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FORBIDDEN THETA GRAPH, BOUNDED SPECTRAL RADIUS AND SIZE OF NON-BIPARTITE GRAPHS

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Abstract. Zhai and Lin recently proved that if G is an n-vertex connected $\theta(1,2,r+1)$-free graph, then for odd r and $n \geqslant 10r$, or for even r and $n \geqslant 7r$, one has $\rho(G) \leq \sqrt{\lfloor \frac{n^2}{4} \rfloor}$, and equality holds if and only if G is $K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$. In this paper, for large enough n, we prove a sharp upper bound for the spectral radius in an n-vertex H-free non-bipartite graph, where H is $\theta(1,2,3)$ or $\theta(1,2,4)$, and we characterize all the extremal graphs. Furthermore, for $n \geqslant 137$, we determine the maximum number of edges in an n-vertex $\theta(1,2,4)$-free non-bipartite graph and characterize the unique extremal graph.

1. Introduction

We start by introducing the background information which will derive our main results. Our main results and some preliminaries will also be given in this section.

1.1. Background

In this paper, we consider only simple, undirected and finite graphs. Let $G = (V(G), E(G))$ be a graph, where $V(G)$ is its vertex set and $E(G)$ is its edge set. The *order* of G is the number $|G|$ (or $|V(G)|$) of its vertices and its *size* is the number $|E(G)|$ of its edges. Denote by P_n, C_n, K_n and $K_{t,n-t}$ the path, the cycle, the complete graph and the complete bipartite graph on n vertices, respectively. The *theta graph* $\theta(i,j,k)$ is formed by connecting two distinct vertices with three independent paths of lengths i, j and k, respectively (length refers to the number of edges). Unless otherwise stated, we follow the traditional notation and terminology; see [3].

Let F be a given graph. We say a graph G is F-*free* if it does not contain F as a subgraph. That is to say, F is *forbidden* in the graph G. The *Turán number*

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of F, written by $\mathrm{ex}(n, F)$, is the maximum size of an n-vertex F-free graph. Mantel and Turán determined this function exactly when $F \cong K_{r+1}$. The research for the Turán numbers attracts much attention, and it has become to be one of the most attractive fundamental problems in extremal graph theory (see [15, 31] for surveys).

The Erdős-Stone-Simonovits theorem [11, 12] gives us the asymptotic behaviour of $\mathrm{ex}(n, F)$ whenever $\chi(F) \geqslant 3$, here $\chi(F)$ is the chromatic number of F. Since then one is interested in considering the Turán problem when F is bipartite. Let $\Theta_{\ell,t}$ be the graph obtained by connecting two distinct vertices by t independent paths of length ℓ. Faudree and Simonovits [13] and Bukh and Tait [7] displayed the asymptotic behaviour of $\mathrm{ex}(n, \Theta_{\ell,t})$. Further on Verstraëte and Williford [34] gave a lower bound of order $n^{5/4}$ on the greatest number of edges of any n-vertex $\Theta_{4,3}$-free graph. Even so it is challenging and interesting to determine the exact values of $\mathrm{ex}(n, F)$.

Let $A(G)$ be the adjacency matrix of a graph G. The largest modulus of all eigenvalues of $A(G)$ is called the *spectral radius* of G and denoted by $\lambda(G)$. In 2010, Nikiforov [30] proposed a spectral analogue of Turán type problem: what is the maximal spectral radius of an F-free graph on n vertices? This is also called the Brualdi-Solheid-Turán type problem. This problem attracts more and more researchers' attention. For example, one may see $F \cong K_r$ [6, 26, 27, 35], $F \cong K_{s,t}$ [2, 27, 29, 41], $F \cong P_k, \bigcup_{i=1}^{k} P_{a_i}$ or $\bigcup_{i=1}^{k} K_{1,d_i}$ [8, 9, 30], and $F \cong C_4, C_6$ or C_{2k+1} [27, 30, 39, 42]. For more information, we refer the reader to [1, 10, 20, 22–24, 31, 33]. Motivated by these works, the other purpose of ours is to study the spectral Turán type problem.

We pay attention to one mathematical phenomenon: In some Turán type problems the corresponding extremal graphs are certain bipartite graphs; see Mantel Theorem [25], Zhai, Fang, and Shu [38], and Füredi and Gunderoson [14], whereas in some spectral Turán type problems the corresponding extremal graphs are also bipartite graphs; see Nikiforov [28], Nosal [32], and Zhai and Lin [40]. Based on these observations, we consider both the Turán type problem and the spectral Turán type problem among non-bipartite graphs in this paper. Notice that there are only specific families of non-bipartite graphs whose extremal graphs are known; see [4, 5, 16–18, 21, 23].

In this paper, we determine the exact value of Turán number of $\theta(1, 2, 4)$ whose host graph is non-bipartite. We also consider the Brualdi-Solheid-Turán type problem on $\theta(1, 2, 3)$-free/$\theta(1, 2, 4)$-free non-bipartite graphs with fixed order.

1.2. Main results

Our first two main results determine the unique graph having the maximum spectral radius among $\theta(1, 2, 3)$-free and $\theta(1, 2, 4)$-free non-bipartite graphs, respectively. Let $SK_{a,b}$ denote the graph obtained from $K_{a,b}$ by subdividing an edge, and let $K_{a,b} \bullet K_3$ be the graph obtained by identifying an edge of $K_{a,b}$ with an edge of K_3; see Figure 1.

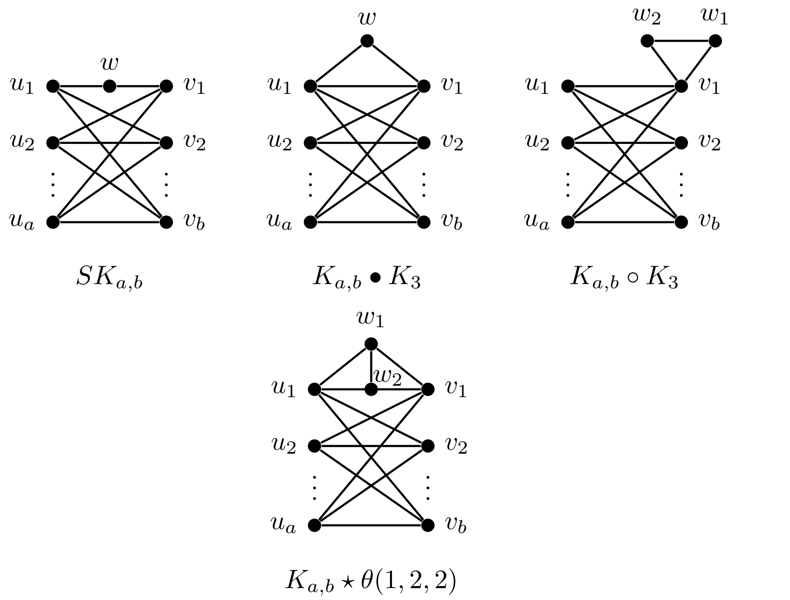

FIGURE 1. The graphs $SK_{a,b}$, $K_{a,b} \bullet K_3$, $K_{a,b} \circ K_3$ and $K_{a,b} \star \theta(1,2,2)$.

Theorem 1.1. *Let G be a non-bipartite graph with order $n \geqslant 20$. If G is $\theta(1,2,3)$-free, then*

$$\lambda(G) \leqslant \lambda(SK_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor}).$$

Equality holds if and only if $G \cong SK_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor}$.

Theorem 1.2. *Let G be a non-bipartite graph with order $n \geqslant 21$. If G is $\theta(1,2,4)$-free, then*

$$\lambda(G) \leqslant \lambda(K_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor} \bullet K_3).$$

Equality holds if and only if $G \cong K_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor} \bullet K_3$.

For convenience, let

$$\mathrm{ex}_{nb}(n, H) = \max\{|E(G)| : G \text{ is an } H\text{-free non-bipartite graph with order } n\}.$$

Bataineh, Jaradat and Al-Shboul [5] obtained $\mathrm{ex}_{nb}(n, \theta(1,2,3)) = \lfloor \frac{(n-1)^2}{4} \rfloor + 1$ for $n \geqslant 9$ (see Lemma 1.10 below). Motivated by this result, our next result determines the exact value of $\mathrm{ex}_{nb}(n, \theta(1,2,4))$ for $n \geqslant 137$.

Theorem 1.3. *Let $n \geqslant 137$ be an integer. Then*

$$\mathrm{ex}_{nb}(n, \theta(1,2,4)) = \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 2.$$

The only extremal graph is $K_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor} \bullet K_3$.

The remainder of this paper is organized as follows. In the rest of this section, we give some preliminary results, which will be used in the subsequent sections. In Section 2, we give the proof of Theorem 1.1. In Section 3, we present the proofs of Theorems 1.2 and 1.3. Some concluding remarks are given in the last section.

1.3. Preliminaries

In this subsection, we describe some known results, which play an important role in the subsequent sections.

Lemma 1.4 ([3]). *Let G be a connected graph and let H be a proper subgraph of G. Then $\lambda(H) < \lambda(G)$.*

Let G be a connected graph on n vertices. Then $A(G)$ is irreducible and nonnegative. From the Perron-Frobenius Theorem, we know that $\lambda(G)$ is the largest eigenvalue of $A(G)$ and there exists a unique positive unit eigenvector $\mathbf{x} := (x_1, \ldots, x_n)^T$ of $A(G)$ corresponding to $\lambda(G)$. We call $\mathbf{x}$ the *Perron vector* of G. It will be convenient to associate a labeling of vertices of G (with respect to $\mathbf{x}$) in which x_v is a label of the vertex v.

The set of neighbors of a vertex u is denoted by $N_G(u)$. Let $N_G[u] = N_G(u) \cup \{u\}$. The *degree* $d_G(u)$ of a vertex u (in G) is the cardinality of $N_G(u)$. If $U \subset V(G)$, then we write $G[U]$ to denote the induced subgraph of G with vertex set U. An induced subgraph of G obtained by deleting a set of vertices $V' \subset V(G)$ is denoted by $G - V'$. Similarly, $G - E'$ designates the deletion of a subset of edges E'. By $G + e$ we denote a graph obtained from G by inserting a single edge.

Lemma 1.5 ([36]). *Let G be a connected graph and let $\mathbf{x}$ be the Perron vector of G. Assume that u and v are two distinct vertices of G with $x_u \geqslant x_v$ and $\{v_i : 1 \leqslant i \leqslant s\} \subseteq N_G(v) \setminus N_G[u]$. If $G' = G - \{vv_i : 1 \leqslant i \leqslant s\} + \{uv_i : 1 \leqslant i \leqslant s\}$, then $\lambda(G') > \lambda(G)$.*

Let H be a real square matrix, whose columns and rows are indexed by $U = \{1, 2, \ldots, n\}$. Assume that $\pi := U_1 \cup U_2 \cup \cdots \cup U_t$ is a partition of U. Then H can be partitioned based on π as follows.

$$H = \begin{pmatrix} H_{11} & \cdots & H_{1t} \\ \vdots & \ddots & \vdots \\ H_{t1} & \cdots & H_{tt} \end{pmatrix},$$

where H_{ij} denotes the submatrix of H, indexed by the rows and columns of U_i and U_j, respectively. Let π_{ij} be the average row sum of H_{ij} for $1 \leqslant i, j \leqslant t$.

Usually, the matrix $H^\pi = (\pi_{ij})$ is called the *quotient matrix* of H. Moreover, if the row sum of H_{ij} is constant for $1 \leqslant i, j \leqslant t$, then we call π an *equitable partition.*

Lemma 1.6 ([37])**.** *Let H be a real square matrix with an equitable partition π, and let H^π be the corresponding quotient matrix. Then every eigenvalue of H^π is an eigenvalue of H. In addition, if $H = A(G)$ for some graph G, then the spectral radius of G is equal to the largest eigenvalue of H^π.*

Denote by $K_{a,b} \circ K_3$ the graph obtained by identifying a vertex of $K_{a,b}$ belonging to the part of size b and a vertex of K_3; see Figure 1.

Lemma 1.7 ([40])**.** *Let $a + b = n - 2$ and $a \geqslant b \geqslant 2$. If $n \geqslant 10$, then $\lambda(K_{a,b} \circ K_3) \leqslant \lambda(K_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor} \circ K_3)$ with equality if and only if $K_{a,b} \circ K_3 \cong K_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor} \circ K_3$.*

Lemma 1.8 ([23])**.** *Let G be a C_3-free non-bipartite graph with order n. Then $\lambda(G) \leqslant \lambda(SK_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor})$ with equality if and only if $G \cong SK_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor}$.*

Lemma 1.9 ([40])**.** *Let G be a $\theta(1, 2, r + 1)$-free graph with order n. Then $\lambda(G) \leqslant \sqrt{\lfloor \frac{n^2}{4} \rfloor}$ for $n \geqslant 10r$ if r is odd and $n \geqslant 7r$ if r is even. Equality holds if and only if $G \cong K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$.*

Lemma 1.10 ([5])**.** *Let $n \geqslant 9$ be an integer. Then* $\mathrm{ex}_{nb}(n, \theta(1, 2, 3)) = \lfloor \frac{(n-1)^2}{4} \rfloor + 1$.

2. Proof of Theorem 1.1

In this section, we give the proof of Theorem 1.1, which characterizes the unique graph having the maximum spectral radius among $\theta(1, 2, 3)$-free non-bipartite graphs of given order. Before giving the proof, we need the following key lemma.

Let $K_{a,b} \star \theta(1, 2, 2)$ be the last graph depicted in Figure 1. Clearly, $K_{a,b} \star \theta(1, 2, 2)$ can be obtained from $K_{a,b}$ by replacing one edge with $\theta(1, 2, 2)$. In the following lemma, we adopt the labels for vertices in Figure 1.

Lemma 2.1. *For $n \geqslant 20$, we have*

$$\lambda(K_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor} \star \theta(1, 2, 2)) < \lambda(K_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor} \circ K_3) < \lambda(SK_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor}).$$

Proof. Firstly, we prove $\lambda(K_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor} \star \theta(1, 2, 2)) < \lambda(K_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor} \circ K_3)$. Clearly, $\pi_1 := \{w_1, w_2\} \cup \{u_1\} \cup \{v_1\} \cup \{v_2, \ldots, v_{\lfloor \frac{n-2}{2} \rfloor}\} \cup \{u_2, \ldots, u_{\lceil \frac{n-2}{2} \rceil}\}$ is an equitable partition of $A(K_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor} \star \theta(1, 2, 2))$. Hence the quotient matrix corresponding to π_1 can be written as follows.

$$A(K_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor} \star \theta(1, 2, 2))^{\pi_1} = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 0 & 0 & \lfloor \frac{n}{2} \rfloor - 2 & 0 \\ 2 & 0 & 0 & 0 & \lceil \frac{n}{2} \rceil - 2 \\ 0 & 1 & 0 & 0 & \lceil \frac{n}{2} \rceil - 2 \\ 0 & 0 & 1 & \lfloor \frac{n}{2} \rfloor - 2 & 0 \end{pmatrix}.$$

Therefore, the characteristic polynomial of $A(K_{\lceil\frac{n-2}{2}\rceil,\lfloor\frac{n-2}{2}\rfloor}\star\theta(1,2,2))^{\pi_1}$ is

$$f(x)=\begin{cases} x^5-x^4-(\frac{n^2}{4}-n+4)x^3+(\frac{n^2}{4}-n)x^2+(\frac{5n^2}{4}-8n+12)x-\frac{5n^2}{4}+10n-20, & \text{if } n \text{ is even;}\\ x^5-x^4-(\frac{n^2+15}{4}-n)x^3+(\frac{n^2-1}{4}-n)x^2+(\frac{5n^2+43}{4}-8n)x-\frac{5n^2+75}{4}+10n, & \text{if } n \text{ is odd.}\end{cases}$$

Similarly, one may see that $\pi_2:=\{w_1,w_2\}\cup\{v_1\}\cup\{u_1\}\cup\{u_2,\ldots,u_{\lceil\frac{n-2}{2}\rceil}\}\cup\{v_2,\ldots,v_{\lfloor\frac{n-2}{2}\rfloor}\}$ is an equitable partition of $A(K_{\lceil\frac{n-2}{2}\rceil,\lfloor\frac{n-2}{2}\rfloor}\circ K_3)$. Then the corresponding quotient matrix can be given as

$$A(K_{\lceil\frac{n-2}{2}\rceil,\lfloor\frac{n-2}{2}\rfloor}\circ K_3)^{\pi_2}=\begin{pmatrix} 1 & 1 & 0 & 0 & 0\\ 2 & 0 & 1 & \lceil\frac{n}{2}\rceil-2 & 0\\ 0 & 1 & 0 & 0 & \lfloor\frac{n}{2}\rfloor-2\\ 0 & 1 & 0 & 0 & \lfloor\frac{n}{2}\rfloor-2\\ 0 & 0 & 1 & \lceil\frac{n}{2}\rceil-2 & 0\end{pmatrix}.$$

Consequently, the characteristic polynomial of $A(K_{\lceil\frac{n-2}{2}\rceil,\lfloor\frac{n-2}{2}\rfloor}\circ K_3)^{\pi_2}$ is

$$g(x)=\begin{cases} x^5-x^4-(\frac{n^2}{4}-n+3)x^3+(\frac{n^2}{4}-n+1)x^2+(\frac{n^2}{2}-3n+4)x, & \text{if } n \text{ is even;}\\ x^5-x^4-(\frac{n^2+11}{4}-n)x^3+\frac{3}{4}x^2+(\frac{n^2+5}{2}-3n)x, & \text{if } n \text{ is odd.}\end{cases}$$

In view of Lemma 1.6, one obtains that $\lambda(K_{\lceil\frac{n-2}{2}\rceil,\lfloor\frac{n-2}{2}\rfloor}\star\theta(1,2,2))$ and $\lambda(K_{\lceil\frac{n-2}{2}\rceil,\lfloor\frac{n-2}{2}\rfloor}\circ K_3)$ equal the largest roots of $f(x)=0$ and $g(x)=0$, respectively. Together with Lemmas 1.4 and 1.9, we know that the largest root $f(x)=0$ (resp. $g(x)=0$) lie in the interval $\left(\sqrt{\lfloor\frac{(n-3)^2}{4}\rfloor},\sqrt{\lfloor\frac{n^2}{4}\rfloor}\right)$ (resp. $\left(\sqrt{\lfloor\frac{(n-2)^2}{4}\rfloor},\sqrt{\lfloor\frac{n^2}{4}\rfloor}\right)$).

By some calculations, we find that

$$f(x)-g(x)=\begin{cases} -x^3-x^2+(\frac{3n^2}{4}-5n+8)x-\frac{5n^2}{4}+10n-20, & \text{if } n \text{ is even;}\\ -x^3-x^2+(\frac{3n^2+33}{4}-5n)x-\frac{5n^2+75}{4}+10n, & \text{if } n \text{ is odd.}\end{cases}$$

By using Mathematica 9.0, we get

$$\min\left\{f(x)-g(x):\sqrt{\lfloor\frac{(n-3)^2}{4}\rfloor}<x<\sqrt{\lfloor\frac{n^2}{4}\rfloor},\, n\geqslant 20\right\}>0.$$

It follows that the largest root of $f(x)=0$ is less than that of $g(x)=0$. That is, $\lambda(K_{\lceil\frac{n-2}{2}\rceil,\lfloor\frac{n-2}{2}\rfloor}\star\theta(1,2,2))<\lambda(K_{\lceil\frac{n-2}{2}\rceil,\lfloor\frac{n-2}{2}\rfloor}\circ K_3)$, as desired.

Next, we show $\lambda(K_{\lceil\frac{n-2}{2}\rceil,\lfloor\frac{n-2}{2}\rfloor}\circ K_3)<\lambda(SK_{\lceil\frac{n-1}{2}\rceil,\lfloor\frac{n-1}{2}\rfloor})$. Clearly, $\pi_3:=\{u_1\}\cup\{w\}\cup\{v_1\}\cup\{u_2,\ldots,u_{\lceil\frac{n-1}{2}\rceil}\}\cup\{v_2,\ldots,v_{\lfloor\frac{n-1}{2}\rfloor}\}$ is an equitable partition of $A(SK_{\lceil\frac{n-1}{2}\rceil,\lfloor\frac{n-1}{2}\rfloor})$. Hence the corresponding quotient matrix is

$$A(SK_{\lceil\frac{n-1}{2}\rceil,\lfloor\frac{n-1}{2}\rfloor})^{\pi_3}=\begin{pmatrix} 0 & 1 & 0 & 0 & \lfloor\frac{n-1}{2}\rfloor-1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & \lceil\frac{n-1}{2}\rceil-1 & 0 \\ 0 & 0 & 1 & 0 & \lfloor\frac{n-1}{2}\rfloor-1 \\ 1 & 0 & 0 & \lceil\frac{n-1}{2}\rceil-1 & 0 \end{pmatrix}.$$

Therefore, we obtain the characteristic polynomial of $A(SK_{\lceil\frac{n-1}{2}\rceil,\lfloor\frac{n-1}{2}\rfloor})^{\pi_3}$ as

$$h(x)=\begin{cases} x^5-\frac{n^2-2n+4}{4}x^3+\frac{3n^2-14n+12}{4}x-\frac{n^2-6n+8}{2}, & \text{if } n \text{ is even;} \\ x^5-\frac{n^2-2n+5}{4}x^3+\frac{3n^2-14n+15}{4}x-\frac{n^2-6n+9}{2}, & \text{if } n \text{ is odd.} \end{cases}$$

Combining with Lemma 1.6, one has that $\lambda(SK_{\lceil\frac{n-1}{2}\rceil,\lfloor\frac{n-1}{2}\rfloor})$ is equal to the largest root of $h(x)=0$.

By some calculations, we see that

$$g(x)-h(x)=\begin{cases} -x^4+\frac{n-4}{2}x^3+\frac{n^2-4n+4}{4}x^2-\frac{n^2-2n-4}{4}x+\frac{n^2-6n+8}{2}, & \text{if } n \text{ is even;} \\ -x^4+\frac{n-3}{2}x^3+\frac{n^2-4n+3}{4}x^2-\frac{n^2-2n+5}{4}x+\frac{n^2-6n+9}{2}, & \text{if } n \text{ is odd.} \end{cases}$$

Applying Mathematica 9.0 again yields

$$\min\left\{g(x)-h(x):\sqrt{\lfloor\frac{(n-2)^2}{4}\rfloor}<x<\sqrt{\lfloor\frac{n^2}{4}\rfloor},\ n\geqslant 20\right\}>0.$$

It follows that the largest root of $g(x)=0$ is less than that of $h(x)=0$, which implies $\lambda(K_{\lceil\frac{n-2}{2}\rceil,\lfloor\frac{n-2}{2}\rfloor}\circ K_3)<\lambda(SK_{\lceil\frac{n-1}{2}\rceil,\lfloor\frac{n-1}{2}\rfloor})$, as desired. $\square$

For a given graph G, let S and T be subgraphs and/or vertex subsets of G. Define $E_G(S,T)$ to be the set of edges with one endpoint in S and the other in T. Then denote $e(S,T):=|E_G(S,T)|$. In particular, $E_G(S,S)$ and $e(S,S)$ are simplified by $E_G(S)$ and $e(S)$, respectively. Furthermore, if $T=\{v\}$, then denote $d_S(v):=e(S,\{v\})$.

For $k\geqslant 2$, we use $N_G^k(u)$ to denote the set of vertices at distance k from u. Let W be a subgraph or a vertex subset of G. Then denote by $N_G(W)$ the set of neighbors of vertices in W. In the whole context, when there is no scope for ambiguity, we always suppress the graph name from our notation.

Now, we are ready to give the proof of Theorem 1.1.

Proof of Theorem 1.1. Let G^* be a $\theta(1,2,3)$-free non-bipartite graph of order n having the maximum spectral radius. For convenience, denote $\lambda^*=\lambda(G^*)$. It is routine to check that $SK_{\lceil\frac{n-1}{2}\rceil,\lfloor\frac{n-1}{2}\rfloor}$ is a $\theta(1,2,3)$-free non-bipartite graph with order n. Together with the choice of G^* and Lemma 2.1, we get that

$$\begin{aligned}\lambda^* &\geqslant \lambda(SK_{\lceil\frac{n-1}{2}\rceil,\lfloor\frac{n-1}{2}\rfloor})>\lambda(K_{\lceil\frac{n-2}{2}\rceil,\lfloor\frac{n-2}{2}\rfloor}\circ K_3)\\ &>\lambda(K_{\lceil\frac{n-2}{2}\rceil,\lfloor\frac{n-2}{2}\rfloor})=\sqrt{\left\lfloor\frac{(n-2)^2}{4}\right\rfloor}. \qquad (2.1)\end{aligned}$$

If G^* is C_3-free, then by Lemma 1.8 one has $\lambda^* \leqslant \lambda(SK_{\lceil\frac{n-1}{2}\rceil,\lfloor\frac{n-1}{2}\rfloor})$ with equality if and only if $G \cong SK_{\lceil\frac{n-1}{2}\rceil,\lfloor\frac{n-1}{2}\rfloor}$, as desired.

So, in what follows, we just consider the case that C_3 is a subgraph of G^*. In view of Lemma 1.4 and the choice of G^*, we know that G^* is connected. Let $\mathbf{x}$ be the Perron vector of G^* and u^* be a vertex of G^* such that $x_{u^*} = \max\{x_v : v \in V(G^*)\}$. Recall that G^* is $\theta(1,2,3)$-free. Then $G^*[N(u^*)]$ is P_4-free. It follows that each component of $G^*[N(u^*)]$ is in $\bigcup_{i=0}^{3} T_i$, where

(i) T_0 consists of all trivial components;
(ii) T_1 is the disjoint union of P_2;
(iii) T_2 is the disjoint union of stars with order at least three;
(iv) T_3 is the disjoint union of K_3.

Denote $U_0 = N(T_0)\cap N^2(u^*)$ and $U(T) = N(T)\cap N^2(u^*)$ for each nontrivial subgraph T of $G^*[N(u^*)]$. Applying the fact that G^* is $\theta(1,2,3)$-free again, we obtain the following claim.

Claim 2.2. *The following items hold*:

(i) $U(T_i)\cap U(T_j) = \emptyset$ *for* $0 \leqslant i < j \leqslant 3$;
(ii) $U(T_1^1)\cap U(T_1^2) = \emptyset$ *for any two components* T_1^1 *and* T_1^2 *in* T_1;
(iii) $e(v, N(u^*)) = 1$ *for any vertex* $v \in U(T_2)\cup U(T_3)$;
(iv) *either* $|N(v_1)\cap N(v_2)\cap N(u^*)| = 0$, *or* $|(N(v_1)\cup N(v_2))\cap N(u^*)| = 1$ *holds for each edge* $v_1v_2 \in E(N^2(u^*))$.

Based on (2.1), one has

$$\begin{aligned}\left\lfloor\frac{(n-2)^2}{4}\right\rfloor x_{u^*} < {\lambda^*}^2 x_{u^*} &= \sum_{v\in V(G)} a^{(2)}_{vu^*} x_v\\ &= d(u^*)x_{u^*} + \sum_{v\in N(u^*)\setminus V(T_0)} d_{N(u^*)}(v)x_v + \sum_{w\in N^2(u^*)} d_{N(u^*)}(w)x_w\\ &\leqslant \big(|N(u^*)| + 2e(N(u^*)) + e(N(u^*), N^2(u^*))\big)\, x_{u^*},\end{aligned} \tag{2.2}$$

where $a^{(2)}_{vu^*}$ denotes the number of walks of length 2 from v to the vertex u^*. Let $\gamma(u^*) = |N(u^*)| + 2e(N(u^*)) + e(N(u^*), N^2(u^*))$. Then (2.2) gives

$$\gamma(u^*) > \left\lfloor\frac{(n-2)^2}{4}\right\rfloor, \text{ i.e., } \gamma(u^*) \geqslant \left\lfloor\frac{(n-2)^2}{4}\right\rfloor + 1. \tag{2.3}$$

Denote the number of components of T_2 by c. Notice that $|T_1| = 2e(T_1)$, $|T_2| = e(T_2) + c$, and $|T_3| = e(T_3)$. Hence

$$e(N(u^*)) = \frac{|T_1|}{2} + |T_2| - c + |T_3|. \tag{2.4}$$

Based on Claim 2.2, one has

$$e(N(u^*), N^2(u^*)) = \sum_{i=0}^{3} |E(T_i, U(T_i))|$$

$$\leqslant |T_0||U_0| + 2|U(T_1)| + |U(T_2)| + |U(T_3)|. \tag{2.5}$$

Furthermore,

$$\sum_{i=0}^{3}(|T_i| + |U(T_i)|) \leqslant n-1 \text{ and so } |T_2| + |T_3| \leqslant n-1-|T_0|-|U_0|. \tag{2.6}$$

Together with (2.4)-(2.6), we obtain that

$$\begin{aligned}
\gamma(u^*) &= |N(u^*)| + 2e(N(u^*)) + e(N(u^*), N^2(u^*)) \\
&\leqslant |N(u^*)| + |T_1| + 2|T_2| - 2c + 2|T_3| + |T_0||U_0| \\
&\quad + 2|U(T_1)| + |U(T_2)| + |U(T_3)| \\
&\leqslant 2(n-1) + |T_2| + |T_3| - 2c + (|T_0|-2)|U_0| - |T_0| - |U(T_2)| - |U(T_3)| \\
&\leqslant 3(n-1) - 2c + (|T_0|-3)|U_0| - 2|T_0| - |U(T_2)| - |U(T_3)| \\
&\leqslant 3(n-1) + (|T_0|-3)|U_0| - 2|T_0| \\
&\leqslant 3(n-1) + (|T_0|-3)(|U_0|-2) - 6 \\
&\leqslant \frac{(|T_0|+|U_0|-5)^2}{4} + 3(n-3).
\end{aligned}$$

Together with (2.3) we obtain

$$\begin{aligned}
\frac{(|T_0|+|U_0|-5)^2}{4} &\geqslant \lfloor \frac{(n-2)^2}{4} \rfloor - 3(n-3) + 1 \\
&\geqslant \frac{(n-2)^2-1}{4} - 3n + 10 \\
&= \frac{(n-8)^2-21}{4} \\
&> \frac{(n-9)^2}{4},
\end{aligned}$$

and the last inequality follows by $n \geqslant 20$. Thus, $n-3 \leqslant |T_0| + |U_0| \leqslant n-1$.

In what follows, we proceed by considering the following three cases with respect to the value of $|T_0| + |U_0|$.

Case 1. $|T_0| + |U_0| = n-1$. In this case, $V(T_0) = N(u^*)$. Since G^* is non-bipartite, one has $e(U_0) \geqslant 1$. Recall that $x_{u^*} = \max\{x_v : v \in V(G^*)\}$. Hence $|T_0| \geqslant 2$. We distinguish the proof into the following two subcases.

Subcase 1.1. $e(U_0) = 1$. Note that G^* contains C_3 as a subgraph. Then the two vertices of the unique edge in $E(U_0)$ have a common neighbor in T_0. Together with Lemma 1.4 and Claim 2.2(iv), we get $G^* \cong K_{a,b} \circ K_3$ for some positive integers a and b. Notice that $a, b \geqslant 2$. Otherwise, we can add an edge between two pendant vertices of G^* to get a $\theta(1,2,3)$-free non-bipartite graph with larger spectral radius, a contradiction. It follows from Lemma 1.7 that $G^* \cong K_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor} \circ K_3$. In view of Lemma 2.1, one has $\lambda^* < \lambda(SK_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor})$, which contradicts the choice of G^*.

Subcase 1.2. $e(U_0) \geqslant 2$. Firstly, we consider the case that $G^*[N^2(u^*)]$ contains a triangle $C_3 = w_1w_2w_3w_1$. Then based on Claim 2.2(iv), one has

$$\gamma(u^*) \leqslant |T_0|+|T_0|+1+|T_0|(|U_0|-3) = |T_0|(|U_0|-1)+1 \leqslant \left\lfloor \frac{(n-2)^2}{4} \right\rfloor+1. \tag{2.7}$$

Together with (2.3), one has $\gamma(u^*) = \lfloor \frac{(n-2)^2}{4} \rfloor + 1$, that is to say, all equalities in (2.7) hold. Then we have

(i) there exist two vertices w_i and w_j in C_3 which are adjacent to exactly one common vertex, say w, in T_0;

(ii) $w_l\,(l \neq i, j)$ is adjacent to all vertices in $V(T_0) \setminus \{w\}$;

(iii) each vertex in $U_0 \setminus \{w_1, w_2, w_3\}$ is adjacent to all vertices in T_0;

(iv) one of $|T_0|$ and $|U_0| - 1$ equals $\lfloor \frac{n-2}{2} \rfloor$, the other is $\lceil \frac{n-2}{2} \rceil$.

Thus, $G^* \cong K_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor} \star \theta(1, 2, 2)$. By Lemma 2.1 and the choice of G^*, we get a contradiction.

Next, we assume $G^*[N^2(u^*)]$ is triangle-free. Notice that G^* contains C_3 as a subgraph. Hence there exists an edge, say uv, in $E(U_0)$ such that u and v have a common neighbor in T_0. Suppose that there is an edge in $E(U_0)$ which is incident to neither u nor v. Together with Claim 2.2(iv), we obtain

$$\gamma(u^*) \leqslant |T_0| + 2 + |T_0| + |T_0|(|U_0| - 4) = |T_0|(|U_0| - 2) + 2 \leqslant \left\lfloor \frac{(n-3)^2}{4} \right\rfloor + 2,$$

which contradicts (2.3). Hence each edge in $E(U_0)$ is incident to u or v. Let wu be an arbitrary edge of $E(U_0)$, where $w \neq v$. Then w has at most $|T_0| - 1$ neighbors in T_0. It follows that

$$\begin{aligned} \gamma(u^*) &\leqslant |T_0| + 2 + |T_0|(|U_0| - 2) - (e(U_0) - 1) \qquad (2.8)\\ &= |T_0|(|U_0| - 1) - e(U_0) + 3 \\ &\leqslant \left\lfloor \frac{(n-2)^2}{4} \right\rfloor + 1. \qquad (2.9) \end{aligned}$$

Together with (2.3), one has $\gamma(u^*) = \lfloor \frac{(n-2)^2}{4} \rfloor + 1$. Thus, equalities in (2.8) and (2.9) hold. By a similar discussion as that of (2.7), we get that G^* is a graph obtained from $K_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor} \star \theta(1, 2, 2)$ by deleting an edge. Together with Lemmas 1.4 and 2.1, we get $\lambda^* < \lambda(K_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor} \star \theta(1, 2, 2)) < \lambda(SK_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor})$, a contradiction.

Case 2. $|T_0| + |U_0| = n - 2$. In this case, $V(T_0) = N(u^*)$ and $|N^3(u^*)| = 1$. Since G^* is non-bipartite, one has $e(U_0) \geqslant 1$. Let uv be an edge of $G^*[U_0]$. In view of Claim 2.2(iv), one has $e(\{u, v\}, T_0) \leqslant |T_0|$. Hence

$$\gamma(u^*) \leqslant |T_0| + |T_0| + |T_0|(|U_0| - 2) = |T_0||U_0| \leqslant \left\lfloor \frac{(n-2)^2}{4} \right\rfloor,$$

which contradicts (2.3).

Case 3. $|T_0|+|U_0| = n-3$. In this case, either $|T_1| = 2$ or $|V(G^*)\setminus(N[u^*]\cup N^2(u^*))| = 2$ holds. We claim that $e(U_0) = 0$. In fact, if $e(U_0) \geqslant 1$, then together with Claim 2.2(iv) one has

$$\gamma(u^*) \leqslant |T_0| + 4 + |T_0| + |T_0|(|U_0| - 2) = |T_0||U_0| + 4 \leqslant \left\lfloor \frac{(n-3)^2}{4} \right\rfloor + 4,$$

which contradicts (2.3).

If $|T_1| = 2$, then by Lemmas 1.4, 1.7 and the choice of G^*, we obtain $G^* \cong K_{\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor} \circ K_3$. By Lemma 2.1, we get a contradiction.

If $|V(G^*) \setminus (N[u^*] \cup N^2(u^*))| = 2$, then

$$\gamma(u^*) \leqslant |T_0| + |T_0||U_0| \leqslant \left\lfloor \frac{(n-2)^2}{4} \right\rfloor,$$

which also contradicts (2.3).

Together with Cases 1-3, we obtain $G^* \cong SK_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor}$. This completes the proof. □

3. Proofs of Theorems 1.2 and 1.3

In this section, we give the proofs of Theorems 1.2 and 1.3, which characterize the graph having the largest spectral radius and size among $\theta(1,2,4)$-free non-bipartite graphs with order n, respectively.

A *cut-vertex* of a graph is a vertex whose deletion increases the number of components. A maximal connected subgraph without a cut-vertex is called a *block*. The *double star* $D_{i,j}$ consists of two stars $K_{1,i+1}$ and $K_{1,j+1}$ joined together so that they share an edge.

Firstly, we present the proof of Theorem 1.2.

Proof of Theorem 1.2. Let G^* be a $\theta(1,2,4)$-free non-bipartite graph of order n with the maximum spectral radius. For convenience, denote $\lambda^* = \lambda(G^*)$. Notice that $K_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor} \bullet K_3$ is a non-bipartite $\theta(1,2,4)$-free graph. Hence together with Lemma 1.4 one has

$$\lambda^* \geqslant \lambda(K_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor} \bullet K_3) > \lambda(K_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor}) = \sqrt{\left\lfloor \frac{(n-1)^2}{4} \right\rfloor} \geqslant 10. \tag{3.1}$$

If G^* is C_3-free, then by Lemma 1.8 one has $\lambda^* \leqslant \lambda(SK_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor})$. Notice that $SK_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor}$ is a proper subgraph of $K_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor} \bullet K_3$. Then Lemma 1.4 implies $\lambda^* < \lambda(K_{\lceil \frac{n-1}{2} \rceil, \lfloor \frac{n-1}{2} \rfloor} \bullet K_3)$, a contradiction.

So, in what follows, we consider the case that C_3 is a subgraph of G^*. In view of Lemma 1.4 and the choice of G^*, we know that G^* is connected. Let $\mathbf{x}$ be the Perron vector of G^* and $x_{u^*} = \max\{x_v : v \in V(G^*)\}$. The next claim characterizes the local structures of G^*.

Claim 3.1. *Any vertex in $V(G^*)\setminus\{u^*\}$ cannot be a cut vertex; hence $d(u) \geqslant 2$ for any $u \in V(G^*) \setminus N[u^*]$.*

Proof of Claim 3.1. Suppose to the contrary that there exists a cut vertex, say w, in $V(G^*) \setminus \{u^*\}$. Let B be a block of G^* with $w \in V(B)$ and $u^* \notin V(B)$. Then we consider a new graph $G_1 = G^* - \{wu : u \in V(B)\} + \{u^*u : u \in V(B)\}$. It is easy to see that G_1 is a $\theta(1,2,4)$-free non-bipartite graph with order n. On the other hand, by Lemma 1.5, one has $\lambda(G_1) > \lambda^*$, which contradicts the choice of G^*. □

Recall that G^* is $\theta(1,2,4)$-free. Then $G^*[N(u^*)]$ is P_5-free. Hence each component of $G^*[N(u^*)]$ is in $\bigcup_{i=0}^{5} H_i$, where

(i) H_0 consists of all trivial components;
(ii) H_1 is the disjoint union of stars $K_{1,r}$ for $r \geqslant 1$;
(iii) H_2 is the disjoint union of double stars $D_{a,b}$ for $a, b \geqslant 1$;
(iv) H_3 is the disjoint union of K_3;
(v) H_4 is the disjoint union of C_4, $C_4 + e$ and K_4;
(vi) H_5 is the disjoint union of $K_{1,r} + e$ for $r \geqslant 3$.

Define $U_0 = N^2(u^*) \cap N(H_0)$ and $U(H) = N^2(u^*) \cap N(H)$ for each subgraph H of $G^*[N(u^*)]$. Applying the fact that G^* is $\theta(1,2,4)$-free yields $U(H) \cap U(H') = \emptyset$ for any two distinct components H and H' of $G^*[N(u^*)]$ unless H is an isolated vertex and H' is a star $K_{1,r}$, where $K_{1,0}$ denotes an isolated vertex (in particular, the vertex in H' which has a common neighbor with the vertex in H must be its central vertex). For any nontrivial component H of $G^*[N(u^*)]$, we define

$$\eta(H) = \sum_{v \in V(H)} (d_H(v) - 1)x_v + \sum_{u \in U(H) \setminus U_0} d_H(u)x_u \text{ and } \zeta(H) = |H| + 2|U(H) \setminus U_0|.$$

Now, we are to establish the relationship between $\eta(H)$ and $\zeta(H)$ for each nontrivial component H of $G^*[N(u^*)]$.

Claim 3.2. *Let H be a nontrivial component of $G^*[N(u^*)]$. Then the following items hold.*

(i) *If H is a component of H_1, then $\eta(H) < \zeta(H)x_{u^*}$;*
(ii) *If H is a component of H_2, then $\eta(H) < \zeta(H)x_{u^*}$;*
(iii) *If H is a component of H_3, then $\eta(H) \leqslant (\zeta(H) + 1)x_{u^*}$;*
(iv) *If H is a component of H_4, then $\eta(H) \leqslant (\zeta(H) + 2)x_{u^*}$;*
(v) *If H is a component of H_5, then $\eta(H) \leqslant \zeta(H)x_{u^*}$.*

Proof of Claim 3.2. (i) Assume that $H \cong K_{1,r}$ for some $r \geqslant 1$. Then $e(H) = |H| - 1$. If $e(U(H) \setminus U_0, V(H)) \leqslant 2|U(H) \setminus U_0|$, then

$$\begin{aligned}\eta(H) &\leqslant (2e(H) - |H| + e(U(H) \setminus U_0, V(H)))x_{u^*} \\ &\leqslant (|H| - 2 + 2|U(H) \setminus U_0|)x_{u^*} < \zeta(H)x_{u^*},\end{aligned}$$

as desired.

Next, we assume that $e(U(H) \setminus U_0, V(H)) > 2|U(H) \setminus U_0|$. Then there exists a vertex, say w, in $U(H) \setminus U_0$ such that $d_H(w) \geqslant 3$. It follows that $|H| \geqslant 3$. If $|H| \geqslant 4$, then it is routine to check that $\theta(1,2,4)$ is a subgraph of G^*, a contradiction. Hence $|H| = 3$ and $H \cong K_{1,2}$. Applying the fact that G^* is $\theta(1,2,4)$-free yields $d_H(w') = 1$ for each $w' \in U(H) \setminus (U_0 \cup \{w\})$. Recall that $e(U(H) \setminus U_0, V(H)) > 2|U(H) \setminus U_0|$. Then $U(H) \setminus U_0 = \{w\}$. Therefore,

$$\eta(H) \leqslant (2e(H) - |H| + e(U(H) \setminus U_0, V(H)))x_{u^*} = 4x_{u^*} < \zeta(H)x_{u^*},$$

as desired.

(ii) Let H be a component of H_2. Then $U(H) \cap U_0 = \emptyset$ and $d_{N(u^*)}(u) = 1$ for any $u \in U(H)$. It follows that $e(U(H), V(H)) = |U(H)|$. Clearly, $e(H) = |H| - 1$. Thus,

$$\eta(H) \leqslant (2e(H) - |H| + e(U(H), V(H)))x_{u^*} = (|H| - 2 + |U(H)|)x_{u^*} < \zeta(H)x_{u^*},$$

as desired.

(iii) Let H be a component of H_3, i.e., $H \cong C_3$. Notice that $U(H) \cap U_0 = \emptyset$ and $e(H) = |H|$. If $|U(H)| = 0$, then

$$\eta(H) \leqslant (2e(H) - |H|)x_{u^*} = |H|x_{u^*} = \zeta(H)x_{u^*},$$

as desired.

If $|U(H)| = 1$, then let $u \in U(H)$. We may assume, without loss of generality, that $V(H) = \{v_1, v_2, v_3\}$ and $x_{v_1} = \max\{x_{v_i} : i = 1,2,3\}$. Then $v_1 \in N(u)$ and $e(U(H), V(H)) \leqslant 3$. It follows that

$$\eta(H) \leqslant (2e(H) - |H| + e(U(H), V(H)))x_{u^*} \leqslant (|H| + 3)x_{u^*} = (\zeta(H) + 1)x_{u^*},$$

as desired.

If $|U(H)| \geqslant 2$, then together with the fact that G^* is $\theta(1,2,4)$-free, one of the followings holds:

♣ $U(H)$ contains exactly one vertex having three neighbors in $V(H)$ and all other vertices have only one neighbor in $V(H)$;

♣ all vertices of $U(H)$ have at most two neighbors in $V(H)$.

In both cases, we get that $e(U(H), V(H)) \leqslant 2|U(H)|$. Thus,

$$\eta(H) \leqslant (2e(H) - |H| + e(U(H), V(H)))x_{u^*} \leqslant (|H| + 2|U(H)|)x_{u^*} = \zeta(H)x_{u^*},$$

as desired.

(iv) Assume H is a component of H_4. Notice that $U(H) \cap U_0 = \emptyset$. Since G^* is $\theta(1,2,4)$-free, we have $d_{N(u^*)}(u) = 1$. If $|U(H)| = 0$, then let $x_v = \max\{x_u : u \in V(H)\}$. Hence $\lambda^* x_v \leqslant x_{u^*} + 3x_v$, that is, $x_v \leqslant \frac{x_{u^*}}{\lambda^* - 3} \leqslant \frac{x_{u^*}}{7}$. Therefore,

$$\eta(H) \leqslant (2e(H) - |H|)x_v \leqslant \frac{8}{7}x_{u^*} < (\zeta(H) + 2)x_{u^*},$$

as desired.

If $|U(H)| = 1$, then let $U(H) = \{u\}$. Let v be a vertex in H such that $uv \in E(G^*)$. Assume that $V(H) = \{v, v_1, v_2, v_3\}$ and $x_{v_1} = \max\{x_{v_i} : i = 1,2,3\}$. Then $\lambda^* x_{v_1} \leqslant x_{u^*} + 2x_{v_1} + x_v \leqslant 2(x_{u^*} + x_{v_1})$, i.e., $x_{v_1} \leqslant \frac{2}{\lambda^* - 2}x_{u^*} \leqslant \frac{1}{4}x_{u^*}$. Therefore,

$$\eta(H) \leqslant 6x_{v_1} + 2x_v + |U(H)|x_{u^*} \leqslant \left(\frac{7}{2} + |U(H)|\right)x_{u^*} < (\zeta(H) + 2)x_{u^*},$$

as desired.

If $|U(H)| \geqslant 2$, then

$$\eta(H) \leqslant (2e(H) - |H| + |U(H)|)x_{u^*} \leqslant (|H| + 4 + |U(H)|)x_{u^*} \leqslant (\zeta(H) + 2)x_{u^*},$$

as desired.

(v) Let H be a component of H_5. Then $U(H) \cap U_0 = \emptyset$ and $d_{N(u^*)}(u) = 1$ for any $u \in U(H)$. Hence $e(U(H), V(H)) = |U(H)|$. Together with the fact that $e(H) = |H|$, we have

$$\eta(H) \leqslant (2e(H) - |H| + e(U(H), V(H)))x_{u^*} = (|H| + |U(H)|)x_{u^*} \leqslant \zeta(H)x_{u^*},$$

as desired. □

With Claim 3.2 in hand, we are ready to give a lower bound on $|U_0| + |H_0|$. Let c_3 and c_4 denote the numbers of components of H_3 and H_4, respectively. Since each vertex in U_0 has at most two neighbors in $N(u^*) \setminus V(H_0)$, one has $\sum_{w \in U_0} d_{N(u^*)}(w) \leqslant |U_0||H_0| + 2|U_0|$. We use $H \in H_i$ to denote that H is a component of H_i for $i \in \{0, 1, \ldots, 5\}$. Together with Claim 3.2 and some calculation we find that

$$\begin{aligned}
(3.2) \qquad & (\lambda^{*2} - \lambda^*)x_{u^*} \\
&= |N(u^*)|x_{u^*} + \sum_{v \in N(u^*) \setminus V(H_0)} (d_{N(u^*)}(v) - 1)x_v \\
&\quad + \sum_{w \in N^2(u^*)} d_{N(u^*)}(w)x_w \\
&\leqslant |N(u^*)|x_{u^*} + \sum_{i=1}^{5} \sum_{H \in H_i} \eta(H) + \sum_{w \in U_0} d_{N(u^*)}(w)x_w \\
&\leqslant \left(|N(u^*)| + \sum_{i=1}^{5} \sum_{H \in H_i} \zeta(H) + (c_3 + 2c_4) + (|U_0||H_0| + 2|U_0|) \right) x_{u^*} \\
&= \left(|N(u^*)| + \sum_{i=1}^{5} \sum_{H \in H_i} (|H| + 2|U(H) \setminus U_0|) + (c_3 + 2c_4) + (|U_0||H_0| + 2|U_0|) \right) x_{u^*} \\
&= \big(|N(u^*)| + (|N(u^*)| - |H_0|) + 2(|N^2(u^*)| - |U_0|) + (c_3 + 2c_4) + |U_0|(|H_0| + 2) \big) x_{u^*} \\
(3.3) \quad &\leqslant \big(2(n-1) + (c_3 + 2c_4) + (|U_0| - 1)|H_0| \big) x_{u^*}.
\end{aligned}$$

In view of (3.1), one has

$$\lambda^{*2} - \lambda^* > \left\lfloor \frac{(n-1)^2}{4} \right\rfloor - \sqrt{\left\lfloor \frac{(n-1)^2}{4} \right\rfloor} > \frac{(n-1)^2 - 1}{4} - \frac{n}{2}. \tag{3.4}$$

If $|U_0| \leqslant 1$, then together with (3.3) and (3.4) one has

$$\frac{(n-1)^2 - 1}{4} - \frac{n}{2} < 2(n-1) + (c_3 + 2c_4) < 3n - 2,$$

which implies that $n \leqslant 16$, a contradiction. Hence $|U_0| \geqslant 2$ and $|H_0| \geqslant 1$. Assume that $|U_0| + |H_0| = n - 1 - 3c_3 - 4c_4 - t$. Then $t \leqslant n - 4 - 3c_3 - 4c_4$. Combining with (3.3) and (3.4), we get

$$\begin{aligned}\frac{(n-1)^2-1}{4} - \frac{n}{2} &< 2(n-1) + (c_3+2c_4) + (|U_0|-1)|H_0| \\ &\leqslant 2(n-1) + (c_3+2c_4) + \frac{(n-2-3c_3-4c_4-t)^2}{4},\end{aligned}$$

which is equivalent to

$$\begin{aligned}&-t^2-4t+2tn-8n+4 \\ &< 9c_3^2+16c_4^2+24c_3c_4-6\left(n-\frac{8}{3}-t\right)c_3-8(n-3-t)c_4. \qquad (3.5)\end{aligned}$$

Next, we proceed by considering the following five possible subcases.

♠ $c_3 = c_4 = 0$. Then $n \geqslant 3c_3 + 4c_4 + t + 4 = t + 4$ and (3.5) becomes

$$-t^2-4t+2tn-8n+4<0.$$

Clearly, $-t^2-4t+2tn-8n+4$ is an increasing function in t with $t \in [5, n-4]$. Therefore, $-t^2-4t+2tn-8n+4 \geqslant 2n-41 > 0$ if $n \geqslant 21$, a contradiction. Thus, $t \in \{0,1,2,3,4\}$ and so $n-5 \leqslant |U_0|+|H_0| \leqslant n-1$.

♠ $c_3 = 1$ and $c_4 = 0$. Then $n \geqslant 3c_3 + 4c_4 + t + 4 = t + 7$ and (3.5) becomes

$$-t^2-4t+2tn-8n+4<25+6t-6n, \text{ i.e., } -t^2-10t+2tn-2n-21<0.$$

Obviously, $-t^2-10t+2tn-2n-21$ is an increasing function in t with $t \in [3, n-7]$. Hence, $-t^2-10t+2tn-2n-21 \geqslant 4n-60 \geqslant 0$ if $n \geqslant 15$, a contradiction. Thus, $t \in \{0,1,2\}$. It follows that $n-6 \leqslant |U_0|+|H_0| \leqslant n-4$.

♠ $c_3 = 0$ and $c_4 = 1$. Then $n \geqslant 3c_3 + 4c_4 + t + 4 = t + 8$ and (3.5) becomes

$$-t^2-4t+2tn-8n+4<40+8t-8n, \text{ i.e., } -t^2-12t+2tn-36<0.$$

Clearly, $-t^2-12t+2tn-36$ is an increasing function in t with $t \in [2, n-8]$. Hence $-t^2-12t+2tn-36 \geqslant 4n-64 \geqslant 0$ if $n \geqslant 16$, a contradiction. Therefore $t \in \{0,1\}$, which implies $n-6 \leqslant |U_0|+|H_0| \leqslant n-5$.

♠ $c_3 = c_4 = 1$. Then $n \geqslant 3c_3 + 4c_4 + t + 4 = t + 11$ and (3.5) becomes

$$-t^2-4t+2tn-8n+4<89+14t-14n, \text{ i.e., } -t^2-18t+2tn+6n-85<0.$$

It is routine to check that $-t^2-18t+2tn+6n-85$ is an increasing function in t with $t \in [0, n-11]$. Therefore, $-t^2-18t+2tn+6n-85 \geqslant 6n-85 \geqslant 0$ if $n \geqslant 15$, which is also a contradiction.

♠ $c_3 \geqslant 2$ or $c_4 \geqslant 2$. Then $n \geqslant 3c_3 + 4c_4 + t + 4 \geqslant t + 10$. Let $\varphi(x,y) = 9x^2+16y^2+24xy-6(n-\frac{8}{3}-t)x-8(n-3-t)y$ be a real function in x, y for $x \in [0,+\infty)$, $y \in [0,+\infty)$ with $n \geqslant 3x+4y+t+3$. It is routine to check that the derivative functions of $\varphi(x,y)$ with respect to x and y are, respectively,

$$\frac{d(\varphi(x,y))}{dx} = 18x+24y-6\left(n-\frac{8}{3}-t\right) = 6\left(3x+4y+t+\frac{8}{3}-n\right) < 0$$

and

$$\frac{d(\varphi(x,y))}{dy} = 32y + 24x - 8\,(n-3-t) = 8\,(3x+4y+t+3-n) \leqslant 0.$$

It follows that $\varphi(x,y)$ is a decreasing function for x (resp. y).

If $c_3 \geqslant 2$, then

$$\varphi(c_3,c_4) \leqslant \varphi(2,0) = 68 + 12t - 12n.$$

Together with (3.5), one has

$$-t^2 - 4t + 2tn - 8n + 4 < 68 + 12t - 12n, \text{ i.e., } -t^2 - 16t + 2tn + 4n - 64 < 0.$$

On the other hand, it is easy to check that $-t^2-16t+2tn+4n-64 \geqslant 4n-64 > 0$ for $t \in [0, n-10]$ and $n \geqslant 21$, a contradiction.

For $c_4 \geqslant 2$, by a similar discussion as that of $c_3 \geqslant 2$, we may get a contradiction.

Together with the discussion as above, we have if $n \geqslant 21$, then $(c_3,c_4) \in \{(0,0),(0,1),(1,0)\}$ and

$$|U_0| + |H_0| \in \begin{cases} [n-5, n-1], & \text{if } (c_3,c_4) = (0,0); \\ [n-6, n-4], & \text{if } (c_3,c_4) = (1,0); \\ [n-6, n-5], & \text{if } (c_3,c_4) = (0,1). \end{cases} \tag{3.6}$$

Similar to (2.2), one has

$$\left\lfloor \frac{(n-1)^2}{4} \right\rfloor < \lambda^{*2} \leqslant |N(u^*)| + 2e(N(u^*)) + e(N(u^*), N^2(u^*)).$$

Denote $\beta(u^*) = |N(u^*)| + 2e(N(u^*)) + e(N(u^*), N^2(u^*))$. Hence

$$\beta(u^*) > \left\lfloor \frac{(n-1)^2}{4} \right\rfloor, \text{ i.e., } \beta(u^*) \geqslant \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1. \tag{3.7}$$

Bear in mind that G^* is $\theta(1,2,4)$-free. For each edge $uv \in E(N^2(u^*))$, one has $|N(u) \cap N(v) \cap N(u^*)| \leqslant 2$. Moreover, if $|N(u) \cap N(v) \cap N(u^*)| = 2$, then $|(N(u) \cup N(v)) \cap N(u^*)| = 2$. That is to say,

$$e(\{u,v\}, N(u^*)) \leqslant |N(u^*)| + 1 \text{ if } |N(u^*)| \geqslant 3. \tag{3.8}$$

Now, we distinguishing our proof into the following four possible case with respect to the value of $|U_0| + |H_0|$.

Case 1. $|U_0| + |H_0| = n - 1$. In this case, $V(G^*) = \{u^*\} \cup V(H_0) \cup U_0$. If $|H_0| \leqslant 2$, then

$$\beta(u^*) \leqslant |H_0| + |U_0||H_0| \leqslant 2n - 4 < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,$$

a contradiction to (3.7). Hence $|H_0| \geqslant 3$.

Since G^* is non-bipartite, one has $e(U_0) \geqslant 1$. If $G^*[U_0]$ contains a $C_3 = w_1w_2w_3w_1$, then all vertices of C_3 must share a unique common neighbor in H_0. Otherwise, G^* contains $\theta(1,2,4)$ as a subgraph, a contradiction. Hence

$$\begin{aligned}\beta(u^*) &\leqslant |H_0| + 3 + |H_0|(|U_0| - 3) = |H_0|(|U_0| - 2) + 3\\ &\leqslant \left\lfloor \frac{(n-3)^2}{4} \right\rfloor + 3 < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,\end{aligned}$$

a contradiction. Thus, $G^*[U_0]$ is C_3-free. Notice that G^* contains C_3 as a subgraph. Then there exists an edge, say uv, in $G^*[U_0]$ such that u and v have a common neighbor, say w, in H_0.

Next, we show that $e(U_0) = 1$. Suppose to the contrary that $e(U_0) \geqslant 2$. Let $u'v'$ be an edge other than uv in $G^*[U_0]$. If $u'v'$ is incident to neither u nor v, then in view of (3.8) one has

$$\begin{aligned}\beta(u^*) &\leqslant |H_0| + 2(|H_0| + 1) + |H_0|(|U_0| - 4) = |H_0|(|U_0| - 1) + 2\\ &\leqslant \left\lfloor \frac{(n-2)^2}{4} \right\rfloor + 2 < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,\end{aligned}$$

a contradiction. Hence each edge in $G^*[N(u^*)]$ is adjacent to either u or v. Without loss of generality, we assume that $u = u'$. Since G^* is $\theta(1,2,4)$-free, one has $N(v') \cap (N(u^*) \setminus \{w\}) = \emptyset$. Together with the proof of (3.8), we have

$$\begin{aligned}\beta(u^*) &\leqslant |H_0| + |H_0| + 2 + |H_0|(|U_0| - 3) = |H_0|(|U_0| - 1) + 2\\ &\leqslant \left\lfloor \frac{(n-2)^2}{4} \right\rfloor + 2 < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,\end{aligned}$$

which is also a contradiction. Therefore, $e(U_0) = 1$.

If $|N(u) \cap N(v) \cap N(u^*)| = 2$, then

$$\begin{aligned}\beta(u^*) &\leqslant |H_0| + 4 + |H_0|(|U_0| - 2) = |H_0|(|U_0| - 1) + 4\\ &\leqslant \left\lfloor \frac{(n-2)^2}{4} \right\rfloor + 4 < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,\end{aligned}$$

a contradiction. Hence $|N(u) \cap N(v) \cap N(u^*)| = 1$. In view of Lemma 1.4, one has $(N(u) \cup N(v)) \cap N(u^*) = N(u^*)$ and $N(w') \cap N(u^*) = N(u^*)$ for each $w' \in U_0 \setminus \{u, v\}$. Assume, without loss of generality, that $x_u \geqslant x_v$. Then $N(v) \cap N(u^*) = \{w\}$. Otherwise, let $G' = G^* - \{vv' : v' \in N(u^*) \setminus \{w\}\} + \{uv' : v' \in N(u^*) \setminus \{w\}\}$. Clearly, G' is a non-bipartite $\theta(1,2,4)$-free graph with order n. By Lemma 1.5, one has $\lambda^* < \lambda(G')$, which contradicts the choice of G^*. It follows that $N_{G^*}(u^*) \subsetneq N_{G^*}(u)$, which implies $x_u > x_{u^*}$, a contradiction.

Case 2. $|U_0| + |H_0| = n - 2$. In this case, $V(G^*) = \{u^*\} \cup V(H_0) \cup U_0 \cup N^3(u^*)$ and $|N^3(u^*)| = 1$. Then

$$\beta(u^*) \leqslant |H_0| + |H_0||U_0| = |H_0|(|U_0| + 1) \leqslant \left\lfloor \frac{(n-1)^2}{4} \right\rfloor < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,$$

a contradiction.

Case 3. $|U_0|+|H_0| = n-3$. In this case, either $|V(G^*)\backslash(N[u^*]\cup N^2(u^*))| = 2$ or $G^*[N(u^*)]$ contains exactly one edge. If $|H_0| \leqslant 2$, then

$$\beta(u^*) \leqslant |H_0| + 4 + |U_0|(|H_0| + 2) \leqslant 4n - 14 < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,$$

a contradiction. Hence $|H_0| \geqslant 3$.

Firstly, we assume $|V(G^*) \setminus (N[u^*] \cup N^2(u^*))| = 2$. Then

$$\beta(u^*) \leqslant |H_0| + |U_0||H_0| \leqslant \left\lfloor \frac{(n-2)^2}{4} \right\rfloor < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,$$

a contradiction.

In what follows, we consider the case that $G^*[N(u^*)]$ contains one edge w_1w_2. Then we have the following claim.

Claim 3.3. $e(U_0) = 0$.

Proof of Claim 3.3. Suppose that $e(U_0) \geqslant 1$ and let uv be an edge in $G^*[U_0]$. Define

$$A_i = \{w \in U_0 \setminus \{u,v\} : N(w) \cap \{w_1, w_2\} = \{w_i\}\} \text{ for } i \in \{1,2\}$$

and

$$A_3 = \{w \in U_0 \setminus \{u,v\} : N(w) \cap \{w_1, w_2\} = \{w_1, w_2\}\}.$$

Based on the fact that G^* is $\theta(1,2,4)$-free, one has $N(A_1) \cap N(A_2 \cup A_3) \cap V(H_0) = \emptyset$ and $N(A_2) \cap N(A_1 \cup A_3) \cap V(H_0) = \emptyset$. Moreover, each pair of vertices in A_3 have no common neighbor in $V(H_0)$. Denote $s_i = |\{u : u \in N(A_i) \cap V(H_0)\}|$ for $i \in \{1,2,3\}$. Then $s_1 + s_2 + s_3 \leqslant |H_0|$. We may assume $s_1 \geqslant s_2$.

If $s_1 \geqslant 1$ and $|H_0| \geqslant s_1 + 1$, then $|A_1 \cup A_2 \cup A_3| \geqslant 1$. Hence together with (3.8), one has

$$\begin{aligned}
\beta(u^*) &\leqslant |H_0| + 4 + \sum_{i=1}^{2} |A_i|(s_i + 1) + 2|A_3| + s_3 \\
&\quad + (|U_0| - |A_1 \cup A_2 \cup A_3| - 2)|H_0| + |H_0| + 3 \\
&\leqslant (|A_1| + |A_2|)(s_1 + 1) + 2|A_3| + (|H_0| - s_1) \\
&\quad + (|U_0| - |A_1 \cup A_2 \cup A_3|)|H_0| + 7 \\
&= (|A_1| + |A_2| - 1)(s_1 + 1) + 2|A_3| \\
&\quad + (|U_0| - |A_1 \cup A_2 \cup A_3| + 1)|H_0| + 8 \\
&\leqslant (|A_1 \cup A_2 \cup A_3| - 1)(s_1 + 1) + (|U_0| - |A_1 \cup A_2 \cup A_3| + 1)|H_0| + 8 \\
&= |U_0||H_0| - (|A_1 \cup A_2 \cup A_3| - 1)(|H_0| - s_1 - 1) + 8 \\
&\leqslant |U_0||H_0| + 8 \leqslant \left\lfloor \frac{(n-3)^2}{4} \right\rfloor + 8 < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1, \qquad (3.9)
\end{aligned}$$

a contradiction. Therefore, either $s_1 = 0$ or $|H_0| = s_1$ holds.

If $s_1 = 0$, then $s_2 = 0$ and (3.9) becomes

$$\begin{aligned}\beta(u^*) &\leqslant |H_0| + 4 + \sum_{i=1}^{2} |A_i| + 2|A_3| + s_3 \\ &\quad + (|U_0| - |A_1 \cup A_2 \cup A_3| - 2)|H_0| + |H_0| + 3 \\ &\leqslant (|A_1| + |A_2|) + 2|A_3| + (|U_0| - |A_1 \cup A_2 \cup A_3| + 1)|H_0| + 7 \\ &\leqslant 2(|A_1 \cup A_2 \cup A_3| - 1) + (|U_0| - |A_1 \cup A_2 \cup A_3| + 1)|H_0| + 9 \\ &\leqslant |U_0||H_0| - (|A_1 \cup A_2 \cup A_3| - 1)(|H_0| - 2) + 9 \\ &\leqslant |U_0||H_0| + |H_0| - 2 + 9 \\ &\leqslant \left\lfloor \frac{(n-2)^2}{4} \right\rfloor + 7 < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,\end{aligned}$$

a contradiction.

If $|H_0| = s_1$, then $s_2 = s_3 = 0$ and (3.9) becomes

$$\begin{aligned}\beta(u^*) &\leqslant |H_0| + 4 + |A_1|(|H_0| + 1) + |A_2| + 2|A_3| \\ &\quad + (|U_0| - |A_1 \cup A_2 \cup A_3| - 2)|H_0| + |H_0| + 3 \\ &= |A_1| + |A_2| + 2|A_3| + (|U_0| - |A_2 \cup A_3|)|H_0| + 7 \\ &\leqslant |U_0| + |A_3| + (|U_0| - |A_2 \cup A_3|)|H_0| + 7 \\ &\leqslant |U_0|(|H_0| + 1) - |A_2 \cup A_3|(|H_0| - 1) + 7 \\ &\leqslant |U_0|(|H_0| + 1) + 7 \\ &\leqslant \left\lfloor \frac{(n-2)^2}{4} \right\rfloor + 7 < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,\end{aligned}$$

which also contradicts (3.7). Thus, $e(U_0) = 0$.

This completes the proof of Claim 3.3. □

Now, we define

$$A'_i = \{w \in U_0 : N(w) \cap \{w_1, w_2\} = \{w_i\}\} \text{ for } i \in \{1, 2\}$$

and

$$A'_3 = \{w \in U_0 : N(w) \cap \{w_1, w_2\} = \{w_1, w_2\}\}.$$

Since G^* is $\theta(1, 2, 4)$-free, one has $N(A'_1) \cap N(A'_2 \cup A'_3) \cap V(H_0) = \emptyset$ and $N(A'_2) \cap N(A'_1 \cup A'_3) \cap V(H_0) = \emptyset$. Moreover, each pair of vertices in A'_3 have no common neighbor in H_0. Assume $s'_i = |\{u : u \in N(A'_1) \cap V(H_0)\}|$ for $i \in \{1, 2, 3\}$ and $s'_1 \geqslant s'_2$. If $s'_1 \geqslant 1$ and $|H_0| \geqslant s'_1 + 1$, then $|A'_1 \cup A'_2 \cup A'_3| \geqslant 1$. By a similar discussion as (3.9), one has

$$\begin{aligned}\beta(u^*) &\leqslant |H_0| + 4 + \sum_{i=1}^{2} |A'_i|(s'_i + 1) + 2|A'_3| + s'_3 + (|U_0| - |A'_1 \cup A'_2 \cup A'_3|)|H_0| \\ &\leqslant (|U_0| + 1)|H_0| + 5 \leqslant \left\lfloor \frac{(n-2)^2}{4} \right\rfloor + 5 < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,\end{aligned}$$

a contradiction. Therefore, either $s_1'=0$ or $|H_0|=s_1'$ holds.

If $s_1'=0$, then $s_2'=0$. Together with Claim 3.1, we get $|A_1'|=|A_2'|=0$. If $|A_3'|\geqslant 1$, then

$$\begin{aligned}\beta(u^*) &\leqslant |H_0|+4+2|A_3'|+s_3'+(|U_0|-|A_3'|)|H_0|\\ &=(|U_0|+1)|H_0|+(2-|H_0|)|A_3'|+s_3'+4\\ &\leqslant |U_0||H_0|+s_3'+6\leqslant |U_0||H_0|+|U_0|+6\\ &\leqslant \left\lfloor\frac{(n-2)^2}{4}\right\rfloor+6<\left\lfloor\frac{(n-1)^2}{4}\right\rfloor+1,\end{aligned}$$

a contradiction. Hence $|A_3'|=0$. Together with Lemmas 1.4 and 1.7, we have $G^*\cong K_{\lceil\frac{n-2}{2}\rceil,\lfloor\frac{n-2}{2}\rfloor}\circ K_3$. Applying Lemmas 1.4 and 2.1 one has

$$\lambda^*<\lambda(SK_{\lceil\frac{n-1}{2}\rceil,\lfloor\frac{n-1}{2}\rfloor})<\lambda(K_{\lceil\frac{n-1}{2}\rceil,\lfloor\frac{n-1}{2}\rfloor}\bullet K_3),$$

a contradiction to (3.1).

If $|H_0|=s_1'$, then $s_2'=s_3'=0$. In view of Claims 3.1 and 3.3, we get $|A_2'|=0$. If $|A_3'|\geqslant 1$, then

$$\begin{aligned}\beta(u^*) &\leqslant |H_0|+4+|A_1'|(|H_0|+1)+2|A_3'|+(|U_0|-|A_1'\cup A_3'|)|H_0|\\ &=(|U_0|+1)|H_0|+|A_1'|+|A_3'|(2-|H_0|)+4\\ &\leqslant |U_0||H_0|+|A_1'|+6\leqslant |U_0||H_0|+|U_0|+6\\ &\leqslant \left\lfloor\frac{(n-2)^2}{4}\right\rfloor+6<\left\lfloor\frac{(n-1)^2}{4}\right\rfloor+1,\end{aligned}$$

which also contradicts (3.7). Therefore, $|A_3'|=0$. Together with Lemma 1.4, we have $G^*\cong K_{a,b}\bullet K_3$ with $a=|H_0|+1$ and $b=|U_0|+1$. Without loss of generality, assume that $a\geqslant b$. We claim $a=\lceil\frac{n-1}{2}\rceil$ and $b=\lfloor\frac{n-1}{2}\rfloor$. Otherwise,

$$\begin{aligned}\beta(u^*)&=a+3+a(b-1)=ab+3\\ &\leqslant\left(\left\lceil\frac{n-1}{2}\right\rceil+1\right)\left(\left\lfloor\frac{n-1}{2}\right\rfloor-1\right)<\left\lfloor\frac{(n-1)^2}{4}\right\rfloor+1,\end{aligned}$$

a contradiction. Hence $G^*\cong K_{\lceil\frac{n-1}{2}\rceil,\lfloor\frac{n-1}{2}\rfloor}\bullet K_3$, as desired.

Case 4. $n-6\leqslant |U_0|+|H_0|\leqslant n-4$. Then $N(u^*)\setminus V(H_0)\neq\emptyset$. Otherwise, $N^2(u^*)=U_0$. Hence

$$\beta(u^*)\leqslant |H_0|+|U_0||H_0|=(|U_0|+1)|H_0|\leqslant\left\lfloor\frac{(n-3)^2}{4}\right\rfloor<\left\lfloor\frac{(n-1)^2}{4}\right\rfloor+1,$$

a contradiction to (3.7).

Let H be a nontrivial component of $G^*[N(u^*)]$. In view of (3.6), one has

$$H\in\{P_2,K_{1,2},K_{1,3},P_4,C_3,C_4,C_4+e,K_4,K_{1,3}+e\}.$$

If $H\in\{K_{1,2},K_{1,3}\}$, then $n-5\leqslant |U_0|+|H_0|\leqslant n-1-|H|\leqslant n-4$ (based on (3.6)) and so H is the unique nontrivial component of $G^*[N(u^*)]$. Note that each vertex in U_0 is adjacent to at most one vertex in H and each vertex in $U(H)$ is adjacent to at most three vertices in H. Hence

$$\begin{aligned}
\beta(u^*) &\leqslant |H_0| + 4 + 6 + |U_0||H_0| + |U_0| + 3(n - |U_0| - |H_0| - 4)\\
&\leqslant \begin{cases} (|U_0|+1)(|H_0|+1) + 12, & \text{if } |U_0| + |H_0| = n-5;\\ (|U_0|+1)(|H_0|+1) + 9, & \text{if } |U_0| + |H_0| = n-4, \end{cases}\\
&\leqslant \begin{cases} \left\lfloor \dfrac{(n-3)^2}{4} \right\rfloor + 12, & \text{if } |U_0| + |H_0| = n-5;\\ \left\lfloor \dfrac{(n-2)^2}{4} \right\rfloor + 9, & \text{if } |U_0| + |H_0| = n-4, \end{cases}\\
&< \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,
\end{aligned}$$

a contradiction.

If $H \in \{P_4, C_4, C_4+e, K_4, K_{1,3}+e\}$, then in view of (3.6) one has that H is the unique nontrivial component of $G^*[N(u^*)]$ and $|U_0|+|H_0| \in \{n-6, n-5\}$. Notice that $U_0 \cap U(H) = \emptyset$ and each vertex in $U(H)$ is adjacent to exactly one vertex in H. It follows that

$$\begin{aligned}
\beta(u^*) &\leqslant |H_0| + 4 + 2|E(H)| + |U_0||H_0| + (n - |U_0| - |H_0| - 5)\\
&\leqslant \begin{cases} \left\lfloor \dfrac{(n-5)^2}{4} \right\rfloor + 17, & \text{if } |U_0| + |H_0| = n-6;\\ \left\lfloor \dfrac{(n-4)^2}{4} \right\rfloor + 16, & \text{if } |U_0| + |H_0| = n-5, \end{cases}\\
&< \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,
\end{aligned}$$

a contradiction.

If $H \cong C_3$ and H is the unique nontrivial component of $G^*[N(u^*)]$, then $U_0 \cap U(H) = \emptyset$ and by (3.6) one has $|U_0| + |H_0| \in [n-6, n-4]$. Therefore,

$$\begin{aligned}
\beta(u^*) &\leqslant |H_0| + 3 + 6 + |U_0||H_0| + 3(n - |U_0| - |H_0| - 4)\\
&\leqslant \begin{cases} \left\lfloor \dfrac{(n-5)^2}{4} \right\rfloor + 15, & \text{if } |U_0| + |H_0| = n-6;\\ \left\lfloor \dfrac{(n-4)^2}{4} \right\rfloor + 12, & \text{if } |U_0| + |H_0| = n-5;\\ \left\lfloor \dfrac{(n-3)^2}{4} \right\rfloor + 9, & \text{if } |U_0| + |H_0| = n-4, \end{cases}\\
&< \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,
\end{aligned}$$

a contradiction.

Together with the discussion above, we know that $G^*[N(u^*)] - H_0 \in \{P_2, 2P_2, P_2 \cup C_3\}$. We proceed by distinguishing the following three subcases.

Subcase 4.1. $|U_0| + |H_0| = n - 4$. In this subcase, $G^*[N(u^*)] - H_0 \cong P_2$. By a similar discussion as Case 3, we can get a contradiction. The detailed proof is given in the Appendix.

Subcase 4.2. $|U_0| + |H_0| = n - 5$. Notice that each vertex in U_0 is adjacent to at most two vertices in $N(u^*) \setminus V(H_0)$. Hence

$$\begin{aligned}\beta(u^*) &\leqslant |H_0| + 4 + 4 + |U_0|(|H_0| + 2) = (|U_0| + 1)(|H_0| + 2) + 6 \\ &\leqslant \left\lfloor \frac{(n-2)^2}{4} \right\rfloor + 6 < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,\end{aligned}$$

a contradiction.

Subcase 4.3. $|U_0| + |H_0| = n - 6$. In view of (3.6), we know that $G^*[N(u^*)]$ contains C_3 as a component. Then $G^*[N(u^*)] - H_0 \cong P_2 \cup C_3$ and $V(G^*) = N[u^*] \cup U_0$. Hence each vertex in U_0 is adjacent to at most two vertices in $N(u^*) \setminus V(H_0)$. Therefore,

$$\begin{aligned}\beta(u^*) &\leqslant |H_0| + 5 + 8 + |U_0|(|H_0| + 2) = (|U_0| + 1)(|H_0| + 2) + 11 \\ &\leqslant \left\lfloor \frac{(n-3)^2}{4} \right\rfloor + 11 < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,\end{aligned}$$

which also contradicts (3.7).

This completes the proof. □

We close this section by giving the proof of Theorem 1.3, which determines the maximum possible size of a $\theta(1,2,4)$-free non-bipartite graph with given order. Recall that Zhai, Fang and Shu [38] established the following result.

Theorem 3.4 ([38])**.** *Let $q, r \geqslant 2$ be two integers such that qr is even. Let $k = q + r$ and $n \geqslant 9k^2 - 3k$. Then*

$$\mathrm{ex}(n, \theta(1,q,r)) = \left\lfloor \frac{n^2}{4} \right\rfloor.$$

The only extremal graph is $K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$.

In fact, if we put $p = 2$ and $q = 4$, then by the proof of Theorem 3.4, we may get a result as follows.

Corollary 3.5. *Let $n \geqslant 132$ be an integer. Then*

$$\mathrm{ex}(n, \theta(1,2,4)) = \left\lfloor \frac{n^2}{4} \right\rfloor.$$

The only extremal graph is $K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$.

Now, we are ready to give the proof of Theorem 1.3.

Proof of Theorem 1.3. Let G^* be an n-vertex $\theta(1,2,4)$-free non-bipartite graph having the largest number of edges. Notice that $K_{\lceil \frac{n-1}{2}\rceil,\lfloor \frac{n-1}{2}\rfloor}\bullet K_3$ is a $\theta(1,2,4)$-free non-bipartite graph with order n. Hence

$$|E(G^*)| \geqslant |E(K_{\lceil \frac{n-1}{2}\rceil,\lfloor \frac{n-1}{2}\rfloor}\bullet K_3)| \geqslant \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 2.$$

If G^* is also $\theta(1,2,3)$-free, then by Lemma 1.10, one has $|E(G^*)| \leqslant \lfloor \frac{(n-1)^2}{4} \rfloor + 1 < \lfloor \frac{(n-1)^2}{4} \rfloor + 2$, a contradiction. Hence G^* contains $\theta(1,2,3)$ as a subgraph.

Let $H \cong \theta(1,2,3)$ be a subgraph of G^* with $V(H) = \{v_1, v_2, v_3, v_4, v_5\}$ and $E(H) = \{v_i v_{i+1} : 1 \leqslant i \leqslant 5\} \cup \{v_1 v_3\}$, taking subscripts modulo 5. Since G^* is $\theta(1,2,4)$-free, one has that each vertex in $V(G^*) \setminus V(H)$ has at most two neighbors in $V(H)$. Let $G' = G^* - V(H)$. Notice that G' is also $\theta(1,2,4)$-free and $|V(G')| \geqslant 132$. By Corollary 3.5, one has $|E(G')| \leqslant \lfloor \frac{(n-5)^2}{4} \rfloor$. Hence

$$\begin{aligned} |E(G^*)| &= |E(G')| + e(V(H), V(G')) + |E(H)| \\ &\leqslant \left\lfloor \frac{(n-5)^2}{4} \right\rfloor + 2(n-5) + 6 = \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 2. \end{aligned} \tag{3.10}$$

In what follows, we prove the second part of Theorem 1.3. The necessity part is obvious, so we only give the proof of the sufficiency part.

Sufficiency. Assume that the equality in (3.10) holds. Then $|E(G')| = \lfloor \frac{(n-5)^2}{4} \rfloor$ and each vertex in G' has exactly two neighbors in H. In view of Corollary 3.5, one has $G' \cong K_{\lceil \frac{n-5}{2}\rceil,\lfloor \frac{n-5}{2}\rfloor}$.

For $1 \leqslant i, j \leqslant 5$, denote

$$U_{i,j} = \{w \in V(G^*) \setminus V(H) : N(w) \cap V(H) = \{v_i, v_j\}\}.$$

Without loss of generality, assume that $|U_{1,4}| \geqslant |U_{3,5}|$. Based on G^* is $\theta(1,2,4)$-free, one has the following assertions.

(i) $U_{i,j} \neq \emptyset$ only if $(i,j) \in \{(1,3),(1,4),(3,5)\}$;
(ii) $e(U_{1,3}, U_{1,4} \cup U_{3,5}) = 0$;
(iii) For all $i, j \in \{1,2,3,4,5\}$, $U_{i,j}$ is an independent set of G^*.

Then (i) implies $V(G') = U_{1,3} \cup U_{1,4} \cup U_{3,5}$. Together with $G' \cong K_{\lceil \frac{n-5}{2}\rceil,\lfloor \frac{n-5}{2}\rfloor}$ and (ii)-(iii), we have $U_{1,3} = \emptyset$. Moreover, (iii) also implies that $|U_{1,4}| = \lceil \frac{n-5}{2} \rceil$, $|U_{3,5}| = \lfloor \frac{n-5}{2} \rfloor$ and each vertex in $U_{1,4}$ is adjacent to all vertices in $U_{3,5}$. It follows that $G^* \cong K_{\lceil \frac{n-1}{2}\rceil,\lfloor \frac{n-1}{2}\rfloor}\bullet K_3$, as desired. □

4. Concluding remarks

In this paper, we first determine the unique graph among the set of $\theta(1,2,3)$-free non-bipartite graphs with order $n \geqslant 20$ having the maximum spectral radius. Then we characterize the unique graph among the set of $\theta(1,2,4)$-free non-bipartite graphs with order $n \geqslant 21$ having the largest spectral radius. At last we identify the unique graph among $\theta(1,2,4)$-free non-bipartite graphs on $n \geqslant 137$ vertices having the maximum number of edges. Unfortunately, all the problems considered in this paper are not completely solved for smaller order n. Probably, with the help of computer we may solve them.

Recently, Zhai and Lin [40] showed that $K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$ is the unique graph among the n-vertex $\theta(1,2,r)$-free graphs having the largest spectral radius for sufficiently large n. Therefore, one sees the extremal graph is independent of the parity of r for sufficiently large n. On the other hand, comparing Theorem 1.1 with Theorem 1.2 gives us that the graph among the n-vertex $\theta(1,2,3)$-free non-bipartite graphs having the largest spectral radius is not the same as that among the n-vertex $\theta(1,2,4)$-free non-bipartite having the largest spectral radius. So, it is more interesting and challenging to determine the $\theta(1,2,k)$-free non-bipartite graphs having the largest spectral radius, $k \geqslant 5$. So we propose the following problem.

Problem 1. How to characterize all the graphs among $\theta(1,2,k)$-free non-bipartite graphs with given order having the largest spectral radius for $k \geqslant 5$?

One may wonder whether the method in this paper can be used to solve Problem 1 or not. In fact, our idea for proving Theorems 1.1 and 1.2 is as follows. Firstly, choose a non-bipartite graph G^* such that its spectral radius is as large as possible. Clearly, G^* is connected and there is a Perron vector of G^*, say $\mathbf{x}$. Then let u^* be a vertex of G^* such that $x_{u^*} = \max\{x_v : v \in V(G^*)\}$. The most important step is to analyze the structures of $G^*[N(u^*)]$, $G^*[N^2(u^*)]$ and $E(N(u^*), N^2(u^*))$. To show this, we repeatedly use the property that G^* does not contain $\theta(1,2,3)$ or $\theta(1,2,4)$ as a subgraph. In fact, when r is large, it is hard to determine whether $\theta(1,2,r)$ is a subgraph of G^*. So, it is necessary to develop some other techniques to solve Problem 1.

Let $\theta(k) = \{\theta(1,i,j) : i+j = k\}$. Notice that Lan, Shi and Song [19] studied the planar Turán number of $\theta(k)$ for $k \in \{4,5,6\}$. It encourages us to consider the spectral Turán type problem among the set of planar graphs as follows.

Problem 2. How to characterize all the graphs among $\theta(k)$-free (resp. $\theta(1,2,k)$-free) planar graphs with given order having the largest spectral radius for a positive integer k?

We will develop the above study in the near future.

Appendix

The proof of Subcase 4.1. In this subcase, we know that $P_2 = w_1w_2$ is the unique nontrivial component of $G^*[N(u^*)]$ and $|V(G^*) \setminus (N[u^*] \cup U_0)| = 1$. We also find that $|H_0| \geqslant 3$. Otherwise, we have

$$\begin{aligned} \beta(u^*) &\leqslant |H_0| + 4 + |U_0|(|H_0| + 2) + 2 = (|U_0| + 1)(|H_0| + 2) + 4 \\ &\leqslant 4(n-6) + 8 < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1, \end{aligned}$$

a contradiction.

Next we show the following claim.

Claim 4.1. $e(U_0) = 0$.

Proof of Claim 4.1. Suppose that $e(U_0) \geqslant 1$ and let uv be an edge in $G^*[U_0]$. Define

$$B_i = \{w \in U_0 \setminus \{u, v\} : N(w) \cap \{w_1, w_2\} = \{w_i\}\} \text{ for } i \in \{1, 2\}$$

and

$$B_3 = \{w \in U_0 \setminus \{u, v\} : N(w) \cap \{w_1, w_2\} = \{w_1, w_2\}\}.$$

Denote $t_i = |\{u : u \in N(B_1) \cap V(H_0)\}|$ for $i \in \{1, 2, 3\}$ and assume $t_1 \geqslant t_2$. If $|B_1 \cup B_2 \cup B_3| = 0$, then by (3.8), one has

$$\begin{aligned}\beta(u^*) &\leqslant |H_0| + 4 + (|U_0| - 2)|H_0| + |H_0| + 3 + 2 = |U_0||H_0| + 9\\ &\leqslant \left\lfloor \frac{(n-4)^2}{4} \right\rfloor + 9 < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,\end{aligned}$$

a contradiction to (3.7). Thus, $|B_1 \cup B_2 \cup B_3| \geqslant 1$. Therefore, together with (3.8) one has

$$\begin{aligned}\beta(u^*) &\leqslant |H_0| + 4 + \sum_{i=1}^{2} |B_i|(t_i + 1) + 2|B_3| + t_3\\ &\quad + (|U_0| - |B_1 \cup B_2 \cup B_3| - 2)|H_0| + |H_0| + 3 + 2\\ &\leqslant (|B_1 \cup B_2 \cup B_3| - 1)(t_1 + 1) + |B_3|\\ &\quad + (|U_0| - |B_1 \cup B_2 \cup B_3| + 1)|H_0| + 10\\ &\leqslant |U_0||H_0| - (|B_1 \cup B_2 \cup B_3| - 1)(|H_0| - t_1 - 1) + |B_3| + 10\\ &\leqslant |U_0||H_0| + (|B_1 \cup B_2 \cup B_3| - 1) + |B_3| + 10\\ &\leqslant |U_0||H_0| + 2|U_0| + 9\\ &\leqslant \left\lfloor \frac{(n-2)^2}{4} \right\rfloor + 9 < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,\end{aligned}$$

a contradiction. It follows that $e(U_0) = 0$. □

Together with Claim 4.1 and the fact that G^* is $\theta(1, 2, 4)$-free, one has $e(N^2(u^*)) = 0$. Let

$$B_i' = \{w \in U_0 : N(w) \cap \{w_1, w_2\} = \{w_i\}\} \text{ for } i \in \{1, 2\}$$

and

$$B_3' = \{w \in U_0 : N(w) \cap \{w_1, w_2\} = \{w_1, w_2\}\}.$$

Denote $t_i' = |\{u : u \in N(B_1') \cap V(H_0)\}|$ for $i \in \{1, 2, 3\}$ and assume $t_1' \geqslant t_2'$. By a similar discussion as above, one has $|B_1' \cup B_2' \cup B_3'| \geqslant 1$. If $t_1' \geqslant 1$, then

$$\begin{aligned}\beta(u^*) &\leqslant |H_0| + 4 + \sum_{i=1}^{2} |B_i'|(t_i' + 1) + 2|B_3'| + t_3'\\ &\quad + (|U_0| - |B_1' \cup B_2' \cup B_3'|)|H_0| + 2\\ &\leqslant (|U_0| + 1)|H_0| - (|B_1' \cup B_2' \cup B_3'| - 1)(|H_0| - t_1' - 1) + 7\end{aligned}$$

$$\begin{aligned}
&\leqslant (|U_0|+1)|H_0| + (|B_1' \cup B_2' \cup B_3'| - 1) + 7 \\
&\leqslant (|U_0|+1)(|H_0|+1) + 6 \\
&\leqslant \left\lfloor \frac{(n-2)^2}{4} \right\rfloor + 6 < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,
\end{aligned}$$

a contradiction. Therefore, $t_1' = 0$ and so $t_2' = 0$. Together with Claim 3.1 and $e(N^2(u^*)) = 0$, one has $|B_1'| = |B_2'| = 0$. Recall that $|H_0| \geqslant 3$. Thus,

$$\begin{aligned}
\beta(u^*) &\leqslant |H_0| + 4 + 2|B_3'| + t_3' + (|U_0| - |B_3'|)|H_0| + 2 \\
&\leqslant (|U_0|+1)|H_0| + |B_3'|(2 - |H_0|) + t_3' + 6 \\
&\leqslant (|U_0|+1)|H_0| + t_3' + 6 \\
&\leqslant (|U_0|+1)(|H_0|+1) + 5 \\
&\leqslant \left\lfloor \frac{(n-2)^2}{4} \right\rfloor + 5 < \left\lfloor \frac{(n-1)^2}{4} \right\rfloor + 1,
\end{aligned}$$

which is also a contradiction. □

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