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On the spectral characterization of theta graphs

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Abstract

The *θ-graph*, denoted by $\theta_{i,j,k}$, is a graph consisting of two given vertices joined by three paths whose order is $i+2$, $j+2$ and $k+2$ respectively, with any two of these paths having only the given vertices in common. It is well-know that the problem of spectral characterization is related to the Hückel theory from Chemistry. In the paper we will show that the θ-graphs containing odd cycles and without no 4-cycles and the θ-graphs with minimal spectral radius are determined by the adjacency spectrum.

1 Introduction

We first introduce the background of the paper. Two non-isomorphic graphs are said to be *cospectral* if they have equal spectrum (i.e., equal characteristic polynomial). A graph G is said to be *determined by the spectrum* (or G is a *DS-graph* for short) if there is no other non-isomorphic graph with the same spectrum.

It is well-known that the theory of graph spectra is related to the Chemistry through the HMO (Hückel Molecular Orbital) Theory (see [12], for example). At an early stage, it was supposed that HMO Theory could be reduced to the study of graph spectra of the adjacency matrix of molecular graphs (Chemical Graph Theory). In fact in 1956, Günthard and Primas [16] posed the question in a paper that

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relates the theory of graph spectra to the Hückel Theory (see also Chapter 8 in [3] or [4]). From that moment it was believed that each (molecular) graph is determined by the spectrum (of the adjacency matrix), since different physical properties of molecules would take to different values of the spectra. In 1957, Collatz and others (see Chapter 6 in [3] or Section 4.6 in [10]) reported several examples of non isomorphic graphs having the same spectrum (later such pairs were called PINGs, Pair of Isospectral Non-isomorphic Graphs) and in 1973 Živković (see also [23]) found the first PING based on chemical graphs: 1,4-divinylbenzene and 2-phenylbutadiene have all 10 eigenvalues equal when looking to the adjacency matrix of corresponding molecular graphs (with hydrogen atoms suppressed). Then the question "which graphs are determined by their spectrum" dates from about half a century and it originates from Chemistry. Actually, there are few results known about DS-graphs, and determining what kinds of graphs are DS is yet far from resolved. The recent developments about DS-graphs are summarized in two excellent surveys in [5, 6].

In the paper all graphs considered are simple and undirected. Let $G = (V(G), E(G))$ be a graph with vertex set $V(G) = \{v_1, v_2, \cdots, v_n\}$ and edge set $E(G)$, where its order and size are $|V(G)| = n(G) = n$ and $|E(G)| = m(G) = m$ respectively. Let matrix $A(G)$ be the (0,1)-*adjacency matrix* of G and $d_G(v_k) = d_k$ the degree of the vertex v_k. The polynomial $\phi(G, \lambda) = \mathrm{d}et(\lambda I - A(G))$ or simply $\phi(G)$, where I is the identity matrix, is defined as the *characteristic plolynomial* of the graph G. Since matrix $A(G)$ is real and symmetric, its eigenvalues are all real numbers. Assume that $\lambda_1(G) \geq \lambda_2(G) \cdots \geq \lambda_n(G)$ are the *adjacency eigenvalues* of the graph G, where the maximum eigenvalue $\lambda_1(G)$ is called the *spectral radius* or *index* of G. The *adjacency spectrum* (or simply *adj-spectrum*) of a graph G, denoted by Spec(G), is the multiset of its adjancency eigenvalues. By $[G]_\phi$ we denote the *cospectral class* consisting of the graphs cospectral with a given graph G. Now, we pose the Spectral Characterization Problem (SCP) of a graph G as follows:

SCP1 : *Is G a DS-graph?*

SCP2 : *If G is not a DS-graph, can we determine $[G]_\phi$?*

As far as we know, there are fewer results about SCP2 of graphs. The authors of [27, 28] obtained the cospectral classes of some special graphs. In this paper, we pose our attention on SCP1 of θ-graphs, and prove that the θ-graphs containing odd cycles (i.e., cycles with odd order) and without 4-cycles and the θ-graphs with minimal index are determined by the adj-spectrum. Some other notations and terminology are also needed:

(i) let C_n, P_n and W_n be respectively the *cycle*, the *path* and the *double-snake* of order n. C_n is called a n*-cycle*.

(ii) The θ*-graph*, denoted by $\theta_{i,j,k}$ is a graph consisting of two given vertices joined by three paths whose order is $i+2$,$j+2$ and $k+2$ respectively, with any two of these paths having only the given vertices in common (see Fig. 1). Due to the symmetry, let us consider $k \geq j \geq i \geq 0$, with $(i,j) \neq (0,0)$.

(iii) The *dumbbell graph*, denoted by $D_{a,b,c}$, consists of two vertex-disjoint cycles C_a, C_b and a path P_{c+1} joining them having only its end-vertices in common with the cycles (see Fig. 1). By symmetry, consider $b \geq a \geq 3$ and $c \geq -1$.

(iv) The *lollipop graph*, denoted by $H_{n,p}$, is obtained by appending a cycle C_p to a pendant vertex of a path P_{n-p} (see Fig. 1).

(v) For two graphs G and H, $G \cup H$ denotes the disjoint union of G and H, and kG stands for the disjoint union of k copies of G.

(vi) Let $T_{a,b,c}$ denote the tree with exactly one vertex v having maximum degree 3 such that $T_{a,b,c} - v = P_a \cup P_b \cup P_c$.

(vii) A property of a graph G is called a *cospectral invariant* if $\phi(H) = \phi(G)$ implies that the graph H shares the same property.

(viii) A graph G is said to be *bicyclic* if it contains only two independent cycles. If G is connected, then G is bicyclic if and only if $m(G) = n(G) + 1$.

(ix) A graph G is $(r, r+1)$-*almost regular* if $V(G)$ can be partitioned into two subsets V_1 and V_2 such that $d(v_i) = r$ for $v_i \in V_1$ and $d(v_i) = r+1$ for $v_i \in V_2$.

The graphs belonging to Fig.1 are relevant in Chemistry. For instance, some chemical graphs are θ-graphs: $\theta_{0,4,4}$ is the naphithalene graph, $\theta_{0,3,5}$ is the azulene graph, $\theta_{0,3,3}$ is the pentalene graph, $\theta_{0,5,5}$ is the heptalene graph. θ-graphs are also considered in [7]. Dumbbells were studied in several papers (see, for example, [7, 9]). A spectral characterization for dumbbells containing an odd cycle is given in [29]; in [15] it was conjectured that the dumbbell graphs with two hexagons has maximal *energy* (sum of the absolute values of the eigenvalues) among all bicyclic molecular graphs; a partial proof of the latter fact is given in [21]. Spectral properties of lollipops are studied in several recent papers [1, 17, 32]. Lollipops emerged in chemical graph theory in the study of unicyclic graphs with maximal energy. It was empirically found in [2] that among n-vertex connected unicyclic bipartite graphs the lollipop with a hexagon has greatest energy, except for n=10 when cycle C_{10} has greatest energy. In [14, 19] it was exactly proven that among n-vertex connected unicyclic bipartite graphs either the lollipop with a hexagon, or the cycle has greatest energy. Until now nobody succeeded to prove that the energy of the lollipop with a hexagon exceeds the energy of the cycle (except for $n = 10$). Other relevant papers concerning lollipops are [7, 8, 13, 20, 26, 31]. In this paper we will study the spectral characterization of a large subset of θ-graphs.

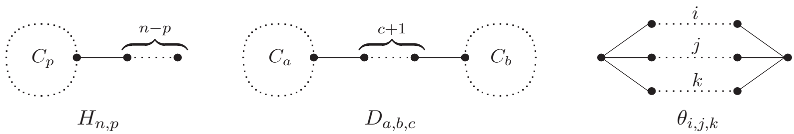


Fig. 1

This paper is organized as follows. In Section 2, some known lemmas will be summarized. In Section 3, a cospectral invariant for $(r, r+1)$-almost regulars will be given. In Section 4, some preparations for the main result will be done. In Section 5, we will prove that the θ-graphs containing odd cycles and without 4-cycles, and that the θ-graphs with minimal index are determined by the adj-spectrum. Finally, in Section 6, we give a conjecture about the spectral characterization of θ-graphs not considered above and a remark on chemical graphs characterized by adj-spectrum.

2 Basic results

Some useful established results about the spectrum are presented in this section, which will play an important role throughout this paper.

Lemma 2.1. [3] *Let H be a proper subgraph of a connected graph G, then $\lambda_1(H) < \lambda_1(G)$.*

Lemma 2.2. [3] *Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1}$ be the eigenvalues of G and $G - v$, respectively. Then $\lambda_1 \geq \mu_1 \geq \lambda_2 \geq \mu_2 \geq \cdots \geq \mu_{n-1} \geq \lambda_n$.*

Lemma 2.3. [3] *Let G be a (simple) graph. Denote by $\mathscr{C}(v)$ ($\mathscr{C}(e)$) the set of all cycles in G containing a vertex v (resp. an edge $e = uv$). Then we have:*

(i) $\phi(G,\lambda) = \lambda\phi(G-v,\lambda) - \sum_{w\sim v}\phi(G-v-w,\lambda) - 2\sum_{C\,\in\,\mathscr{C}(v)}\phi(G-V(C),\lambda);$

(ii) $\phi(G,\lambda) = \phi(G-e,\lambda) - \phi(G-v-u,\lambda) - 2\sum_{C\,\in\,\mathscr{C}(e)}\phi(G-V(C),\lambda).$

We assume that $\phi(G,\lambda) = 1$ if G is the empty graph (i.e. with no vertices).

Lemma 2.4. [5] *For $n \times n$ matrices A and B, the following are equivalent:*

(i) *A and B are cospectral;*

(ii) *A and B have the same characteristic polynomial;*

(iii) $\mathrm{tr}(A^i) = \mathrm{tr}(B^i)$ *for $i = 1, 2, \cdots, n$.*

Lemma 2.5. [3] *Let G be a graph with $\phi(G,\lambda) = \lambda^n + a_1(G)\lambda^{n-1} + \cdots + a_n(G)$. Then the length g of a shortest odd cycle in G is equal to the index of the first non-vanishing coefficient among $a_1(G), a_3(G), a_5(G), \cdots$. The number of shortest odd cycle is equal to $-\frac{1}{2}a_g(G)$.*

If two graphs G and H are cospectral, then by Lemma 2.4 we get $\phi(G) = \phi(H)$ which implies $a_i(G) = a_i(H)$ for $1 \leq i \leq n(G)$. Thus the following corollary follows from Lemma 2.5:

Corollary 2.1. *Let two graphs G and H be cospectral. Then both the length and the number of shortest odd cycles in G and H are the same.*

With respect to the cospectral invariants, we have the following result besides Corollary 2.1:

Lemma 2.6. [5] *Let G and H be two graphs such that $\phi(G) = \phi(H)$. Then*

(i) *$n(G) = n(H)$ and $m(G) = m(H)$;*

(ii) *G is bipartite if and only if H is bipartite;*

(iii) *G is k-regular if and only if H is k-regular;*

(iv) *G is k-regular with girth g if and only if H is k-regular with girth g;*

(v) *G and H have the same number of closed walks of any fixed length.*

Lemma 2.7. [30] *Let r_i and s_i $(i = 1, 2)$ be non-negative integers such that $0 \leq r_1 \leq r_2$, $r_1 \leq s_1 \leq s_2$ and $r_1 + r_2 = s_1 + s_2$. Then*

$$\phi(P_{r_1})\phi(P_{r_2}) - \phi(P_{s_1})\phi(P_{s_2}) = -\phi(P_{s_1-r_1-1})\phi(P_{s_2-r_1-1}).$$

Lemma 2.8. *Let G be a graph of order n, size m and degree sequence $(d_1, d_2, \cdots, d_n)$. If $n_G(C_4)$ denotes the number of cycles C_4 in G, then the number of closed walks of length 4 is*

$$W_4(G) = 2\sum_{i=1}^{n} d_i^2 - 2m + 8n_G(C_4).$$

Proof. Let $n_G(P_3)$ be the number of paths P_3 in G. Then $W_4(G) = 2m + 4n_G(P_3) + 8n_G(C_4)$. Substituting $n_G(P_3) = \sum_{i=1}^{n} \binom{d_i}{2}$ and $\sum_{i=1}^{n} d_i = 2m$, by direct calculation we get the result. $\square$

Simić studied the index of bicyclic graphs in [24, 25]. Next lemma is a subcase of Theorem 1 in [25], it will be useful for proving some main theorems in Section 5.

Lemma 2.9. *Let $n(\theta_{i,j,k})$ and k be fixed. Then $\lambda_1(\theta_{i,j,k})$ is an increasing function in $j - i$.*

Lemma 2.10. [24] *Among all the connected bicyclic graphs of order n, there are precisely two graphs whose index is minimal: one of both is $D_{k,k,n-2k-1}$, while the other is $\theta_{k-1,k-1,n-2k}$, where $k = \lceil \frac{n}{3} \rceil$ and $n \geq 7$.*

The following lemma, reported here in a weaker variant, can be found in [3] p. 58. To state it, we need more definitions. An *internal path* in some graph, denoted by $v_0, v_1, \ldots, v_{k-1}, v_k$, is a path joining vertices v_0 and v_k which are both of degree greater than two (not necessarily distinct), while all other vertices (i.e. $v_1, \ldots, v_{k-1}$) are of degree equal to two.

Lemma 2.11. *Let G' be a graph obtained from a connected graph G by inserting in an edge e, which lies on an internal path, a vertex of degree two. Then, if G is not the tree W_n, $\lambda_1(G') < \lambda_1(G)$. If $G = W_n$, then $\lambda_1(G') = \lambda_1(G) = 2$.*

In view of Lemma 2.11, Lemma 2.10 becomes:

Corollary 2.2. *Among all the connected bicyclic graphs of order less than or equal to n, there are precisely two graphs whose index is minimal: one of both is $D_{k,k,n-2k-1}$, while the other is $\theta_{k-1,k-1,n-2k}$, where $k = \lceil \frac{n}{3} \rceil$ and $n \geq 7$.*

3 A cospectral invariant for $(r, r+1)$-almost regular graphs

To prove that a graph is determined by the spectrum, it is helpful to know more about cospectral invariants. In this section, we provide a new one for $(r, r+1)$-almost regular graphs. The following lemma and theorem were proved in [29] by Lagrange multiplier method and by the coefficients of characteristic polynomial, respectively. Here, by the number of closed walks, we provide another proof for Theorem 3.1.

Lemma 3.1. [29] *Let $(d_1, d_2, \cdots, d_n)$ be the degree sequence of a graph of order n and size m, and $\overline{d}$ the average degree. Then $\sum_{i=1}^{n} d_i^2$ is minimum if and only if*

$$d_1 = \cdots = d_t = \lfloor \overline{d} \rfloor + 1 \quad \textit{and} \quad d_{t+1} = \cdots = d_n = \lfloor \overline{d} \rfloor,$$

where $t = \sum_{i=1}^{n} d_i - n\lfloor \overline{d} \rfloor$. In addition, the minimum value of $\sum_{i=1}^{n} d_i^2$ is $2m\overline{d}$, and it is reachable iff the graph is a regular or $(\lfloor \overline{d} \rfloor, \lfloor \overline{d} \rfloor + 1)$-almost regular graph.

Theorem 3.1. *Let G be a $(r, r+1)$-almost regular graph without cycle C_4 as its subgraph. If H is a graph such that* $\mathrm{Spec}(H) = \mathrm{Spec}(G)$, *then*

(i) *H contains no cycle C_4 as its subgraph;*

(ii) *H is a $(r, r+1)$-almost regular graph with the same degree sequence as G.*

Proof. Since $\mathrm{Spec}(H) = \mathrm{Spec}(G)$, by Lemma 2.6 we get $n(G) = n(H) = n$, $m(G) = m(H) = m$ and $W_4(G) = W_4(H)$, where $W_4(G)$ is the number of closed walks of length 4. Note that G does not contain C_4 as subgraph. By Lemma 2.8 we have

$$2\sum_{i=1}^{n} d_G(v_i)^2 = 2\sum_{i=1}^{n} d_H(v_i)^2 + 8n_H(C_4). \tag{1}$$

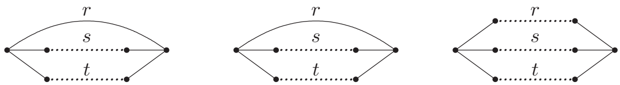
Since G is a $(r, r+1)$-almost regular graph, from Lemma 3.1 we know that the left of (1) is minimum, which implies $n_H(C_4)$ must be zero. Then H does not contain C_4 as its subgraph too, and, by Lemma 3.1, H is a regular or $(r, r+1)$-almost regular graph with the same degree sequence as G. From Lemma 2.6(iii) H cannot be a regular graph. Hence the required result follows. □

4 Structural properties of θ-graphs

The following lemma is trivial but fundamental, it follows from simple observations. It classifies all the θ-graphs $\theta_{r,s,t}$ (recall that $(r,s) \neq (0,0)$) by the number of the shortest odd cycles contained in $\theta_{r,s,t}$. Note that $\theta_{r,s,t}$ contains no odd cycles iff r, s and t have the same parity; $\theta_{r,s,t}$ contains two odd cycles in the remaining cases.

Lemma 4.1. *Under the convention that $t \geq s \geq r \geq 0$, graph $\theta_{r,s,t}$ contains at most two shortest odd cycles C_g. In addition,*

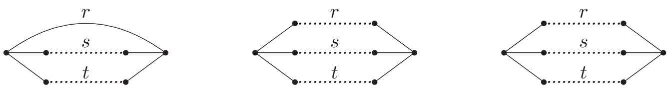
(i) *The θ-graphs containing exactly one shortest odd cycle C_g are graphs $\theta_{r,s,t}$ depicted below:*



$r = 0 < s < t$, $s = g-2$, Type A | $r = 0 < s < t$, $t = g-2$, Type B | $0 < r < s < t$, Condition *1*, Type C

where s and t have the opposite parity in Type B and Condition *1 means that $r+s+2 = g$ (or $r+t+2 = g$, when r and s have the same parity).*

(ii) *The θ-graphs containing two shortest odd cycles C_g are graphs $\theta_{r,s,t}$ depicted below:*



$r = 0 < s = t$, $s = g-2$, Type D | $0 < r = s < t$, $r+t+2 = g$, Type E | $0 < r < s = t$, $r+s+2 = g$, Type F

Lemma 4.2. [11] *$\phi(P_n, 2) = n+1$ and $\phi(T_{a,b,c}, 2) = a+b+c+2-abc$.*

Lemma 4.3. *Let $k \geq j \geq i \geq 0$, then $2 \in \mathrm{Spec}(\theta_{i,j,k})$ if and only if $(i,j,k) \in \mathscr{S} =$* $\{(2,6,41),(2,7,23),(2,8,17),(2,9,14),(2,11,11),(3,4,19),(3,5,11),(3,7,7),$ $(4,4,9),(5,5,5)\}$.

In addition, 2 is a simple root.

Proof. By Lemma 2.3 we get that

$$\phi(\theta_{i,j,k}) = \lambda\phi(T_{i,j,k}) - (\phi(T_{i-1,j,k}) + \phi(T_{i,j-1,k}) + \phi(T_{i,j,k-1})) - 2(\phi(P_i) + \phi(P_j) + \phi(P_k)),$$

which implies from Lemma 4.2 that

$$\phi(\theta_{i,j,k}, 2) = ijk - (ij + ik + jk) - 3(i + j + k) - 5. \tag{2}$$

Thus, $2 \in \mathrm{Spec}(\theta_{i,j,k})$ iff $ijk - (ij + ik + jk) - 3(i + j + k) - 5 = 0$ which leads to

$$k = \frac{ij + 3(i + j) + 5}{ij - (i + j) - 3} = \frac{1 + 3(\frac{1}{i} + \frac{1}{j}) + \frac{5}{ij}}{1 - (\frac{1}{i} + \frac{1}{j}) - \frac{3}{ij}} \tag{3}$$

implying that k is the strictly decrease function of i and j. Thus, for $k \geq j \geq i \geq 6$, we obtain that the maximum of k is attained when $i = j = 6$. From (3) we get $k \leq 77/21 \approx 3.7$ contradicting $k \geq 6$, then $2 \notin \mathrm{Spec}(\theta_{i,j,k})$. Next we only need to consider the cases $0 \leq i \leq 5$:

Case 1. $i = 0$. By (2) we get $\phi(\theta_{0,j,k}, 2) = -jk - 3(j + k) - 5 < 0$ and so $2 \notin \mathrm{Spec}(\theta_{0,j,k})$.

Case 2. $i = 1$. By (2) we get $\phi(\theta_{1,j,k}, 2) = -2j - 2 < 0$ and so $2 \notin \mathrm{Spec}(\theta_{1,j,k})$.

Case 3. $i = 2$. By (3) we get $k = \frac{5j+11}{j-5}$ which, together with $k \geq j \geq 2$, implies that $j^2 - 10j - 11 \leq 0$, i.e., $2 \leq j \leq 11$. Note that j and k are integers. A direct calculation shows that $(2, 6, 41), (2, 7, 23), (2, 8, 17), (2, 9, 14), (2, 11, 11) \in \mathscr{S}$.

Case 4. $i = 3$. By (3) we get $k = \frac{3j+7}{j-3}$ which, together with $k \geq j \geq 3$, implies that $j^2 - 6j - 7 \leq 0$, i.e., $3 \leq j \leq 7$. A direct calculation shows that $(3, 4, 19), (3, 5, 11), (3, 7, 7) \in \mathscr{S}$.

Case 5. $i = 4$. By (3) we get $k = \frac{7j+17}{3j-7}$ which, together with $k \geq j \geq 4$, implies that $3j^2 - 14j - 17 \leq 0$, i.e., $4 \leq j \leq 17/3$. A direct calculation shows that $(4, 4, 9) \in \mathscr{S}$.

Case 6. $i = 5$. By (3) we get $k = \frac{2j+5}{j-2}$ which, together with $k \geq j \geq 5$, implies that $j^2 - 4j - 5 \leq 0$, i.e., $j = 5$. Thus, $k = 5$ and so $(5, 5, 5) \in \mathscr{S}$.

Now we show the second assertion. Let u and v denote the vertices of degree 3 in $\theta_{i,j,k}$ respectively. By Lemma 2.2 we get

$$\lambda_1(\theta_{i,j,k}) \geq \lambda_1(\theta_{i,j,k} - u) \geq \lambda_2(\theta_{i,j,k}) \geq \lambda_2(\theta_{i,j,k} - u) \geq \lambda_3(\theta_{i,j,k})$$

and

$$\lambda_3(\theta_{i,j,k}) \leq \lambda_2(\theta_{i,j,k} - u) \leq \lambda_1(\theta_{i,j,k} - u - v) = \lambda_1(P_i \cup P_j \cup P_k).$$

Since $\theta_{i,j,k}$ contains cycles (whose index is 2) as its proper subgraphs and $\lambda_1(P_n) < 2$, from the above two inequalities and Lemma 2.1 we have $\lambda_1(\theta_{i,j,k}) > \lambda_2(\theta_{i,j,k}) = 2 > \lambda_3(\theta_{i,j,k})$. This completes the proof. □

Lemma 4.4. $\mathrm{Spec}(\theta_{0,j,k}) = \mathrm{Spec}(\theta_{0,s,t})$ *if and only if* $(j,k) = (s,t)$.

Proof. We need only to show the necessary condition. Assume, for contradiction, that $(j,k) \neq (s,t)$. Since $\phi(\theta_{0,j,k}) = \phi(\theta_{0,s,t})$, from Lemma 2.6(i) we get $j+k = s+t$. Without loss of generality, set $j > s$ and so $s < j \leq k < t$. By Lemma 2.3 we have

$$\phi(\theta_{0,j,k}) = \phi(C_{j+k+2}) - \phi(P_j)\phi(P_k) - 2(\phi(P_j) + \phi(P_k)),$$

and

$$\phi(\theta_{0,s,t}) = \phi(C_{s+t+2}) - \phi(P_s)\phi(P_t) - 2(\phi(P_s) + \phi(P_t)).$$

From the above two equalities, it follows that

$$\phi(P_s)\phi(P_t) - \phi(P_j)\phi(P_k) = 2(\phi(P_j) + \phi(P_k) - \phi(P_s) - \phi(P_t)),$$

which implies from Lemma 2.7 that

$$\phi(P_{j-s-1})\phi(P_{k-s-1}) = 2(\phi(P_t) + \phi(P_s) - \phi(P_k) - \phi(P_j)).$$

Note, the degree of both sides of above equality is equal and so $j + k - 2s - 2 = t$ which, together with $j + k = s + t$, leads to $s = -2$. This is impossible. □

Lemma 4.5. *If* $\theta_{0,j,k}$ *is the graph of Type A or B, then* $\mathrm{Spec}(\theta_{0,j,k}) \neq \mathrm{Spec}(\theta_{r,s,t})$, *where* $r > 0$.

Proof. We only consider $\theta_{0,j,k}$ as a graph of Type A, i.e., $\theta_{0,j,k} = \theta_{0,g-2,k}$ (the other case can be proved similarly). Assume, for contradiction, that $\mathrm{Spec}(\theta_{0,j,k}) = \mathrm{Spec}(\theta_{r,s,t})$. Under the hypothesis, we get that $\theta_{0,j,k}$ contains exactly one shortest odd g-cycle, so $\theta_{r,s,t}$ does by Corollary 2.1, and thus $\theta_{r,s,t}$ is of Type C by Lemma 4.1, where $r + s + 2 = g$ (or $r + t + 2 = g$). If $r + s + 2 = g$ (or $r + t + 2 = g$), from $g + k = n(\theta_{0,j,k}) = n(\theta_{r,s,t}) = g + t$ (or $g + s$) we have $k = t$ (or $k = s$). Since $g - 2 = r + s > s - r$ (or $g - 2 = r + t > t - r$), by Lemma 2.9 we conclude that $\lambda_1(\theta_{0,g-2,k}) > \lambda_1(\theta_{r,s,k})$ (or $\lambda_1(\theta_{0,g-2,k}) > \lambda_1(\theta_{r,k,t})$), a contradiction. □

Lemma 4.6. *Suppose that $\theta_{i,j,k}$ contains at least one odd cycle of length g, then* $\mathrm{Spec}(\theta_{i,j,k}) \neq \mathrm{Spec}(D_{a,b,c})$.

Proof. Assume, for contradiction, that $\mathrm{Spec}(\theta_{i,j,k}) = \mathrm{Spec}(D_{a,b,c})$. By Lemma 2.6 we get that $\theta_{i,j,k}$ and $D_{a,b,c}$ have the same order and the same number of closed walks of a given length l (such a closed walk is called a *l-tour* in [17]). Since $\theta_{i,j,k}$ has at most two shortest odd cycles C_g (see Lemma 4.1), by Corollary 2.1 it is also true for the graph $D_{a,b,c}$, and so we can set $b \geq a = g$.

There are two types of $(g+2)$-tours in $D_{g,b,c}$. Tours around the cycle C_g where one edge is used three times (there are precisely $2g^2$ (if $b \neq g$) or $4g^2$ (if $b = g$) of these), and tours around C_g that go one step up and down the edge $e = uv$, where e is the edge not contained in C_g such that $d(u) = 3$, $u \in V(C_g)$ and $v \notin V(C_g)$ (there are $2(g+2)$ such $(g+2)$-tours if $b \neq g$ or $4(g+2)$ if $b = g$). Thus the total number τ of $(g+2)$-tours in $D_{g,b,c}$ is

$$\tau_1 = \begin{cases} 2g^2 + 2(g+2) & \text{if } b \neq g; \\ 4g^2 + 4(g+2) & \text{if } b = g. \end{cases} \tag{4}$$

With the similar method, the number of $(g+2)$-tours in the θ-graphs $\theta_{i,j,k}$ is

$$\tau_2 = \begin{cases} 2g^2 + 4(g+2) & \text{if } \theta_{i,j,k} \text{ contains one } C_g; \\ 4g^2 + 8(g+2) & \text{if } \theta_{i,j,k} \text{ contains two } C_g. \end{cases} \tag{5}$$

Obviously, $\tau_1 \neq \tau_2$ which is a contradiction. □

Lemma 4.7. *For $l \geq 1$,* $\mathrm{Spec}(\theta_{l,l,l}) \neq \mathrm{Spec}(D_{l+1,l+1,l-1})$.

Proof. Assume, for contradiction, that $\phi(D_{l+1,l+1,l-1}) = \phi(\theta_{l,l,l})$. Thus

$$\phi(D_{l+1,l+1,l-1}, 2) = \phi(\theta_{l,l,l}, 2). \tag{6}$$

By Lemma 2.3 we get that

$$\phi(D_{l+1,l+1,l-1}) = \phi(C_{l+1})\phi(H_{2l+1,l+1}) - \phi(P_l)\phi(C_{l+1})\phi(P_{l-1}) + \phi(P_l)^2\phi(P_{l-2})$$

and

$$\phi(\theta_{l,l,l}) = \lambda\phi(T_{l,l,l}) - 3\phi(T_{l-1,l,l}) - 6\phi(P_l),$$

which shows from Lemma 4.2 that

$$\phi(D_{l+1,l+1,l-1},2) = (l+1)^2(l-1) \quad \text{and} \quad \phi(\theta_{l,l,l},2) = l^3 - 3l^2 - 9l - 5. \tag{7}$$

By (6) and (7) we get $(l+1)^2(l-1) = l^3 - 3l^2 - 9l - 5$ which implies that $l = -1$, a contradiction. This completes the proof. □

5 Main results

5.1 The θ-graphs containing odd cycles and without 4-cycles are determined by the adj-spectrum

The main results of this subsection is the following theorem:

Theorem 5.1. *The θ-graphs containing odd cycles and without 4-cycles are determined by the adj-spectrum.*

We prove the above theorem in two steps . Firstly, we show that the θ-graphs with eigenvalue 2 are determined by the adj-spectrum (see Theorem 5.2). Secondly, we show that the θ-graphs without eigenvalue 2 are determined by the adj-spectrum (see Theorems 5.3-5.6). The following lemma restricts the structure of graphs cospectral with θ-graphs:

Lemma 5.1. *Let G be a graph cospectral with $\theta_{i,j,k}$ not containing C_4, then $G \cong D_{a,b,c} \bigcup_{z\in Z} C_z$ or $G \cong \theta_{r,s,t} \bigcup_{z\in Z} C_z$, where Z is a finite subset of $\{n \in \mathbb{N} \mid n \geq 3\}$.*

Proof. If G is a graph cospectral with $\theta_{i,j,k}$ then $m(G) = m(\theta_{i,j,k})$ and $n(G) = n(\theta_{i,j,k})$, so we get that $m(G) = n(G) + 1$. Since $\theta_{i,j,k}$ is a $(2,3)$-almost regular graph, then G is a $(2,3)$-almost regular graph by Theorem 3.1. By combining the above facts we get the assertion. □

Theorem 5.2. *Let $(i,j,k) \in \mathscr{S} \backslash \{(3,5,11),(3,7,7),(5,5,5)\}$, where $\mathscr{S}$ is defined in Lemma 4.3. Then $\theta_{i,j,k}$ is determined by the adj-spectrum.*

Proof. We just prove the case $(i,j,k) = (4,4,9)$. The remaining cases can be proved similarly. Let G be any graph cospectral with $\theta_{4,4,9}$, so by Lemma 5.1 G consists of a θ-graph with some cycles or a dumbbell graph with some cycles and C_4 is not a subgraph in both cases. From Lemma 4.3, we know that $2 \in \mathrm{Spec}(\theta_{4,4,9})$ with multiplicity one. Then G is one of the following graphs:

$$G \cong D_{a,b,c} \cup hC_z \quad \text{or} \quad G \cong \theta_{r,s,t} \cup hC_z, \tag{8}$$

where h is an integer with $h \leq 1$. Using the computer package *NewGraph* [22] (or similar programs), we find that $-2 \notin \mathrm{Spec}(\theta_{4,4,9})$, and thus C_z is odd cycle (i.e., z is odd). Since $\theta_{4,4,9}$ contains two shortest odd cycle C_{15}, so G does by Corollary 2.1. Thus, $15 \leq z < n(G) = 19$. Using *NewGraph* again, we obtain for $z = 15, 17$ that $\phi(C_z) \not| \phi(\theta_{4,4,9})$ which implies that $h = 0$. Thus $G \cong D_{a,b,c}$ or $G \cong \theta_{r,s,t}$ by (8). Note that G and $\theta_{4,4,9}$ have the same number of 17-tours. Then $G \cong D_{a,b,c}$ is impossible by (4) and (5). For the case $G \cong \theta_{r,s,t}$, since $2 \in \mathrm{Spec}(G) = \mathrm{Spec}(\theta_{r,s,t})$, then $\theta_{r,s,t}$ is one of the graphs in the set $\mathscr{S}$, and thus $\theta_{r,s,t} \cong \theta_{4,4,9}$ by $n(G) = 19$.

This completes the proof. $\square$

Theorem 5.3. *Let $\theta_{0,j,k}$ be the graph of Type A or B. If it contains no 4-cycles, then it is determined by the adj-spectrum.*

Proof. Let G be an any graph cospectral with $\theta_{0,j,k}$, so G is a graph of Lemma 5.1. In addition, G and $\theta_{0,j,k}$ have the same number of l-tours and does not have cycle C_4 as its subgraph, since $\theta_{0,j,k}$ is such a graph. Furthermore, by Lemma 4.3, $\theta_{0,j,k}$ does not have 2 as eigenvalue, then G must be one of the following graphs:

$$G \cong D_{a,b,c} \quad \text{or} \quad G \cong \theta_{r,s,t}.$$

By Lemma 4.6 we know that the former case cannot hold. For the latter case, since $\theta_{0,j,k}$ merely contains one shortest odd g-cycle, then by Corollary 2.1 we have that $\theta_{r,s,t}$ also has one g-cycle, and thus $\theta_{r,s,t}$ is one of the graphs shown in Lemma 4.1(i). If $\theta_{r,s,t}$ is of Type A or B, then by Lemma 4.4 we obtain that $\theta_{r,s,t} \cong \theta_{0,j,k}$. If $\theta_{r,s,t}$ is of Type C, by Lemma 4.5 we know that it is impossible. $\square$

Theorem 5.4. *Let $\theta_{0,j,k}$ be the graph of Type D (i.e, $j = k = g - 2$). If it contains no 4-cycles, then it is determined by the adj-spectrum.*

Proof. Let G be an any graph cospectral with $\theta_{i,j,k}$. By the same analysis as in

Theorem 5.3, we obtain that

$$G \cong D_{a,b,c} \quad \text{or} \quad G \cong \theta_{r,s,t}.$$

By Lemma 4.6 we know that the former case cannot hold. For the latter case, since $\theta_{0,j,k}$ contains two shortest odd g-cycle, then by Corollary 2.1 we have that $\theta_{r,s,t}$ also has two g-cycles, and thus $\theta_{r,s,t}$ is one of the graphs shown in Lemma 4.1(ii). If $\theta_{r,s,t}$ is of Type E (or F), then by $2g-2 = n(\theta_{0,j,k}) = n(\theta_{r,s,t}) = g+s$ (or $g+t$), and so $s = g-2$ (or $t = g-2$) which implies that $t = 0$ (or $r = 0$), a contradiction. If $\theta_{r,s,t}$ is of Type D, then $\theta_{r,s,t} \cong \theta_{0,j,k}$, by Lemma 4.4. This ends the proof. □

Theorem 5.5. *Let $\theta_{i,j,k}$ be a graph of Type C such that $(i,j,k) \notin \mathscr{S}$. If it contains no 4-cycles, then it is determined by the adj-spectrum.*

Proof. Let G be an any graph cospectral with $\theta_{i,j,k}$. By the same analysis as in Theorem 5.3, we get that G is one of the following graphs:

$$G \cong D_{a,b,c} \quad \text{or} \quad G \cong \theta_{r,s,t}.$$

Note that G and $\theta_{i,j,k}$ have the same number of l-tours. Since $\theta_{i,j,k}$ contains exactly one shortest odd g-cycle C_g, so G does. We consider the following two cases:

Case 1. $G \cong D_{a,b,c}$. Since $D_{a,b,c}$ contains one shortest cycle C_g, then $b > a = g$ and thus the number of $(g+2)$-tour is τ_1 which is not equal to τ_2 (see (4) and (5)).

Case 2. $G \cong \theta_{r,s,t}$. Note that $\theta_{i,j,k}$ is the graph of Type C. Then $k > j > i > 0$ and $i+j+2 = g$ or $i+k+2 = g$. Next we only consider $i+j+2 = g$ (the latter case can be proved similarly). Since $\theta_{r,s,t}$ contains one shortest cycle C_g, then $\theta_{r,s,t}$ is one of the graphs shown in Lemma 4.1(i). If $\theta_{r,s,t}$ is a graph of Type A (or B), by Lemma 4.5 we get $\mathrm{Spec}(\theta_{r,s,t}) \neq \mathrm{Spec}(\theta_{i,j,k})$, a contradiction. If $\theta_{r,s,t}$ is the graph of Type C, we get $t > s > r > 0$ and $r+s+2 = g$ (or $r+t+2 = g$). From $g+k = n(\theta_{i,j,k}) = n(G) = g+t$ (or $g+s$) we get $k = t$ (or $k = s$). Since $\lambda_1(\theta_{i,j,k}) = \lambda_1(\theta_{r,s,t})$, then we obtain by Lemma 2.9 that $j-i = s-r$ (or $t-r$) which, together with $j+i = g-2 = s+r$ (or $t+r$), leads to $i = r, j = s$ (or $i = t, j = r$). Thus we get $\theta_{r,s,t} \cong \theta_{i,j,k}$ (or a contradiction, since $j > i$ and $t > r$).

This ends the proof. □

Theorem 5.6. *Let $\theta_{i,j,k}$ be a graph of Type E or F such that $(i,j,k) \notin \mathscr{S}$. If it contains no 4-cycles, then it is determined by the adj-spectrum.*

Proof. We only prove the theorem for Type E (the proof is analogous for Type F). Note, $0 < i = j < k$ and $i + k + 2 = g$. Let G be a graph cospectral with $\theta_{i,i,k}$. By the same analysis as in Theorem 5.3 we get that G is one of the following graphs:

$$G \cong D_{a,b,c} \quad \text{or} \quad G \cong \theta_{r,s,t}.$$

Note that G and $\theta_{i,i,k}$ have the same number of l-tours. Since $\theta_{i,i,k}$ contains exactly two shortest odd g-cycle C_g, so G does. The following cases are taken into account:

Case 1. $G \cong D_{a,b,c}$. Since $D_{a,b,c}$ contains exactly two shortest odd cycles C_g, then $b = a = g$ and thus the number of $(g+2)$-tour is τ_1 which is not equal to τ_2 by (4) and (5).

Case 2. $G \cong \theta_{r,s,t}$. Since $\theta_{r,s,t}$ contains exactly two shortest odd cycles C_g, then $\theta_{r,s,t}$ is the graph of Type E (or F), and so $0 < r = s < t$ and $r + t + 2 = g$ (or $0 < r < s = t$ and $r + s + 2 = g$). By $g + i = n(\theta_{i,i,k}) = n(\theta_{r,s,t}) = g + r$ (or $g + s$), we get that $i = r$ (or $i = s$), and thus $k = t$ (or $k = r$). Hence, we get $\theta_{r,s,t} \cong \theta_{i,i,k}$ (or a contradiction, since $i < k$ and $s > r$). This ends the proof. □

5.2 The θ-graphs with minimal index are determined by the adj-spectrum

Theorem 5.7. *The θ-graphs with minimal index are determined by the adj-spectrum.*

Proof. From Lemma 2.10 we know that, for any fixed order n, the θ-graphs with minimal index are the graphs of type $\theta_{k-1,k-1,n-2k}$, where $k = \lceil \frac{n}{3} \rceil$ and $n \geq 7$. Let G be any graph such that $\phi(G) = \phi(\theta_{k-1,k-1,n-2k})$. Note that $\theta_{k-1,k-1,n-2k}$ contains no cycle C_4 as its subgraph. From Lemma 5.1, we get that:

$$G \cong D_{a,b,c} \bigcup_{z \in Z} C_z \quad \text{or} \quad G \cong \theta_{r,s,t} \bigcup_{z \in Z} C_z, \tag{9}$$

where $|D_{a,b,c}| \leq n$ and $|\theta_{r,s,t}| \leq n$. Since $\theta_{k-1,k-1,n-2k}$ contains a cycle as its proper subgraph, then $\lambda_1(\theta_{k-1,k-1,n-2k}) > 2$, which implies that

$$\lambda_1(G) = \lambda_1(D_{a,b,c}) \quad \text{or} \quad \lambda_1(G) = \lambda_1(\theta_{r,s,t}).$$

Note that $\lambda_1(G) = \lambda_1(\theta_{k-1,k-1,n-2k})$ is minimal among all the bicyclic graphs of order less than or equal to n by Corollary 2.2, which leads to

$$D_{a,b,c} \cong D_{k,k,n-2k-1} \quad \text{or} \quad \theta_{r,s,t} \cong \theta_{k-1,k-1,n-2k}.$$

Since $n(\theta_{k-1,k-1,n-2k}) = n(G) = n$, then $Z = \emptyset$ and

$$G \cong D_{k,k,n-2k-1} \quad \text{or} \quad G \cong \theta_{k-1,k-1,n-2k}.$$

To complete the proof, it is enough to show that the former case is impossible. Let n take over all the integers not less than 7, i.e., $n \in \{3l, 3l+1, 3l+2\}$.

Let $n = 3l$ or $3l+1$. It is easy to see that $\theta_{k-1,k-1,n-2k}$ has the shortest odd cycle C_{2l+1}. By Lemma 2.1 we know that there is such a cycle C_{2l+1} in the graph $D_{k,k,n-2k-1}$. This is impossible, since the longest cycle in $D_{k,k,n-2k-1}$ is C_{l+1}.

Let $n = 3l+2$, then $\theta_{k-1,k-1,n-2k} = \theta_{l,l,l}$ and $G \cong D_{k,k,n-2k-1} \cong D_{l+1,l+1,l-1}$. From Lemma 4.7 we get $\mathrm{Spec}(\theta_{l,l,l}) \neq \mathrm{Spec}(D_{l+1,l+1,l-1})$, a contradiction. $\square$

6 Final remarks

We proved that θ-graphs containing odd cycles and without 4-cycle and θ-graphs with minimal index are determined by the adj-spectrum. Are all of the θ-graphs determined by the adj-spectrum? The answer might be affirmative.

Conjecture 1. *All θ-graphs are determined by the adj-spectrum.*

We observe that by Theorem 5.1 the azulene graph ($\theta_{0,3,5}$), the pentalene graph ($\theta_{0,3,3}$) and the heptalene graph ($\theta_{0,5,5}$) are determined by the adj-spectrum.

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