \cap V(P_{d+1}) = \{u_{\frac{d-1}{2}}, u_{\frac{d+1}{2}}\}$. Let*

$$U_6' = U_6 - \bigcup_{j=2}^{r-3} v_j v_{j+1} - v_1 u_{\frac{d-1}{2}} - v_{r-2} u_{\frac{d+1}{2}} + \bigcup_{j=1}^{\frac{r-2}{2}} v_j u_1 + \bigcup_{j=\frac{r}{2}}^{r-2} v_j u_d.$$

Then, $\varepsilon_1(U_6) < \varepsilon_1(U_6')$.

Proof. To ensure that the diameter of U_6 remains constant d, thus the girth of C_r satisfies $r \leq d + 1$. From graphs U_6 to U_6', assume following the vertex set:

$$W_1 = \{v_1, v_2, \ldots, v_{\frac{r-2}{2}}\} \text{ and } W_2 = \{v_{\frac{r}{2}}, \ldots, v_{r-3}, v_{r-2}\},$$

$$U_1 = \{u_1, u_2, \ldots, u_{\frac{d-1}{2}}\} \text{ and } U_2 = \{u_{\frac{d+1}{2}}, \ldots, u_{d-2}, u_{d-1}\}.$$

Case 1. If $r = d + 1$, then $e_{U_6}(v_{\frac{r-2}{2}}) = e_{U_6}(v_{\frac{r}{2}}) = d$, and $e_{U_6}(w) < d$ for all vertices $w \in (W_1 \cup W_2)\backslash\{v_{\frac{r-1}{2}}, v_{\frac{r}{2}}\}$. For any two vertices $x, y \in V(U_5)$, the element at the xth row and yth column of the matrix $\varepsilon(U_5') - \varepsilon(U_5)$ is

$$\varepsilon(U_6')_{xy} - \varepsilon(U_6)_{xy} = \begin{cases} d - e_{U_6}(x)\,, & \text{if } x \in W_1\,, \text{ and } y \in N_{U_6}(u_{d-1})\backslash\{u_{d-2}\}; \\ e_{U_6}(y)\,, & \text{if } x \in W_1\backslash\{v_{\frac{r-2}{2}}\}\,, \text{ and } y \in U_2; \\ d\,, & \text{if } x \in W_1\,, \text{ and } y \in W_2; \\ d - e_{U_6}(x)\,, & \text{if } x \in W_2\,, \text{ and } y \in N_{U_6}(u_1)\backslash\{u_2\}; \\ e_{U_6}(y)\,, & \text{if } x \in W_2\backslash\{v_{\frac{r}{2}}\}\,, \text{ and } y \in U_1; \\ 0\,, & \text{otherwise.} \end{cases}$$

Case 2. If $r \leq d - 1$, then $e_{U_6}(w) < d$ for all vertices $w \in W_1 \cup W_2$. For any two vertices $x, y \in V(U_5)$, the element at the xth row and yth column of the matrix $\varepsilon(U_5') - \varepsilon(U_5)$ is

$$\varepsilon(U_6')_{xy} - \varepsilon(U_6)_{xy} = \begin{cases} d - e_{U_6}(x)\,, & \text{if } x \in W_1\,, \text{ and } y \in N_{U_6}(u_{d-1})\backslash\{u_{d-2}\}; \\ e_{U_6}(y)\,, & \text{if } x \in W_1\,, \text{ and } y \in U_2; \\ d, & \text{if } x \in W_1\,, \text{ and } y \in W_2; \\ d - e_{U_6}(x)\,, & \text{if } x \in W_2\,, \text{ and } y \in N_{U_6}(u_1)\backslash\{u_2\}; \\ e_{U_6}(y)\,, & \text{if } x \in W_2\,, \text{ and } y \in U_1; \\ 0\,, & \text{otherwise.} \end{cases}$$

Therefore, one has $\varepsilon(U_6) \leq \varepsilon(U_6')$, and $\varepsilon(U_6) \neq \varepsilon(U_6')$. We have $\varepsilon_1(U_6) < \varepsilon_1(U_6')$ by Lemma 2.1 and Theorem 2.1. □

Under condition $|\ V(P_{d+1}) \cap V(C_r)\ | \ = 2$ with even $r \geq 4$, we gradually apply Lemmas 2.11 to 2.15, and eventually obtain a unicyclic graph that is isomorphic to $U_{n,d}^{a,b}$, which causes the ε-spectral radius of unicyclic graphs to increase constantly.

Remark 2.3. *For $|V(C_r) \cap V(P_{d+1})| = 2$ and odd $d \geq 5$, we characterize the extremal graphs with maximum eccentricity spectral radius among n-vertex unicyclic graphs containing an even cycle C_r. However, for unicyclic graphs containing an odd cycle C_r, it seems that this cannot be determined in a way similar to the proof of Theorem* 2.4. *For example, consider the graphs H_1, H_2, H_3, (see Figure 11). The vertices v_1, v_2 in graph H_1; v_1, v_2, v_3, w in graph H_2; and v_1, v_2, v_3, v_4, v_5 in graph H_3 cannot undergo edge-shifting similar to that in Lemmas* 2.12–2.15.

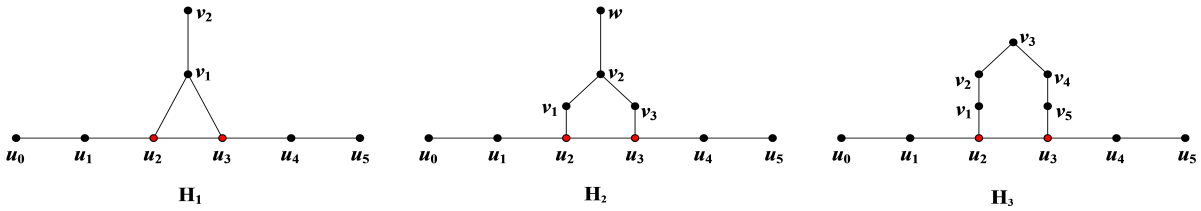


Figure 11. The three graphs contain an odd cycle.

Remark 2.4. *For $|V(C_r) \cap V(P_{d+1})| \geq 3$ and odd $d \geq 5$, the graph-transformation in Lemmas* 2.11 *and* 2.12 *is no longer applicable to graph pairs Q_1, Q_1' , and Q_2, Q_2' , depicted in Figure* 12. *Obviously, $\varepsilon(Q_1)_{v_4y} = d_{Q_1}(v_4, y) = 5 = e_{Q_1'}(v_4) = d_{Q_1'}(v_4, u_5) > d_{Q_1'}(v_4, y)$, and then, $\varepsilon(Q_1)_{v_4y} > 0 = \varepsilon(Q_1')_{v_4y}$. At the same time, $\varepsilon(Q_2)_{w_2u_4} = d_{Q_2}(w_2, u_4) = 7 = \min\{e_{Q_2'}(w_2), e_{Q_2'}(u_4)\} > 6 = d_{Q_2'}(w_2, u_4)$, and then, $\varepsilon(Q_2)_{w_2u_4} > 0 = \varepsilon(Q_2')_{w_2u_4}$. It is necessary to explore new methods, which is an interesting research problem.*

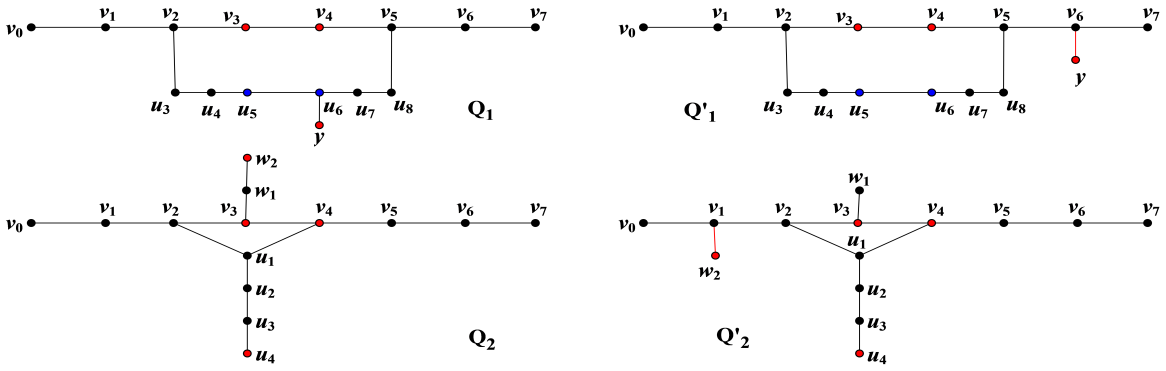


Figure 12. The unicyclic graphs of Remark 2.4.

For the following two classes of unicyclic graphs $G \in U_{n,d}$ with given odd $d \geq 5$,

$$(1)\ |\ V(P_{d+1}) \cap V(C_r)\ |= 1;\ \ (2)\ |\ V(P_{d+1}) \cap V(C_r)\ |= 2 \text{ with even } r \geq 4,$$

where P_{d+1} is one of diametral paths of G, and C_r is the unique cycle of G, and $V(P_{d+1})$ and $V(C_r)$ represent respectively the vertex sets of P_{d+1} and C_r, we obtain finally that the unicyclic graph $U_{n,d}^{a,b}$ (see Figure 2) may achieve the maximum ε-spectral radius by Lemmas 2.8–2.15. Surprisingly, we find that unicyclic graph $U_{n,d}^{a,b}$ and 1-clique tree $T_1(n,d,a,b)$ (or simply a tree) are ε-cospectral with $\varepsilon(U_{n,d}^{a,b}) = \varepsilon(T_1(n,d,a,b))$, where $a+b = n-d-1$, $a \geq 2$, and $b \geq 0$. However, they are not isomorphic.

To make it easier for readers to comprehend, we give the definition of t-clique trees. The graph resulting from substituting each edge of tree G with a clique $K_{t+1}(t \geq 1)$ is called the *t-clique tree* corresponding to G. Denote by $\Phi_t(n', d)$ the set of t-clique trees with order $n' = (n-1)t+1$ and diameter d, where $n \geq 2$, and $t \geq 1$ as in [14]. Deleting an edge $e = x_1x_2$ from the unicyclic graph $U_{n,d}^{a,b}$ in Figure 2 yields the 1-clique tree $T_1(n,d,a,b)$.

Because $\varepsilon(U_{n,d}^{a,b}) = \varepsilon(T_1(n,d,a,b))$, the following conclusion can be obtained easily.

Theorem 2.3. *The unicyclic graph $U_{n,d}^{a,b}$ and clique tree $T_1(n,d,a,b)$ are ε-cospectral, where $a+b = n-d-1$, $a \geq 2$, and $b \geq 0$.*

Let $p, q \in \mathbb{Z}$ (or let p, q be two positive integers). We say that p and q are *coprime* (or *relatively prime*) if their greatest common divisor equals 1, that is, $\gcd(p,q) = 1$. Equivalently, p and q are coprime if and only if there is no integer greater than 1 that divides both p and q. This relation is denoted by $(p,q) = 1$.

Theorem 2.4. *Let unicyclic graph $U \in \mathcal{U}_{n,d}^r$ with order $n \geq d+5$ and fixed odd $d \geq 5$. Denote $\Gamma(d) := \left(\frac{d+1}{2}\right)^2 + \left(\frac{d+3}{2}\right)^2 + \cdots + (d-1)^2 = \frac{d(d-1)(7d-5)}{24}$. Then,*

$$\varepsilon_1(U) \leq \max\left\{\varepsilon_1\left(U_{n,d}^{\lfloor\frac{n-d-1}{2}\rfloor,\lceil\frac{n-d-1}{2}\rceil}\right), \varepsilon_1\left(U_{n,d}^{n-d-1,0}\right)\right\},$$

with equality if and only if $U \cong U_{n,d}^{n-d-1,0}$, $U_{n,d}^{\lfloor\frac{n-d-1}{2}\rfloor,\lceil\frac{n-d-1}{2}\rceil}$ or $U_{n,d}^{\lceil\frac{n-d-1}{2}\rceil,\lfloor\frac{n-d-1}{2}\rfloor}$, based on

$$\varepsilon_1\left(U_{n,d}^{\lceil\frac{n-d-1}{2}\rceil,\lfloor\frac{n-d-1}{2}\rfloor}\right) = \varepsilon_1\left(U_{n,d}^{\lfloor\frac{n-d-1}{2}\rfloor,\lceil\frac{n-d-1}{2}\rceil}\right) \neq \frac{\Gamma(d)}{d} \neq \varepsilon_1\left(U_{n,d}^{n-d-1,0}\right).$$

Hence, the extremal unicyclic graph with fixed odd $d \geq 5$ and $n \geq d+5$ having the maximum eccentricity spectral radius in $\mathcal{U}_{n,d}^r$ is not unique when $\varepsilon_1(U) > \frac{\Gamma(d)}{d}$.

Proof. Let U be the unicyclic graph in $\mathcal{U}_{n,d}^r$ having the maximum eccentricity spectral radius. It is easy to get $U \cong U_{n,d}^{a,b}$ by Lemmas 2.8 to 2.15, as one of diametral paths of $U_{n,d}^{a,b}$ denotes $P_{d+1} = u_0u_1\ldots u_d$, and the unique cycle of $U_{n,d}^{a,b}$ denotes $C_3 = u_1x_1x_2u_1$ in Figure 2.

Denote $X = \{u_0, x_1, x_2, \ldots, x_a\}$ and $Y = \{u_d, y_1, y_2, \ldots, y_b\}$ in Figure 2. Let $\mathbf{x}$ be a Perron eigenvector corresponding to $\rho = \varepsilon_1(U_{n,d}^{a,b})$, whose coordinate with respect to verte v is x_v. Because

$$\rho x_x = \frac{d+1}{2}x_{u_{\frac{d+1}{2}}} + \frac{d+3}{2}x_{u_{\frac{d+3}{2}}} + \cdots + d\sum_{y\in Y} x_y$$

for each $x \in X$, we can obtain $x_x = x_{x'}$ for $\{x, x'\} \subseteq X$. Similarly, $x_y = x_{y'}$ for $\{y, y'\} \subseteq Y$. Therefore, for all $x \in X$, $y \in Y$, we get

$$\rho x_x = \frac{d+1}{2}x_{u_{\frac{d+1}{2}}} + \frac{d+3}{2}x_{u_{\frac{d+3}{2}}} + \cdots + (d-1)x_{u_{d-1}} + d(b+1)x_y;$$

$$\rho x_y = d(a+1)x_x + (d-1)x_{u_1} + (d-2)x_{u_2} + \cdots + \frac{d-1}{2}x_{u_{\frac{d-3}{2}}} + \frac{d+1}{2}x_{u_{\frac{d-1}{2}}};$$

$$\rho x_{u_i} = (b+1)(d-i)x_y \text{ if } i \in \left\{1, 2, \ldots, \frac{d-1}{2}\right\};$$

$$\rho x_{u_j} = (a+1)jx_x \text{ if } j \in \left\{\frac{d+1}{2}, \frac{d+3}{2}, \ldots, d-1\right\}.$$

Hence, we obtain

$$\begin{aligned}\rho^2 x_x &= \frac{d+1}{2}\rho x_{u_{\frac{d+1}{2}}} + \frac{d+3}{2}\rho x_{u_{\frac{d+3}{2}}} + \cdots + (d-1)\rho x_{u_{d-1}} + d(b+1)\rho x_y \\ &= (a+1)\left[\left(\frac{d+1}{2}\right)^2 + \left(\frac{d+3}{2}\right)^2 + \cdots + (d-1)^2\right]x_x + d(b+1)\rho x_y \\ &= (a+1)\Gamma(d)x_x + d(b+1)\rho x_y,\end{aligned}$$

and

$$\begin{aligned}\rho^2 x_y &= d(a+1)\rho x_x + (d-1)\rho x_{u_1} + (d-2)\rho x_{u_2} + \cdots + \frac{d+1}{2}\rho x_{u_{\frac{d-1}{2}}}; \\ &= d(a+1)\rho x_x + (b+1)\left[(d-1)^2 + (d-2)^2 + \cdots + \left(\frac{d+1}{2}\right)^2\right]x_y \\ &= d(a+1)\rho x_x + (b+1)\Gamma(d)x_y.\end{aligned}$$

We immediately obtain the linear equations for x_x and x_y, that is,

$$\begin{cases}\left[\rho^2 - (a+1)\Gamma(d)\right]x_x - d(b+1)\rho x_y &= 0, \\ \left[\rho^2 - (b+1)\Gamma(d)\right]x_y - d(a+1)\rho x_x &= 0.\end{cases}$$

Because $x_x > 0$, and $x_y > 0$, ρ is the largest root of

$$\begin{vmatrix}\rho^2 - (a+1)\Gamma(d) & -d(b+1)\rho \\ -d(a+1)\rho & \rho^2 - (b+1)\Gamma(d)\end{vmatrix} = 0;$$

that is, $\rho^4 - \left[(a+b+2)\Gamma(d) + (a+1)(b+1)d^2\right]\rho^2 + (a+1)(b+1)\Gamma^2(d) = 0$, where $a+b = n-d-1$. Let the function

$$f_{a,b}(\lambda) = \lambda^4 - \left[(a+b+2)\Gamma(d) + (a+1)(b+1)d^2\right]\lambda^2 + (a+1)(b+1)\Gamma^2(d). \tag{2.1}$$

Claim 1. For odd $d \geq 5$ and $n \geq d+5$, $\varepsilon_1(U_{n,d}^{n-d-1,0}) \neq \Gamma(d)/d$.

Based on

$$\begin{aligned} f_{n-d-1,0}\left(\frac{\Gamma(d)}{d}\right) &= \left(\frac{\Gamma(d)}{d}\right)^4 - \left[(n-d+1)\Gamma(d) + (n-d)d^2\right]\left(\frac{\Gamma(d)}{d}\right)^2 + (n-d)\Gamma^2(d) \\ &= \left(\frac{\Gamma(d)}{d}\right)^3 \left[\frac{\Gamma(d)}{d} - (n-d+1)d - \frac{(n-d)d^3}{\Gamma(d)} + \frac{(n-d)d^3}{\Gamma(d)}\right] \\ &= \left(\frac{\Gamma(d)}{d}\right)^3 \left[\frac{\Gamma(d)}{d} - (n-d+1)d\right] \\ &= \left(\frac{\Gamma(d)}{d}\right)^3 \left[\frac{(d-1)(7d-5)}{24} - (n-d+1)d\right], \end{aligned}$$

we obtain $f_{n-d-1,0}\left(\frac{\Gamma(d)}{d}\right) = 0$ if $\varepsilon_1(U_{n,d}^{n-d-1,0}) = \frac{\Gamma(d)}{d}$; that is $\frac{(d-1)(7d-5)}{24} = (n-d+1)d$. Note that $\gcd(d, d-1) = 1$; then, $d \mid (7d-5)$. When $\frac{7d-5}{d} = 7 - \frac{5}{d} \leq 6$ by odd $d \geq 5$, $\frac{24(n-d+1)}{d-1} \geq \frac{24(d+3-d+1)}{d-1} \geq \frac{114}{d-1}$, we get $\frac{24(n-d+1)}{d-1} \geq 36$ and $\frac{7d-5}{d} = 6 \neq \frac{24(n-d+1)}{d-1}$ when $d = 5$, a contradiction. Thus, $\varepsilon_1(U_{n,d}^{n-d-1,0}) \neq \frac{\Gamma(d)}{d}$ for odd $d \geq 5$ and $n \geq d+5$.

Claim 2. $\rho \leq \max\left\{\varepsilon_1\left(U_{n,d}^{n-d-1,0}\right), \varepsilon_1(Q)\right\}$, where $Q \cong U_{n,d}^{\lceil\frac{n-d-1}{2}\rceil,\lfloor\frac{n-d-1}{2}\rfloor}$ or $U_{n,d}^{\lfloor\frac{n-d-1}{2}\rfloor,\lceil\frac{n-d-1}{2}\rceil}$.

Claim 2.1. If $\rho < \frac{\Gamma(d)}{d}$, then $U \cong U_{n,d}^{n-d-1,0}$.

We assume that $a > b \geq 1$. Combining $d\rho - \Gamma(d) < 0$ (here, $\varepsilon_1(U_{n,d}^{a,b}) = \rho$) with $a - b + 1 > 0$, we can get

$$f_{a+1,b-1}(\rho) = f_{a+1,b-1}(\rho) - f_{a,b}(\rho) = (a-b+1)(d\rho - \Gamma(d))(d\rho + \Gamma(d)) < 0.$$

Thus, $\varepsilon_1\left(U_{n,d}^{a,b}\right) < \varepsilon_1\left(U_{n,d}^{a+1,b-1}\right)$, a contradiction. Then, the ε-spectral radius of $U_{n,d}^{a,b}$ when $a = n-d-1$ and $b = 0$, that is, $U \cong U_{n,d}^{n-d-1,0}$.

Claim 2.2. $\rho \neq \frac{\Gamma(d)}{d}$. Assume that $\rho = \varepsilon_1\left(U_{n,d}^{a,b}\right) = \frac{\Gamma(d)}{d}$, then $f_{a,b}(\rho) = 0$. If $a > b \geq 1$, and thus,

$$f_{a+1,b-1}(\rho) = f_{a+1,b-1}(\rho) - f_{a,b}(\rho) = (a-b+1)(d\rho + \Gamma(d))(d\rho - \Gamma(d)) = 0.$$

Therefore, ρ is a root of $f_{a+1,b-1}(\lambda) = 0$. Further, $\varepsilon_1\left(U_{n,d}^{a+1,b-1}\right) = \rho = \frac{\Gamma(d)}{d}$. Continuously making similar changes, we get $\varepsilon_1\left(U_{n,d}^{n-d-1,0}\right) = \rho = \frac{\Gamma(d)}{d}$, which contradicts Claim 1. Therefore, $\rho \neq \frac{\Gamma(d)}{d}$.

Claim 2.3. If $\rho > \frac{\Gamma(d)}{d}$, then U is isomorphic to $U_{n,d}^{\lceil\frac{n-d-1}{2}\rceil,\lfloor\frac{n-d-1}{2}\rfloor}$ or $U_{n,d}^{\lfloor\frac{n-d-1}{2}\rfloor,\lceil\frac{n-d-1}{2}\rceil}$.

Assume that $a > b+1$ and that $a \geq 3$. Combining $\rho = \varepsilon_1\left(U_{n,d}^{a,b}\right) > \frac{\Gamma(d)}{d}$ with $b - a + 1 < 0$, we can get

$$f_{a-1,b+1}(\rho) = f_{a-1,b+1}(\rho) - f_{a,b}(\rho) = (b-a+1)(d\rho - \Gamma(d))(d\rho + \Gamma(d)) < 0.$$

Therefore, $\varepsilon_1(U) = \varepsilon_1\left(U_{n,d}^{a,b}\right) = \rho < \varepsilon_1\left(U_{n,d}^{a-1,b+1}\right)$, a contradiction. Then, $b \leq a \leq b+1$, $\varepsilon_1(U) \leq \varepsilon_1\left(U_{n,d}^{\lceil\frac{n-d-1}{2}\rceil,\lfloor\frac{n-d-1}{2}\rfloor}\right)$. On the other hand, we have $\varepsilon_1\left(U_{n,d}^{\lceil\frac{n-d-1}{2}\rceil,\lfloor\frac{n-d-1}{2}\rfloor}\right) = \varepsilon_1\left(U_{n,d}^{\lfloor\frac{n-d-1}{2}\rfloor,\lceil\frac{n-d-1}{2}\rceil}\right)$ but $U_{n,d}^{\lceil\frac{n-d-1}{2}\rceil,\lfloor\frac{n-d-1}{2}\rfloor} \ncong U_{n,d}^{\lfloor\frac{n-d-1}{2}\rfloor,\lceil\frac{n-d-1}{2}\rceil}$. Clearly, we obtain that U is isomorphic to $U_{n,d}^{\lceil\frac{n-d-1}{2}\rceil,\lfloor\frac{n-d-1}{2}\rfloor}$ or $U_{n,d}^{\lfloor\frac{n-d-1}{2}\rfloor,\lceil\frac{n-d-1}{2}\rceil}$.

If $n \geq d+5$, we get $\varepsilon_1\left(U_{n,d}^{\lceil\frac{n-d-1}{2}\rceil,\lfloor\frac{n-d-1}{2}\rfloor}\right) = \varepsilon_1\left(U_{n,d}^{\lfloor\frac{n-d-1}{2}\rfloor,\lceil\frac{n-d-1}{2}\rceil}\right) \neq \varepsilon_1\left(U_{n,d}^{n-d-1,0}\right)$ by Claims 2.1–2.3. Hence, the extremal unicyclic graph with fixed odd $d \geq 5$ having the maximum eccentricity spectral radius in $\mathcal{U}_{n,d}^r$ is not unique when $\rho > \frac{\Gamma(d)}{d}$.

Combining the above claims, we complete the proof of Theorem 2.4. □

3. Concluding remarks

It is acknowledged that the problem of characterizing graphs whose eccentricity matrices are irreducible remains unresolved. The question of whether the eccentricity matrix of connected graphs containing cycles is reducible or not remains an open problem for researchers to consider. We note that the eccentricity matrices of trees and cycle C_{2n+1} are irreducible, whereas $\varepsilon(C_{2n})$ is reducible. To this end, we prove that the eccentricity matrix of unicyclic graphs (containing at least one pendant vertex) with odd diameter that and $\mid V(P_{d+1}) \cap V(C_r) \mid \leq 2$ is irreducible. Furthermore, an affirmative response can be given to Problem 3 in [20] with regard to unicyclic graphs in $\mathcal{U}^r_{n,d}$. We also characterize extremal unicyclic graphs in $\mathcal{U}^r_{n,d}$ with a maximum eccentricity spectral radius.

What happens, then, to the ε-spectral radius of connected graphs (which include cycles) and trees given other parameters, such as the number of matchings, the number of pendant vertices, or perfect matching? As we know, the extremal graphs for ε-spectral radius are nonunique and irregular. For the general case, they proposed the question ([20], Problem 7): Under what conditions is the diameter of a graph determined by ε-spectrum? This is a profound problem in spectral graph theory.

In the context of odd diameter, for these extremal graphs of trees and unicyclic graphs in $\mathcal{U}^r_{n,d}$ with maximum ε-spectral radius, we find that the extremal graph (see Figure 2) of the latter has only one additional edge x_1x_2 compared to that of the former by Theorem 2.10 (in [24]). Then, can the addition of edges to the trees (the base graph) be achieved in such a manner that the bound of the eccentricity spectral radius of the multicycle graphs obtained remains unchanged? It remains a matter of interest for future study.

Author contributions

Zhengping Qiu: Writing–original draft, Writing–review & editing, Methodology, and Funding acquisition; Zikai Tang: Conceptualization, Validation, Formal analysis, Writing–review and editing; Shilin Zeng: Formal analysis, Software, and Funding acquisition. All authors have read and agreed to the published version of the manuscript.

Use of Generative-AI tools declaration

The authors declare that they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The authors declare that they have no competing interests.

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