axioms

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Spectral Invariants and Their Application on Spectral Characterization of Graphs

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Abstract: In this paper, we give a method to characterize graphs determined by their adjacency spectrum. At first, we give two parameters $\Pi_1(G)$ and $\Pi_2(G)$, which are related to coefficients of the characteristic polynomial of graph G. All connected graphs with $\Pi_1(G) \in \{1, 0, -1, -2, -3\}$ and $\Pi_2(G) \in \{0, -1, -2, -3\}$ are characterized. Some interesting properties of $\Pi_1(G)$ and $\Pi_2(G)$ are also given. We then find the necessary and sufficient conditions for two classes of graphs to be determined by their adjacency spectrum.

Keywords: characteristic polynomial; cospectral graph; invariant

MSC: 05C50

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Citation: Yin, J.; Zhao, H.; Xie, S. Spectral Invariants and Their Application on Spectral Characterization of Graphs. *Axioms* **2022**, *11*, 260. https://doi.org/10.3390/axioms11060260

Academic Editor: Elena Guardo

Received: 29 April 2022
Accepted: 18 May 2022
Published: 29 May 2022

1. Introduction

All graphs considered here are finite and simple. Undefined notations and terminologies will conform to those in [1].

For a graph G with $n(G)$ vertices and $m(G)$ edges, $V(G)$ and $E(G)$ are used to denote the vertex set and the edge set of G, respectively. For $v \in V(G)$, $N_G(v) = \{u | u \in V(G), uv \in E(G)\}$ and $d_G(v)$ (or simple by d_v) be the degree of a vertex v in G. Let $v_1, v_2 \in V(G)$, set $N_G(v_1v_2) = N_G(v_1) \bigcup N_G(v_2) - \{v_1, v_2\}$. If $v_1v_2 \in E(G)$, take $d_G(v_1v_2) = |N_G(v_1v_2)|$. Let $v \in V(G)$, $e \in E(G)$ and $C_k, k \geq 3$ be a cycle of G, use $G - v$, $G - e$ and $G - C_k$ to denote the graphs obtained from G by deleting the vertex v, the edge e and all vertices of C_k, respectively. Let H be a subgraph of G, and $(H)_E$ denotes the subgraph of G induced by the edge set $E(H)$. Let G and H be two graph which we denote by $G \cup H$ as the disjoint union of G and H and by lH the disjoint union of l copies of H.

For a graph G with n vertices, its adjacency matrix $A(G)$ is the $n \times n$ matrix with (i, j)th entry equaling to 1 if vertices i and j are adjacent and equaling to 0 otherwise. $D(G)$ denotes the degrees matrix corresponding to vertices of G on the main diagonal. The Laplacian matrix of G is denoted by $L(G)$, where $L(G) = D(G) - A(G)$. The characteristic polynomial of the adjacency matrix $A(G)$ (respectively, Laplacian matrix $L(G)$) is denoted by $P_A(G, \lambda)$ (respectively, $P_L(G, \mu)$). The eigenvalues of $A(G)$ ($L(G)$) are also called the adjacency (Laplacian) eigenvalues of G. Since both matrices $A(G)$ and $L(G)$ are real symmetric matrices, their eigenvalues are all real numbers. We can therefore assume that $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$ and $\mu_1(G) \geq \mu_2(G) \geq \cdots \mu_{n-1} \geq \mu_n(G)(= 0)$ are adjacency eigenvalues and the Laplacian eigenvalues of G, respectively. The multiset of eigenvalues of $A(G)$ and $L(G)$ are called the adjacency spectrum and Laplacian spectrum of G, respectively. The maximum eigenvalue of $A(G)$ is called the index of G. Two graphs are said to be cospectral with respect to the adjacency (respectively, Laplacian) matrix if they have the same adjacency (respectively, Laplacian) spectrum. A graph is said to be determined

(DS for short) by its adjacency (respectively, Laplacian) spectrum if there is no other non-isomorphic graph with the same spectrum with respect to the adjacency (respectively, Laplacian) matrix.

To date, numerous examples of cospectral but non-isomorphic graphs have been reported. For example, Schwenk showed that the proportion of trees on n vertices which are characterized by their spectra converges towards zero as n increases in [2] and Godsil and Mckay in [3,4] gave some constructions for pairs of cospectral graphs. Recently, many graphs with special structures have been proved to be determined by their spectrum, as can be seen in [5–18]. The authors in [6,7,11] investigated the cospectrality of graphs up to order 11 and gave a survey on the spectral characterizations of graphs. Some results on the Laplacian spectral characterizations of graphs can be found in [19–21].

Here, we list some connected graphs determined by their adjacency spectrum as following:

(i) The path with n vertices P_n and its complement, where $n \geq 2$, the complete graph K_n, the regular complete bipartite graph $K_{m,m}$, the cycle C_n and their complements, some graphs obtained by deleting some edges from K_n are determined by their adjacency spectrum [6–8,22]. We write $\mathcal{P} = \{P_n | n \geq 2\}$ and $\mathcal{C} = \{C_t | t \geq 3\}$.

(ii) Let $T(l_1, l_2, l_3)$ denote a tree with a vertex v of degree 3 such that $T(l_1, l_2, l_3) - v = P_{l_1} \cup P_{l_2} \cup P_{l_3}$. Then, $T(l_1, l_2, l_3)$ is determined by its adjacency spectrum if and only if $(l_1, l_2, l_3) \neq (a, a, 2a - 2)$ for any $a \geq 1$ [14,17]. Write $\mathcal{T}_1 = \{T(l_1, l_2, l_3) | 1 \leq l_1 \leq l_2 \leq l_3\}$.

(iii) A lollipop graph, denoted by $Q(s_1, s_2)$, is obtained by identifying a vertex of C_{s_1} and a vertex of P_{s_2}. Then, the lollipop graph is determined by its adjacency spectrum [5,10].

(iv) All connected graphs with an index in the interval $(2, \sqrt{2 + \sqrt{5}})$ are determined by their adjacency spectrum [9].

(v) The sandglass graph is obtained by appending a triangle to each pendant vertex of a path. Then, the sandglass graph is determined by its adjacency spectrum [12].

(vi) The θ graph, denoted by $\theta(i, j, k)$, is a graph consisting of the two given vertices joined by three paths whose order is $i + 2$, $j + 2$, and $k + 2$, respectively, with any two of these paths only having the given vertices in common. 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. An ∞-graph $B(r, s)$ is a graph consisting of two cycles C_r and C_s with just a vertex in common. The authors in [15,16,23–25] gave some DS-graphs among θ-graphs and all DS-graphs of the dumbbell graphs and ∞-graphs. In [26], the authors proved the θ-graphs without C_4 as its subgraphs are DS.

In this paper, we give two parameters $\Pi_1(G)$ and $\Pi_2(G)$ related to the characteristic polynomial of G. Some properties of $\Pi_1(G)$ and $\Pi_2(G)$ were obtained in Section 3. We characterized all connected graphs with $\Pi_1(G) \in \{1, 0, -1, -2, -3\}$ and $\Pi_2(G) \in \{0, -1, -2, -3\}$. From Section 3, one can see that $\Pi_2(G) \in \{0, -1, -2\}$ for all graphs G in (i)–(vi) as shown above, except for K_n, $K_{m,m}$, $\overline{P_n}$ and $\overline{C_n}$. By applying the results of the parameters $\Pi_1(G)$ and $\Pi_2(G)$ in Section 4, we give the necessary and sufficient conditions for two classes of graphs to be DS with respect to their adjacency spectrum. We also give a method to characterize the graphs determined by their adjacency spectrum in Section 4. Section 5 gives a summary.

2. Some Lemmas

For a graph G, let $P_A(G, \lambda) = \sum\limits_{k=0}^{n} b_k(G)\lambda^{n-k}$ be the characteristic polynomial of G. In this section, we give some basic lemmas.

Lemma 1 ([27])**.** *Let G be a graph with k components $G_1, G_2, \cdots, G_k$. Then*

$$P_A(G, \lambda) = \prod_{i=1}^{k} P_A(G_i, \lambda).$$

Lemma 2 ([27]). *Let G be a graph with the vertex v and the edge e. Denote by $\mathcal{C}(v)(\mathcal{C}(e))$ the set of all cycles in G containing a vertex v (respectively, the edge $e = uv$). We then have*

(1) $P_A(G,\lambda) = \lambda P_A(G-v,\lambda) - \sum_{u\sim v} P_A(G-\{u,v\},\lambda) - 2\sum_{C\in\mathcal{C}(v)} P_A(G-V(C),\lambda)$.

(2) $P_A(G,\lambda) = P_A(G-uv,\lambda) - P_A(G-\{u,v\},\lambda) - 2\sum_{C\in\mathcal{C}(e)} P_A(G-V(C),\lambda)$.

The Sachs graphs of G is the graph with its component being either K_2 or a cycle.

Lemma 3 ([27]). *Let G be a graph on n vertices. Then*

$$b_i(G) = \sum_{U\in\mathcal{U}_i} (-1)^{k(U)} 2^{c(U)},$$

where $\mathcal{U}_i$ denotes the set of the Sachs graphs of G with i vertices, $k(U)$ is the number of components of U and $c(U)$ is the number of cycles contained in U.

Let G be a graph with n vertices and m edges. We denote by $N_G(2,2)$ the number of subgraphs $2K_2$ and by $N_G(2,2,2)$ the number of subgraphs $3K_2$. We denote by $N_G(H)$ the number of subgraphs H in G. Then, the following lemma is found in [28].

Lemma 4 ([28]). *Let G be a graph with n vertices and m edges. Then*

(1) $N_G(2,2) = \binom{m+1}{2} - \frac{1}{2}\sum_{i\in V(G)} d_i^2$.

(2) $N_G(2,2,2) = \frac{m(m^2+3m+4)}{6} - \frac{m+2}{2}\sum_{i\in V(G)} d_i^2 + \frac{1}{3}\sum_{i\in V(G)} d_i^3 + \sum_{ij\in E(G)} d_i d_j - N_G(K_3)$.

From Lemmas 3 and 4, it is easy to obtain the following.

Lemma 5. *Let G be a graph with n vertices and m edges. Then*

(1) $b_0(G) = 1, b_1(G) = 0$,

(2) $b_2(G) = -m, b_3(G) = -2N_G(K_3)$,

(3) $b_4(G) = \binom{m+1}{2} - \frac{1}{2}\sum_{i\in V(G)} d_i^2 - 2N_G(C_4)$,

(4) $-b_6(G) = \frac{m(m^2+3m+4)}{6} - \frac{m+2}{2}\sum_{i\in V(G)} d_i^2 + \frac{1}{3}\sum_{i\in V(G)} d_i^3 + \sum_{ij\in E(G)} d_i d_j - N_G(K_3)$ $-2N_G(K_2\cup C_4) - 4N_G(K_3\cup K_3) + 2N_G(C_6)$.

3. Two Invariants Related to Characteristic Polynomials

In this section, we investigate two invariants related to some coefficients of the characteristic polynomials of G. Then, some properties of the invariants are given.

Definition 1. *Let G be a graph, the parameter $\Pi_1(G)$ is defined by the following*

$$\Pi_1(G) = \begin{cases} 0, & \text{if } m(G) = 0, \\ b_4(G) - \binom{m(G)-1}{2} + 1, & \text{if } m(G) > 0. \end{cases}$$

It is easy to see that if $P_A(G,\lambda) = P_A(H,\lambda)$, then $b_4(G) = b_4(H)$ and $m(G) = m(H)$. Thus, we have:

Theorem 1. *Let G and H be two graphs with $P_A(G,\lambda) = P_A(H,\lambda)$. Then*

$$\Pi_1(G) = \Pi_1(H).$$

Theorem 2. *Let G be a graph with components $G_1, G_2, G_3, \cdots, G_k$. Then*

$$\Pi_1(G) = \sum_{i=1}^{k} \Pi_1(G_i).$$

Proof. It is sufficient to prove the case $k = 2$. Let $G = G_1 \bigcup G_2$, $|V(G_i)| = n_i$ and $|E(G_i)| = m_i$, for $i = 1, 2$. By Lemmas 2 and 5, we have

$$b_4(G_1 \cup G_2) = b_4(G_1) + b_4(G_2) + m_1 m_2 \textit{ and } m(G_1 \cup G_2) = m_1 + m_2.$$

By Definition 1, it follows

$$\begin{aligned}
\Pi_1(G) &= b_4(G_1) + b_4(G_2) + m_1 m_2 - \binom{m_1 + m_2 - 1}{2} + 1 \\
&= b_4(G_1) - \binom{m_1 - 1}{2} + 1 + b_4(G_2) - \binom{m_2 - 1}{2} + 1 \\
&= \Pi_1(G_1) + \Pi_1(G_2).
\end{aligned}$$

□

Theorem 3. *Let G be a graph with n vertices and $uv \in E(G)$. Then*

$$\Pi_1(G) = \Pi_1(G - uv) - |N_G(uv)| - N_{uv}(C_3) - 2N_{uv}(C_4) + 1,$$

where $N_{uv}(C_3)$(respectively, $N_{uv}(C_4)$) denotes the number of triangles (respectively, C_4) containing the edge uv in G.

Proof. Since $n(G) = n(G - uv) = n$ (namely, $V(G) = V(G - uv)$) and $m(G - uv) = m(G) - 1$, by Lemma 5, we have

$$\begin{aligned}
b_4(G - uv) &= \binom{m(G - uv) + 1}{2} - \frac{1}{2} \sum_{i \in V(G)} d^2_{G-uv}(i) - 2N_{G-uv}(C_4) \\
&= \binom{m(G)}{2} - \frac{1}{2} \left(\sum_{i \in V(G) \setminus \{u,v\}} d^2_{G-uv}(i) + d^2_{G-uv}(u) + d^2_{G-uv}(v) \right) \\
&\quad -2N_{G-uv}(C_4).
\end{aligned}$$

Note that $d_{G-uv}(u) = d_G(u) - 1$, $d_{G-uv}(v) = d_G(v) - 1$, $N_{G-uv}(C_4) = N_G(C_4) - N_{uv}(C_4)$ and $d_G(i) = d_{G-uv}(i)$ if $i \notin \{u, v\}$. Since $|N_G(uv)| = d_G(u) + d_G(v) - N_{uv}(C_3) - 2$, we have

$$\begin{aligned}
b_4(G - uv) &= \binom{m(G) + 1}{2} - m(G) - \frac{1}{2} \left(\sum_{i \in V(G)} d^2_G(i) - 2(d_G(u) + d_G(v)) + 2 \right) \\
&\quad -2(N_G(C_4) - N_{uv}(C_4)) \\
&= b_4(G) - m(G) + |N_G(uv)| + N_{uv}(C_3) + 1 + 2N_{uv}(C_4).
\end{aligned}$$

Therefore, it follows

$$\begin{aligned}\Pi_1(G-uv) &= b_4(G-uv) - \binom{m(G)-2}{2} + 1 \\ &= b_4(G) - m(G) + |N_G(uv)| + N_{uv}(C_3) + 1 + 2N_{uv}(C_4) - \binom{m(G)-2}{2} + 1 \\ &= b_4(G) - \binom{m(G)-1}{2} + 1 + |N_G(uv)| + N_{uv}(C_3) + 2N_{uv}(C_4) - 1 \\ &= \Pi_1(G) + |N_G(uv)| + N_{uv}(C_3) + 2N_{uv}(C_4) - 1.\end{aligned}$$

This implies that $\Pi_1(G) = \Pi_1(G-uv) - |N_G(uv)| - N_{uv}(C_3) - 2N_{uv}(C_4) + 1$. □

Note that if G is a connected graph, $|N_G(uv)| \geq 1$, except for $G = K_2$. From Theorem 3, we have:

Corollary 1. *Let G be a connected graph with at least three vertices and $uv \in E(G)$. Then*

(1) $\Pi_1(G) \leq \Pi_1(G-uv)$*, the equality holds if and only if uv is a pendent edge with $d_G(u) = 2$ and $d_G(v) = 1$.*

(2) *If uv is a pendent edge of G and $d_G(v) = 1$, then*

$$\Pi_1(G) = \Pi_1(G-uv) - d_{G-v}(u) + 1.$$

Theorem 4. *Let G be a connected graph. Then:*

(1) $\Pi_1(G) \leq 1$*, and the equality holds if and only if $G \in \mathcal{P}$;*

(2) $\Pi_1(G) = 0$ *if and only if $G \in \{K_1\} \cup \mathcal{C}\backslash\{C_4\} \cup \mathcal{T}_1$.*

Proof. (1) By induction on $m(G)$. Since $\Pi_1(K_1) = 0$ and $\Pi_1(K_2) = 1$, we have (1) holds if $m(G) \leq 1$.

Suppose $m(G) \geq 2$. Choose $e \in E(G)$ such that $G - e = H$ or $H \bigcup K_1$. So, $d_G(e) \geq 1$ and $\Pi_1(G-e) = \Pi_1(H)$. By the induction hypothesis, $\Pi_1(G-e) \leq 1$. By Corollary 1, it is easy to get that $\Pi_1(G) \leq \Pi_1(G-e) \leq 1$ and $\Pi_1(G) = 1$ if and only if $d_G(e) = 1, N_e(C_3) = N_e(C_4) = 0$ and $\Pi_1(G-e) = 1$.

By the induction hypothesis, we have $H \in \mathcal{P}$. Therefore $G \in \mathcal{P}$.

Conversely, since $\Pi_1(P_2) = 1$ and $\Pi_1(G) = \Pi_1(G-e) - d_G(e) - N_e(C_3) - 2N_e(C_4) + 1$, we can show that $\Pi_1(P_n) = \Pi_1(P_{n-1}) = \cdots = \Pi_1(P_2) = 1$.

(2) By induction on $m(G)$. Since $\Pi_1(K_1) = 0$ and $\Pi_1(K_2) = 1$, it is clear that (2) holds if $m(G) \leq 1$.

Suppose $m(G) \geq 2$. Choose $e \in E(G)$ such that H is connected. By Theorem 3, we have

$$\Pi_1(G-e) = d_G(e) + N_e(C_3) + 2N_e(C_4) - 1.$$

Note that $\Pi_1(G) \leq \Pi_1(G-e)$. We consider only the following cases:

Case 1. $\Pi_1(G-e) = 1$.

Note that $d_G(e) + N_e(C_3) + 2N_e(C_4) = 2$ and $d_G(e) \geq 1$. If $N_e(C_3) = 1, d_G(e) = 1$ and $N_e(C_4) = 0$, we have $H \in \mathcal{P}$ by (1). Hence, $G \cong C_3$. If $N_e(C_3) = 0, d_G(e) = 2$ and $N_e(C_4) = 0$, we know that $(G-e)_E \in \mathcal{P}$ by the induction hypothesis. Therefore $G \in \{C_n(n \geq 5)\} \cup \mathcal{T}_1$.

Case 2. $\Pi_1(G-e) = 0$.

Since $d_G(e) + N_e(C_3) + 2N_e(C_4) = 1$ and $d_G(e) \geq 1$, we know that $d_G(e) = 1, N_e(C_3) = N_e(C_4) = 0$. By the induction hypothesis, $H \in \mathcal{C}\backslash\{C_4\} \cup \mathcal{T}_1$. Therefore, $G \in \mathcal{T}_1$.

Conversely, since $\Pi_1(P_n) = 1$ and $\Pi_1(K_1) = \Pi_1(T(1,1,1)) = 0$, we can show that $\Pi_1(C_n) = \Pi_1(P_n) - 1 = 0$ if $n \geq 5$, and $\Pi_1(T(l_1, l_2, l_3)) = \Pi_1(T(1,1,1)) = 0$ and $\Pi_1(C_3) = 0$ by Theorem 3. □

By Theorems 1–3, one can construct all connected graphs G with $\Pi_1(G) = i$. Let $\Gamma_i = \{G | G$ be a connected graph and $\Pi_1(G) = i\}$. By Theorem 4, $\Gamma_1 = \{P_n | n \geq 2\}$ and $K_1 \in \Gamma_0$. Now, we give an algorithm to construct all connected graphs in Γ_i as following.

Algorithm 1: Construction of all connected graphs with $\Pi_1(G) = i$.

(i) Take $\Gamma_1 = \{P_n | n \geq 2\}$ and $\Gamma_0 = \{K_1\}$.
(ii) Let i be an integer, $i \leq 0$,
for $k := 1$ to i (step -1)
  for each $H \in \Gamma_k$
    for each $u, v \in V(H), uv \notin E(H)$
     if $N_H(uv) = k - i - N_{uv}(C_3) - 2N_{uv}(C_4) + 1$
     then $\Gamma_i := \Gamma_i \cup \{H + uv\}$
    end for
    for each $u \in V(H)$
     if $d_H(u) = k - i + 1$
     then $\Gamma_i := \Gamma_i \cup \{H + uv\}$, where $v \notin V(H)$.
    end for
  end for
end for
Note. In the front steps, $N_{uv}(C_3)$ (respectively, $N_{uv}(C_4)$) denotes the number of triangles (respectively, C_4) containing the edge uv in graph $H + uv$.

Lemma 6. *Algorithm 1 achieves completeness, that is, if G is any connected graph with $\Pi_1(G) = i$ and $i \leq 1$, then $G \in \Gamma_i$ by Algorithm 1.*

Proof. By induction on $\Pi_1(G)$ and $m(G)$, by Theorem 4, it is true for $\Pi_1(G) = 1, 0$. Suppose that the algorithm achieves completeness for $\Pi_1(G) > i$. When $\Pi_1(G) = i$, we shall prove the completeness by induction on $m(G)$. □

By the proof of Theorem 4, we have that it is true for $m(G) \leq 1$. Suppose $m(G) \geq 2$, and we consider the following cases:

Case 1. G has a pendant edge, say $e = uv$ and $d_G(v) = 1$. Then, $G - e = H \cup K_1$, where H is connected. By Corollary 1

$$\Pi_1(G) = \Pi_1(H) - d_G(e) + 1 \leq \Pi_1(H).$$

If $d_G(e) = 1$, then $\Pi_1(H) = i$ and $m(H) = m(G) - 1$, so by the induction hypothesis on $m(G)$, $H \in \Gamma_i$. If $d_G(e) \geq 2$, then $\Pi_1(H) > i$, say $\Pi_1(H) = l > i$, and so $H \in \Gamma_l$ by the induction hypothesis on $\Pi_1(G)$. Hence, G must be obtained from H by adding the pendant edge uv from Algorithm 1.

Case 2. G has no any pendant edge. Then, there exists at least an edge $e = uv$ such that $H = G - uv$ is connected. Clearly, $d_G(uv) + N_e(C_3) + 2N_{uv}(C_4) \geq 2$. By Theorem 3,

$$\Pi_1(G) = \Pi_1(H) - d_G(uv) - N_{uv}(C_3) - 2N_{uv}(C_4) + 1 < \Pi_1(H).$$

Hence, $\Pi_1(H) > i$, say $\Pi_1(H) = l > i$. By the induction hypothesis on $\Pi_1(G)$, $H \in \Gamma_l$. Therefore, G must be obtained from H by adding the edge uv by Algorithm 1. This completes the proof of the completeness. □

Note that if $uv \in V(G)$ and $H = G - uv$, then $d_G(uv) = N_H(uv)$. By Lemma 6 and Algorithm 1, we obtain the following theorem. Here, the proof is omitted.

Theorem 5. *Let G be a connected graph. Then:*

(i) $\Pi_1(G) = -1$ *if and only if* $G \in \{G_1, T_2\}$;
(ii) $\Pi_1(G) = -2$ *if and only if* $G \in \{G_2, G_3, C_4, T_3, T_4\}$;

(iii) $\Pi_1(G) = -3$ *if and only if* $G \in \{G_4, G_5, G_6, G_7, G_8, G_9, G_{10}, T_5, T_6, T_7\}$, *where all graphs are listed in Figure 1.*

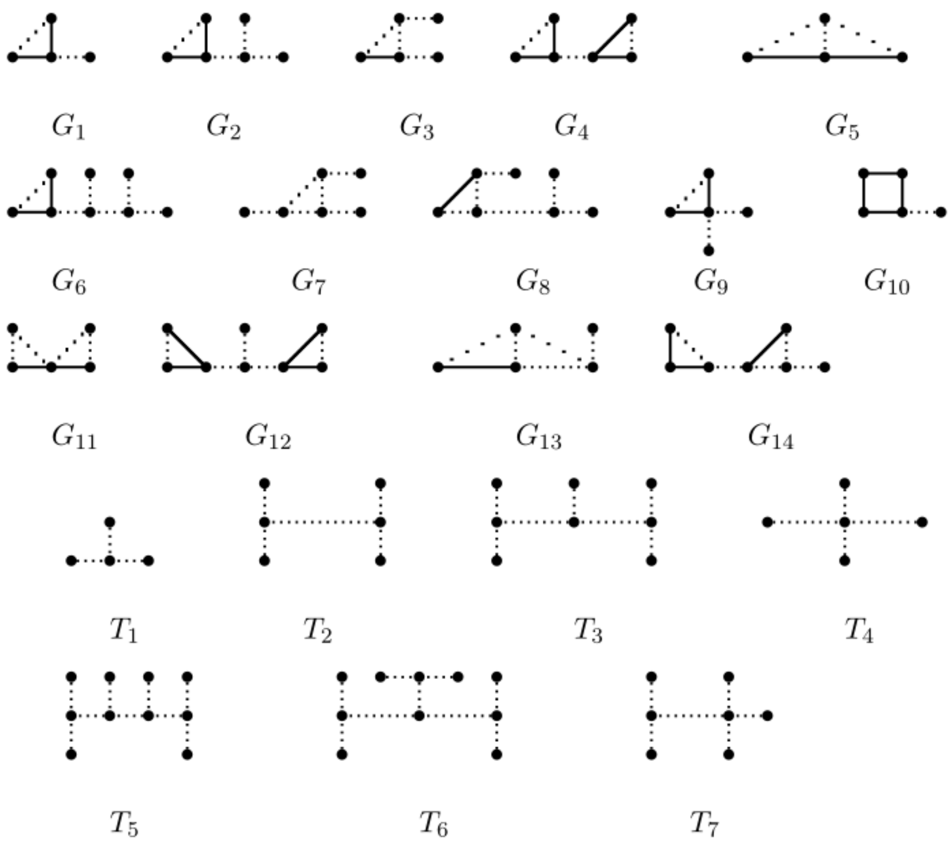

Figure 1. Some connected graphs $\Pi_1 \geq -3$.

Note: G_i in Figure 1, for $1 \leq i \leq 14$ and $i \neq 10$, does not contain C_4 as its subgraphs and all the dot lines of the graphs denote a path with at least two vertices.

Now we give another invariant as follows:

Definition 2. *Let G be a connected graph. Set* $\Pi_2(G) = \Pi_1(G) + m(G) - n(G)$.

From Definitions 1 and 2 and Theorems 1–3, we can easily prove the following:

Theorem 6. *(1) Let G and H be two graphs such that* $P_A(G, \lambda) = P_A(H, \lambda)$. *Then*

$$\Pi_2(G) = \Pi_2(H).$$

(2) Let G be a graph with k components $G_1, G_2, \cdots, G_k$. *Then*

$$\Pi_2(G) = \sum_{i=1}^{k} \Pi_2(G_i).$$

(3) Let G be a connected graph and $e \in E(G)$. *Then*

$$\Pi_2(G) = \Pi_2(G - e) - d_G(e) - 2N_e(C_4) - N_e(C_3) + 2.$$

Theorem 7. *Let G be a connected graph. Then, $\Pi_2(G) \leq 0$, and the equality holds if and only if $G \in \mathcal{P} \cup \mathcal{C} \backslash \{C_4\}$.*

Proof. By induction in $m(G)$, since $\Pi_2(K_1) = -1$ and $\Pi_2(K_2) = 0$, we have (1) which holds when $m(G) \leq 1$.

Suppose $m(G) \geq 2$. Choose $e \in E(G)$ such that $(G-e)_E$ is connected. Clearly, $d_G(e) \geq 1$. We distinguish the three following cases:

Case 1. e is a pendant edge.

Obviously, $G - e = H \cup K_1$, where $H = (G-e)_E$. By Theorem 5 and the induction hypothesis, we have

$$\Pi_2(G-e) = \Pi_2(K_1) + \Pi_2(H) = -1 + \Pi_2(H)$$

and

$$\Pi_2(G) = \Pi_2(H) - d_G(e) - 2N_e(C_4) - N_e(C_3) + 1 \leq \Pi_2(H) \leq 0.$$

Note that $\Pi_2(G) = 0$ if and only if $\Pi_2(H) = 0, d_G(e) = 1$ and $N_e(C_3) = N_e(C_4) = 0$. By the induction hypothesis, $H \in \mathcal{P} \cup \mathcal{C} \backslash \{C_4\}$. Since $G - e = H \cup K_1$ and G is connected, we have $G \in \mathcal{P}$.

Case 2. e is an edge in a triangle.

We know that $G - e$ is connected and $N_e(C_3) \geq 1$. By Theorem 6 (3),

$$\Pi_2(G) = \Pi_2(G-e) - d_G(e) - 2N_e(C_4) - N_e(C_3) + 2 \leq \Pi_2(G-e) \leq 0,$$

and $\Pi_2(G) = 0$ if and only if $\Pi_2(G-e) = 0, N_e(C_3) = d_G(e) = 1$ and $N_e(C_4) = 0$. By the induction hypothesis, $G - e \in \mathcal{P} \cup \mathcal{C} \backslash \{C_4\}$. Thus, $G \cong C_3$(only if $(G-e) \cong P_3$).

Case 3. e is an edge in a cycle whose length is greater than 3.

Clearly, $d_G(e) \geq 2$. By Theorem 6 (3), we have

$$\Pi_2(G) = \Pi_2(G-e) - d_G(e) - 2N_e(C_4) - N_e(C_3) + 2 \leq \Pi_2(G-e) \leq 0$$

and $\Pi_2(G) = 0$ if and only if $\Pi_2(G-e) = 0, d_G(e) = 2$ and $N_e(C_3) = N_e(C_4) = 0$. By the induction hypothesis, $G - e \in \mathcal{P} \cup \mathcal{C} \backslash \{C_4\}$. Hence, $G \in \mathcal{C} \backslash \{C_3, C_4\}$.

Conversely, by Theorem 4 and Definition 2, we can directly verify our findings. □

Let $\Theta_i = \{G | G$ be a connected graph and $\Pi_2(G) = i\}$. Similarly to $\Pi_1(G)$, we construct all connected graphs in Θ_i by the following algorithm.

Lemma 7. *Algorithm 2 is completeness, that is, if G is any connected graph with $\Pi_2(G) = i$ and $i \leq 0$, then $G \in \Theta_i$ by Algorithm 2.*

Proof. By induction in $\Pi_2(G)$ and $m(G)$. By Theorem 7, it is true for $\Pi_2(G) = 0$. Suppose that the algorithm is completeness for $\Pi_2(G) > i$. When $\Pi_2(G) = i$, we shall prove the completeness by induction in $m(G)$.

By the proof of Theorem 7, we have that it is true for $m(G) \leq 1$. Suppose that $m(G) \geq 2$, and we consider the following cases:

Case 1. G has a pendant edge, say $e = uv$ and $d_G(v) = 1$. Then, $G - e = H \cup K_1$, where H is connected. Note that $N_e(C_3) + 2N_{uv}(C_4) = 0$. By the proof of case 1 of Theorem 7, we have

$$\Pi_2(G) = \Pi_2(H) - d_G(e) + 1 \leq \Pi_2(H).$$

If $d_G(e) = 1$, then $\Pi_2(H) = i$ and $m(H) = m(G) - 1$, so by the induction hypothesis on $m(G)$, $H \in \Theta_i$. If $d_G(e) \geq 2$, then $\Pi_2(H) > i$, say $\Pi_2(H) = l > i$, and so $H \in \Theta_l$ by the induction hypothesis on $\Pi_2(G)$. Hence, G must be obtained from H by adding the pendant edge uv from Algorithm 2, where $v \notin V(H)$.

Case 2. G has no any pendant edge. Then, there exists at least an edge $e = uv$ such that $H = G - uv$ is connected. Since $d_G(uv) + N_e(C_3) + 2N_{uv}(C_4) \geq 2$, by Theorem 6 (3) we have

$$\Pi_2(G) = \Pi_2(H) - d_G(uv) - N_{uv}(C_3) - 2N_{uv}(C_4) + 2 \leq \Pi_2(H).$$

If $d_G(uv) + N_e(C_3) + 2N_{uv}(C_4) = 2$, then $\Pi_2(H) = i$ and $m(H) = m(G) - 1$, so by the induction hypothesis on $m(G)$, $H \in \Theta_i$. If $d_G(uv) + N_e(C_3) + 2N_{uv}(C_4) > 2$, then $\Pi_2(H) > i$, say $\Pi_2(H) = l > i$, and so $H \in \Theta_l$ by the induction hypothesis on $\Pi_2(G)$. Hence, G must be obtained from H by adding the edge uv from Algorithm 2. This completes the proof of the completeness. □

Algorithm 2: Construction of all connected graphs with $\Pi_2(G) = i$.

(i) Take $\Theta_0 = \{P_n | n \geq 2\} \cup \{C_3\} \cup \{C_n | n \geq 5\}$ and $\Theta_{-1} = \{K_1\}$.
(ii) Let i be a negative integer, $i \leq 0$,
for $k := 0$ to i (step -1)
  for each $H \in \Theta_k$
    for each $u, v \in V(H), uv \notin E(H)$
      if $N_H(uv) = k - i - N_{uv}(C_3) - 2N_{uv}(C_4) + 2$
      then $\Theta_i := \Theta_i \cup \{H + uv\}$
    end for
    for each $u \in V(H)$
      if $d_H(u) = k - i + 1$
      then $\Theta_i := \Theta_i \cup \{H + uv\}$, where $v \notin V(H)$.
    end for
  end for
end for

Note. In the front steps, $N_{uv}(C_3)$ (respectively, $N_{uv}(C_4)$) denotes the number of triangles (respectively, C_4) containing the edge uv in the graph $H + uv$.

From Lemma 7, Theorems 6 and 7 as well as Algorithm 2, we can prove the following. Here, the proof is omitted.

Theorem 8. *Let G be a connected graph. Then:*

(1) $\Pi_2(G) = -1$ *if and only if* $G \in \{K_1, G_1, T_1\}$;
(2) $\Pi_2(G) = -2$ *if and only if* $G \in \{G_2, G_3, G_4, G_5, C_4, T_2\}$;
(3) $\Pi_2(G) = -3$ *if and only if* $G \in \{G_i, \text{for } 6 \leq i \leq 14, T_3, T_4\}$, *where* G_i, *for* $1 \leq i \leq 14$ *and* $i \neq 10$, *does not contain* C_4 *as its subgraph.*

Remark 1. *The invariants* $\Pi_1(G)$ *and* $\Pi_2(G)$ *are important for determining DS graphs. By Theorems 6 and 7, for each component* G_i *of the cospectral graphs of G, we have that* $\Pi_2(G_i) \geq \Pi_2(G)$, *which gives all possible cospectral graphs of G. It is therefore easy to find all possible cospectral graphs of G. Then, by considering the invariants* $\Pi_1(G)$ *and* $\Pi_2(G)$, *it can be ascertained whether G is determined by its adjacency spectrum.*

Remark 2. *By Algorithms 1 and 2, one can characterize all connected graphs with* $\Pi_1(G) < -k$ *and* $\Pi_2(G) < -k$. *For example,* $k = 4, 5$. *Since there are many classes of graphs with* $\Pi_1(G) = -k$ *and* $\Pi_2(G) = -k$ *for a large positive integer k, it is difficult to characterize all graphs with* $\Pi_1(G) = -k$ *and* $\Pi_2(G) = -k$.

Remark 3. *In this section, we define two invariants for graph G, which satisfies two important properties: component additivity (Theorems 2 and 6 (2)) and boundedness (Theorems 4 and 7).*

In fact, we define some new invariants with component additivity and boundedness. For example, $\Pi_3(G) = \pi_1(G) + N_G(K_3)$ and $\Pi_4(G) = \pi_2(G) + m(G) - n(G)$, which have similar properties and applications of $\Pi_1(G)$ and $\Pi_2(G)$. The readers interested by new invariants may study their properties and find more than DS graphs.

4. Some Graphs Determined by Their Adjacency Spectrum

For convenience, we denote by $\mathcal{G}_i$ the set $\{G_i\}$, for $1 \leq i \leq 14$, and by $\mathcal{T}_i$ the set $\{T_i\}$, for $1 \leq i \leq 4$. In Section 1, we list nearly all connected graphs G determined by their adjacency spectrum, which $\Pi_2(G) \in \{0, -1, -2\}$, except for K_n, $K_{m,m}$, $\overline{P_n}$ and $\overline{C_n}$. In fact, the necessary and sufficient conditions for all connected G with $\Pi_2(G) = 0, -1$ to be DS were found. However, there are a few results on the DS-graphs of the connected graphs G with $\Pi_2(G) \leq -2$, which are some special classes in $\mathcal{G}_3$, $\mathcal{G}_4$ and $\mathcal{T}_2$, seeing [9,15,16,26]. In this section, by using the results of previous sections, we shall give the necessary and sufficient conditions for one class of trees T with $\Pi_2(T) = -3$ and one class of graphs G with $\Pi_2(G) = -2$ to be DS with respect to their adjacency spectrum. In the following text, we use $P_A(G)$ instead of $P_A(G, \lambda)$.

Lemma 8 ([27])**.** *All roots of $P_A(C_n)$ and $P_A(P_n)$ are the following:*

- $P_A(C_n) : 2\cos\frac{2i\pi}{n}, i = 0, 1, \cdots, n-1.$
- $P_A(P_n) : 2\cos\frac{i\pi}{n+1}, i = 1, \cdots, n.$

Let $\lambda = 2\cos\theta$, set $t^{1/2} = e^{i\theta}$, and then it is useful to write the characteristic polynomial of C_n and P_n in the following form:

(1) $P_A(C_n, t^{1/2} + t^{-1/2}) = t^{n/2} + t^{-n/2} - 2,$

(2) $P_A(P_n, t^{1/2} + t^{-1/2}) = t^{-n/2}(t^{n+1} - 1)/(t - 1).$

The following graphs and lemmas are frequently used in following text.

Remark 4. *The parameters of each graph in Figure 2 take the following values: $n \geq 6$ for W_n, $s_2 \geq s_1 \geq 2$ for $W(s_1, s_2)$ and $n \geq 6$ for $T_0(n)$.*

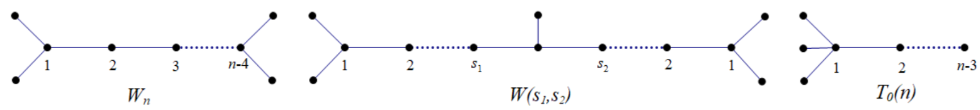

Figure 2. Graphs W_n, $W(s_1, s_2)$ and $T_0(n)$.

Lemma 9 ([27])**.** *(1) Let H be a proper subgraph of a connected graph G, then*

$$\lambda_1(H) < \lambda_1(G).$$

(2) For a graph G of n vertices with $v \in V(G)$, let $H = G - v$, then

$$\lambda_1(G) \geq \lambda_1(H) \geq \lambda_2(G) \geq \lambda_2(H) \geq \cdots \geq \lambda_{n-1}(H) \geq \lambda_n(G).$$

An internal path of G is a walk $v_0v_1 \cdots v_k$ ($k \geq 1$) that the vertices v_1, v_2, $\cdots$, v_k are distinct (v_0, v_k do not need to distinct), $d_G(v_0) \geq 2$, $d_G(v_k) \geq 2$ and $d_G(v_i) = 2$ for $0 < i < k$ [27].

Lemma 10 ([27])**.** *Let G be a connected graph that is not isomorphic to W_n and let G_{uv} be the graph obtained from G by subdividing the edge uv of G. If uv lies on an internal path of G, then $\lambda_1(G_{uv}) < \lambda_1(G)$.*

Lemma 11 ([27])**.** *(1) The connected graphs with index 2 are precisely the graphs below: $C_n (n \geq 3)$, $W_n (n \geq 6)$, $K_{1,4}$ and $T(a, b, c)$ for $(a, b, c) \in \{(2, 2, 2), (1, 2, 5), (1, 3, 3)\}$.*

(2) The connected graphs with an index of less than 2 precisely include the following graphs: $P_n(n \geq 1)$ and $T(a,b,c)$ for $(a,b,c) \in \{(1,2,2),(1,2,3),(1,2,4)\} \cup \{(1,1,n)|n \geq 1\}$.

Woo and Neumaier in [29] gave the structure of graphs with $\sqrt{2+\sqrt{5}} < \lambda_1(G) \leq \frac{3}{2}\sqrt{2}$. An open quipu is a tree G of maximum degree 3 such that all vertices of degree 3 lie on a path and a closed quipu is a connected graph G of maximum degree 3 such that all vertices of degree 3 lie on a circuit and no other circuit exists. The following result can be found in [29].

Lemma 12 ([29])**.** *Let G be a connected graph with $\sqrt{2+\sqrt{5}} < \lambda_1(G) \leq \frac{3}{2}\sqrt{2}$. Then, $\Delta(G) \in \{3,4\}$, where $\Delta(G)$ denotes the maximum degree of G, and:*

(1) If $\Delta(G) = 3$, then G is an open quipu or a closed quipu.
(2) If $\Delta(G) = 4$, then $G \cong T_0(n), n \geq 2$.

Note that if G is an open quipu or a closed quipu, then $\lambda_1(G)$ may not belong to the interval $(\sqrt{2+\sqrt{5}}, \frac{3}{2}\sqrt{2}]$, as can be seen in [29]. For a connected G with $\Pi_2(G) \geq -3$ and $\sqrt{2+\sqrt{5}} < \lambda_1(G) \leq \frac{3}{2}\sqrt{2}$, by Lemma 12 and Theorem 8, we have $G \in \{G_1, G_3, G_7, T_1, T_2, T_3, T_0(n)\}$. The inverse is not true. For example, $\lambda_1(D_4) \simeq 2.17 > \frac{3}{2}\sqrt{2}$, where D_4 is the graph obtained by adding a pendent edge to C_3 and $D_4 \in \mathcal{G}_1$. Now, we consider the spectral characterizations of two classes of trees T such that $\sqrt{2+\sqrt{5}} < \lambda_1(T) \leq \frac{3}{2}\sqrt{2}$ and $\Pi_2(T) = -3$, that is $W(s_1, s_2)$ and $T_0(n)$, as can be seen in Figure 2.

Lemma 13. *Let T be a tree and H be a graph with $m(H) = m(T)$ and $n(H) = n(T)$. If $\Pi_1(H) = \Pi_1(T)$ and H has no C_k as its subgraph, $k = 3,4$, then we have*

$$|b_6(H)| - |b_6(T)| = \frac{1}{3}\sum_{i \in V(H)} d_i^3(H) - \frac{1}{3}\sum_{i \in V(T)} d_i^3(T) + \sum_{ij \in E(H)} d_i d_j - \sum_{ij \in E(T)} d_i d_j + 2N_H(C_6).$$

In particular, if H and G have the same degree sequence, then

$$|b_6(H)| - |b_6(T)| = \sum_{ij \in E(H)} d_i d_j - \sum_{ij \in E(T)} d_i d_j + 2N_H(C_6).$$

Proof. Since $m(H) = m(T)$, $n(H) = n(T)$ and $N_H(C_3) = N_H(C_4) = 0$, by Lemma 5, we have $\sum_{i \in V(H)} d_i^2 = \sum_{i \in V(T)} d_i^2$; thus, the result holds. □

Remark 5. *The parameters of each graph in Figure 3 take the following values: $s_2 \geq s_1 \geq 1$ for G_{31}, $s \geq 1$ for G_{32}, $s_2 \geq s_1 \geq 1$ and $s_3 \geq 3$ for G_{33}, $n_1 \geq 2$ for T_{31}, $s_3 \geq s_1 \geq 3$ and $s_2 \geq 3$ for T_{32}, $s_1 \geq 3$, $s_2 \geq 3$ and $s_3 \geq 3$ for T_{33}. Sometimes, we shall give the parameters of the graphs above, say, $G_{31}(n_1, n_2)$ in Lemma 4.9 and the proof of Theorem 4.1, which are n_1 and n_2 instead of the parameters s_1 and s_2 of G_{31}, respectively.*

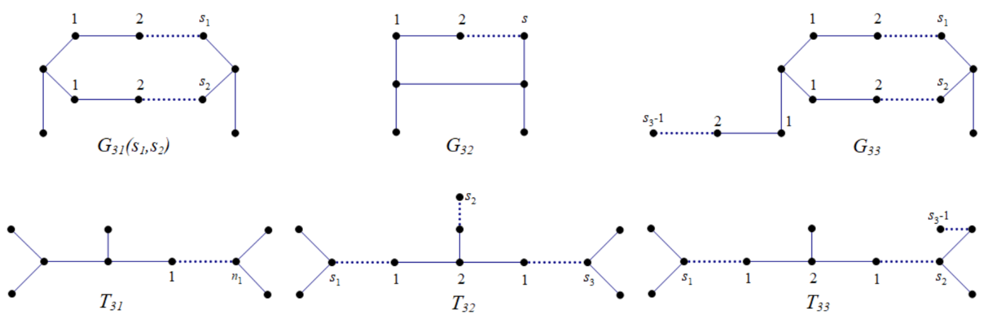

Figure 3. Some graphs in $\mathcal{G}_3$ and $\mathcal{T}_3$.

For a graph G with $uv \in E(G)$, $d_\times(uv) = d_G(u) \times d_G(v)$ is said to be the product degree of the edge uv. We denote by $D_\times(G)$ the sequence of the product degree of G, that is, $D_\times(G) = \{d_\times(e_1), d_\times(e_2), \cdots, d_\times(e_m)\}$, where $E(G) = \{e_1, e_2, \cdots, e_m\}$.

Lemma 14. *Let H be a graph with $m(H) = m(W(s_1,s_2))$ and $n(H) = n(W(s_1,s_2))$. Let $\Pi_i(H) = \Pi_i(W(s_1,s_2))$, $i = 1,2$, then we have:*

(1) If $H = G_{31} \cup T(1,1,1)$, then $|b_6(H)| \geq |b_6(W(s_1,s_2))|$, the equality holds if and only if H does not contain C_6 as its subgraph;

(2) If $H \in \{G_{31} \cup K_1, G_{31} \cup T(1,1,k), k \geq 2, G_{32} \cup T(1,1,1), G_{33} \cup T(1,1,1)\}$, then $|b_6(H)| \geq |b_6(W(s_1,s_2))| + 1$, the equality holds if and only if H does not contain C_6 as its subgraph;

(3) If $H = H_1 \cup H_2$ and H is not a graph in (1) and (2), where $H_1 \in \mathcal{G}_3 \backslash \{G_{3i} | i = 1,2,3\}$ and $H_2 \in \mathcal{T}_1 \cup \{K_1\}$, then $|b_6(H)| \geq |b_6(W(s_1,s_2))| + 2$;

(4) If $H = H_1 \cup H_2$, where $H_1 \in \mathcal{G}_7$ and $H_2 \in \mathcal{P}$, then $|b_6(H)| \geq |b_6(W(s_1,s_2))| + 2$.

Proof. It is easy to see that each H of (1) and (2) and $W(s_1,s_2)$ have the same number of vertices and edges, as well as the same degree sequence. From Lemma 13, by direct computation, we see that (1) and (2) are true.

(3) Here, let G_{3i}, $i = 1,2,3$, which do not contain C_6 as its subgraph. For each graph $F \in \mathcal{G}_3$, by Lemma 4.6 we have $|b_6(G_{32})| = |b_6(G_{33})| = |b_6(G_{31})| + 1$ and $|b_6(F)| > |b_6(G_{32})|$ for all $F \in \mathcal{G}_3 \backslash \{G_{3i} | i = 1,2,3\}$, where $n(F) = n(G_{3i})$, $i = 1,2,3$. One can see that $|b_6(T(l_1,l_2,l_3))| = |b_6(T(1,s_1,s_2))| + 1 = |b_6(T(1,1,k))| + 2$ for $2 \leq l_1 \leq l_2 \leq l_3$, $2 \leq s_1 \leq s_2$ and $2 \leq k$, where $n(T(l_1,l_2,l_3)) = n(T(1,s_1,s_2)) = n(T(1,1,k))$. Therefore, we have the following:

If $H_2 = K_1$, it follows that $|b_6(F \cup K_1)| \geq |b_6(G_{31} \cup K_1)| + 1$ for $F \in \mathcal{G}_3 \backslash \{G_{31}\}$, which implies that (3) is true.

If $H_2 = T(1,1,1)$, it follows that $|b_6(F \cup T(1,1,1))| \geq |b_6(G_{32} \cup T(1,1,1))| + 1$ for $F \in \mathcal{G}_3 \backslash \{G_{3i} | i = 1,2,3\}$. By the (1) and (2) of the lemma, (3) holds.

If $H_2 = T(1,1,k)$, $2 \leq k$, it follows that $|b_6(F \cup T(1,1,k))| \geq |b_6(G_{31} \cup T(1,1,k))| + 1$ for $F \in \mathcal{G}_3 \backslash \{G_{31}\}$. By (2) of the lemma, (3) holds.

If $H_2 = T(1,s_1,s_2)$ with $2 \leq s_1 \leq s_2$, or $H_2 = T(l_1,l_2,l_3)$ with $2 \leq l_1 \leq l_2 \leq l_3$, by the arguments above, we have that (3) holds.

(4) If $H_1 \in \mathcal{G}_7$ and $H_2 \in \mathcal{P}$ and $n(H_1 \cup H_2) = n(W(s_1,s_2))$, one sees that $H_1 \cup H_2$ and $W(s_1,s_2)$ have the same number of edges, the same degree sequence, and the distinct product degree sequence. By the computation of the sum of the product degree, (4) follows from Lemma 13. □

Lemma 15. *Let $H \in \mathcal{T}_3$ and $n(H) = n(T_0(n)) = n$, then we have:*

(1) If $H = W(s_1,s_2)$, then $|b_6(W(s_1,s_2))| = |b_6(T_0(n))| - 1$, for $n \geq 10$;

(2) If $H \in \{T_{31}, T_{32}, T_{33}\}$, then $|b_6(H)| = |b_6(T_0(n))|$, for $n(T_{31}) \geq 9$ and $n(T_{32}) = n(T_{33}) \geq 11$;

(3) If $H \in \mathcal{T}_3 \backslash \{W(s_1,s_2), T_{1i} | i = 1,2,3\}$, then $|b_6(H)| \geq |b_6(T_0(n))| + 1$.

Proof. Note that $s \geq 2$ for T_{31}, $3 \leq s_1 \leq s_3$ and $3 \leq s_2$ for T_{32} and $3 \leq s_1$, $3 \leq s_2$ and $3 \leq s_3$ for T_{33}. By direct computation, (1) follows from Lemma 13.

For each $H \in \mathcal{T}_3$, by Lemma 13, we have that $|b_6(T_{31})| = |b_6(T_{32})| = |b_6(T_{33})| = |b_6(W(s_1,s_2))| + 1$ and $|b_6(H)| \geq |b_6(W(s_1,s_2))| + 2$ for $H \in \mathcal{T}_3 \backslash \{W(s_1,s_2), T_{1i} | i = 1,2,3\}$. By lemma (1), it is easy to see that (2) and (3) hold. □

Lemma 16. *(1) If $H = G_{31}(n_1,n_2) \cup T(1,1,1)$, then H and $W(s_1,s_2)$ are not cospectral, where $2 \leq s_1 \leq s_2$, $1 \leq n_1 \leq n_2$, $n = n(H) = n(W(s_1+s_2))$.*

(2) If $P_A(W(s_1,s_2)) = P_A(W(t_1,t_2))$ with $2 \leq s_1 \leq s_2$ and $2 \leq t_1 \leq t_2$, then $s_1 = t_1$ and $s_2 = t_2$.

Proof. (1) Suppose that $W(s_1, s_2)$ and H are cospectral. Then, $\Pi_1(H) = \Pi_1(W(s_1, s_2))$, $|b_6(H)| = |b_6(W(s_1, s_2))|$ and H does not contain odd circles as its subgraphs. By Theorem 5 and Lemma 14 (1), H does not contain C_4 and C_6 as its subgraphs, which implies that $n_1 + n_2 \geq 6$.

By Lemmas 1 and 2, the characteristic polynomials of $W(s_1, s_2)$ and H can be computed as follows:

$$\begin{aligned} P_A(W(s_1, s_2)) &= \lambda^3 P_A(P_{s_1+s_2+3}) - 2\lambda^3 P_A(P_{s_1+s_2+1}) + \lambda^3 P_A(P_{s_1+s_2-1}) - \\ &\quad \lambda^2 P_A(P_{s_1+1}) P_A(P_{s_2+1}) + \lambda^2 P_A(P_{s_1+1}) P_A(P_{s_2-1}) + \\ &\quad \lambda^2 P_A(P_{s_1-1}) P_A(P_{s_2+1}) - \lambda^2 P_A(P_{s_1-1}) P_A(P_{s_2-1}), \end{aligned}$$

$$P_A(H) = (\lambda P_A(P_3) - \lambda^2)(\lambda^2 P_A(C_{n_1+n_2+2}) - 2\lambda P_A(P_{n_1+n_2+1}) + P_A(P_{n_1}) P_A(P_{n_2})).$$

Since $n = s_1 + s_2 + 6 = n_1 + n_2 + 8 \geq 14$, by Lemma 4.1 and eliminating the same terms from $P_A(W(s_1, s_2), t^{1/2} + t^{-1/2}) t^{\frac{s_1+s_2+6}{2}} (t-1)^2/(t+1)^2$ and $P_A(H, t^{1/2} + t^{-1/2}) t^{\frac{n_1+n_2+8}{2}} (t-1)^2/(t+1)^2$, we can write (using Mathematica5.0) $P_A(W(s_1, s_2))$ and $P_A(H)$, denoted by ϕ_1 and ϕ_2, as follows:

$\phi_1 : -t^4 - t^{2+s_1} + 2t^{3+s_1} - t^{4+s_1} - t^{2+s_2} + 2t^{3+s_2} - t^{4+s_2} - t^{2+s_1+s_2}$,

$\phi_2 : -2t^4 + t^5 + t^6 - t^{3+n_1} + t^{4+n_1} - t^{5+n_1} - 2t^{1+n_1/2+n_2/2} + 2t^{2+n_1/2+n_2/2} + 2t^{3+n_1/2+n_2/2} - 4t^{4+n_1/2+n_2/2} + 2t^{5+n_1/2+n_2/2} + 2t^{6+n_1/2+n_2/2} - 2t^{7+n_1/2+n_2/2} - t^{3+n_2} + t^{4+n_2} - t^{5+n_2} + t^{2+n_1+n_2} + t^{3+n_1+n_2} - 2t^{4+n_1+n_2}$.

Now, we prove the necessity of lemma (1) by comparing the coefficients of the corresponding terms of ϕ_1 and ϕ_2.

Case 1. If $s_1 = s_2$, we have $\phi_1 = -t^4 - 2t^{2+s_1} + 4t^{3+s_1} - 2t^{4+s_1} - t^{2+2s_1}$. Note that $s_1 + s_2 \geq 8$, and one sees $s_1 = s_2 \geq 4$. Then, the least term of ϕ_1 is $-t^4$ while the first term of ϕ_2 is $-2t^4$. Hence, other terms of the same exponents must exist in ϕ_2 such that the sum of the coefficients of which plus -2 equals -1. Since $n_1 + n_2 \geq 6$ and $n_2 \geq n_1$, it is easy to see that all possible candidates are $-t^{3+n_1}$, or $-2t^{1+n_1/2+n_2/2}$. However, the least term of ϕ_1 and ϕ_2 are different, which is a contradiction.

Case 2. If $2 = s_1 < s_2$, substituting $s_1 = 2$ into ϕ_1 and by eliminating the same terms of ϕ_1 and ϕ_2, we have

$\phi_1' : 2t^5 - t^6 - t^{2+s_2} + 2t^{3+s_2}$,

$\phi_2' : t^5 + t^6 - t^{3+n_1} + t^{4+n_1} - t^{5+n_1} - 2t^{1+n_1/2+n_2/2} + 2t^{2+n_1/2+n_2/2} + 2t^{3+n_1/2+n_2/2} - 4t^{4+n_1/2+n_2/2} + 2t^{5+n_1/2+n_2/2} + 2t^{6+n_1/2+n_2/2} - 2t^{7+n_1/2+n_2/2} - t^{3+n_2} + t^{4+n_2} - t^{5+n_2} + t^{2+n_1+n_2} + t^{3+n_1+n_2}$.

Note that $s_1 + s_2 \geq 8$ and $s_2 \geq 6$. Clearly, the least term of ϕ_1' is $2t^5$. Therefore, other terms of the same exponents must exist in ϕ_2' such that the sum of the coefficients of which plus 1 equals 2. Since $n_1 + n_2 \geq 6$ and $n_2 \geq n_1 \geq 1$, it is not hard to see that all possible candidates are $-t^{3+n_1}$, t^{4+n_1}, $-2t^{1+n_1/2+n_2/2}$ and $2t^{2+n_1/2+n_2/2}$. All possible combinations of the terms are : $\{t^5, -t^{3+n_1}, 2t^{2+n_1/2+n_2/2}\}$, or $\{t^5, t^{4+n_1}\}$. For each combination above, we have that the least term of ϕ_2' is $-t^4$ and $-t^4$ does not vanish from ϕ_2', which is a contradiction.

Case 3. If $2 < s_1 < s_2$, the least term of ϕ_1 is $-t^4$. Since the first term of ϕ_2 is $-2t^4$, other terms of the same exponents must exist in ϕ_2 such that the sum of the coefficients of which plus -2 equals -1. Since $n_1 + n_2 \geq 6$ and $n_2 \geq n_1 \geq 1$, it is easy to see that all possible candidates are $-t^{3+n_1}$ and $-2t^{1+n_1/2+n_2/2}$. However, we combine the terms, the coefficient of which plus -2 is not -1, which completes the proof of (1).

(2) Since $s_1 + s_2 = t_1 + t_2$, from ϕ_1, we get

$P_A(W(s_1, s_2))$: $-t^{2+s_1} + 2t^{3+s_1} - t^{4+s_1} - t^{2+s_2} + 2t^{3+s_2} - t^{4+s_2}$,

$P_A(W(t_1, t_2))$: $-t^{2+t_1} + 2t^{3+t_1} - t^{4+t_1} - t^{2+t_2} + 2t^{3+t_2} - t^{4+t_2}$.

Therefore, it follows that $s_1 = t_1$ and $s_2 = t_2$. $\square$

Theorem 9. *Let $2 \leq s_1 \leq s_2$. Then, $W(s_1, s_2)$ is determined by its adjacency spectrum.*

Proof. Let H be cospectral with $W(s_1, s_2)$. Suppose that H has k connected components $H_1, H_2, \cdots, H_k$. By Theorems 3.6–3.8, it is not hard to see that

$$\Pi_2(H) = \sum_{i=1}^{k} \Pi_2(H_i) = \Pi_2(W(s_1, s_2)) = -3.$$

By Theorem 7, $\Pi_2(H_i) \leq 0$, therefore we have $\Pi_2(H_i) \geq -3$ for $1 \leq i \leq k$. Choose the middle vertex v of degree 3 of $W(s_1, s_2)$ such that $W(s_1, s_2) - v = T(1, 1, s_1) \cup T(1, 1, s_2) \cup K_1$. By Lemma 11, $\lambda_1(T(1, 1, n)) < 2$. Thus, by Lemmas 9 and 12 (2), one can see that $\lambda_1(W(s_1, s_2)) > 2$ and $\lambda_2(W(s_1, s_2)) < 2$. On the other hand, it is easy to obtain that $\lambda_1(W_{2,2}) < \frac{3}{2}\sqrt{2}$. By Lemma 10, $\lambda_1(W(s_1, s_2)) < \frac{3}{2}\sqrt{2}$ for all $2 \leq s_1 \leq s_2$. Hence, we know that H only has one component, say H_1, such that $2 < \lambda_1(H_1) \leq \frac{3}{2}\sqrt{2}$ and $\lambda_1(H_i) < 2$ for $2 \leq i \leq k$. Note that $\Pi_2(H_i) \geq -3$, by Lemmas 11, 12 and Theorem 8, we have

$$H_1 \in \mathcal{G}_1 \cup \mathcal{G}_3 \cup \mathcal{G}_7 \cup \mathcal{T}_1 \cup \mathcal{T}_2 \cup \mathcal{T}_3 \cup \{T_0(n) | n \geq 6\}$$

and for $i \geq 2$,

$$H_i \in \mathcal{P} \cup \{T(1, 1, n) | n \geq 1\} \cup \{T(1, 2, k) | k = 2, 3, 4\} \cup \{K_1\}.$$

Clearly, $m(H_1) = n(H_1)$ for each $H_1 \in \mathcal{G}_1 \cup \mathcal{G}_3 \cup \mathcal{G}_7$, $m(H_1) = n(H_1) - 1$ for each $H_1 \in \mathcal{T}_1 \cup \mathcal{T}_2 \cup \mathcal{T}_3 \cup \{T_0(n) | n \geq 6\}$ and $m(H_i) = n(H_i) - 1$ for each $i \geq 2$. Since $m(H) - n(H) = m(W(s_1, s_2)) - n(W(s_1, s_2)) = -1$, we have the following:

(i) $H = H_1 \cup H_2$, where $H_1 \in \mathcal{G}_1 \cup \mathcal{G}_3 \cup \mathcal{G}_7$ and $H_2 \in \mathcal{P} \cup \{T(1, 1, n) | n \geq 1\} \cup \{T(1, 2, k) | k = 2, 3, 4\} \cup \{K_1\}$; or

(ii) $H \in \mathcal{T}_1 \cup \mathcal{T}_2 \cup \mathcal{T}_3 \cup \{T_0(n) | n \geq 6\}$.

Now we distinguish the following cases.

Case 1. $H_1 \in \mathcal{G}_1$. By Theorems 4 and 5, $\Pi_1(H_1) = -1$ and $\Pi_1(H_2) \geq 0$. Then, by Theorem 2, $\Pi_1(H) \geq -1$, which contradicts $\Pi_1(H) = \Pi_1(W(s_1, s_2)) = -2$.

Case 2. $H_1 \in \mathcal{G}_3$. By Theorems 4 and 5, $\Pi_1(H_1) = \Pi_1(W(s_1, s_2)) = -2$. By Theorems 2 and 4, $\Pi_1(H_2) = 0$. By Lemma 14, we have that $|b_6(H)| = |b_6(W(s_1, s_2))|$ if and only if $H = G_{31}(n_1, n_2) \cup T(1, 1, 1)$, where $G_{31}(n_1, n_2)$ does not contain C_6 as its subgraphs. From Lemma 16 (1), $P_A(H) \neq P_A(W(s_1, s_2))$.

Case 3. $H_1 \in \mathcal{G}_7$. By Theorems 4 and Theorem 5, $\Pi_1(H_1) = -3$. Since $\Pi_1(W(s_1, s_2)) = -2$, by Theorems 2 and 4, $\Pi_1(H_2) = 1$, that is $H_2 \cong P_t, t \geq 2$. By Lemma 14 (4), we have that $|b_6(H)| \geq |b_6(W(s_1, s_2))| + 2$, which implies that $P_A(H) \neq P_A(W(s_1, s_2))$.

Case 4. H is a tree, that is $H \in \mathcal{T}_1 \cup \mathcal{T}_2 \cup \mathcal{T}_3 \cup \{T_0(n) | n \geq 6\}$. By Theorem 3.5, $\Pi_1(H) = \Pi_1(W(s_1, s_2)) = -2$. It therefore follows that $H \in \mathcal{T}_3 \cup \{T_0(n) | n \geq 6\}$. By Lemma 15, $H = W_{t_1,t_2}$, where $t_1 + t_2 = s_1 + s_2$. Therefore, $H = W(s_1, s_2)$ from Lemma 16 (2). We complete the proof of the theorem. □

From the proof of Theorem 4.1, we obtain a method to find DS graphs by the following steps.

(i) Characterize all connected graphs with $\Pi_1(G) = i$ and $\Pi_2(G) = j$, where $i \leq 1$ and $j \leq 0$.

(ii) For a given graph G, by applying the properties of invariants, such as $\Pi_1(G)$, $\Pi_2(G)$ and the number of triangles etc., we find all possible cospectral graphs of G.

(iii) Using the results of the eigenvalues, by considering the coefficients of the characteristic polynomial, we give a proof to whether G is determined by its adjacency spectrum.

Here, we give an example to determine whether the graph $F(s_1, s_2)$ (as can be seen in Figure 4) is DS by using the above method.

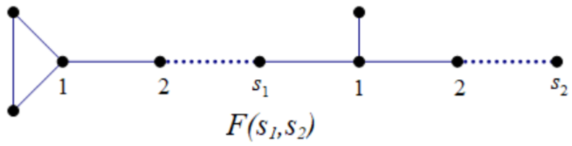

Figure 4. $F(s_1, s_2)$.

Lemma 17 ([21]). *For a graph G, let $TrA(G)^k$ denote the trace of $A(G)^k$ (or the number of close walks of length k in G), then:*

(i) $TrA^3 = 30N_G(K_3)$;

(ii) $TrA^5 = 30N_G(K_3) + 10N_G(C_5) + 10N_G(D_4)$, *where D_4 is the graph obtained from K_3 by adding an edge.*

Suppose that H and $F = F(s_1, s_2)$ are cospectral. At first, we give some invariants. From Lemmas 2, 11 and 17 and Theorems 1 and 6, one can obtain the following invariants.

(i) H and F have the same number of vertices, edges and triangles.

(ii) $N_H(D_4) + N_H(C_5) = N_F(D_4)$.

(iii) $\Pi_i(H) = \Pi_i(F)$, $i = 1, 2$.

(iv) Two is an eigenvalue of F if and only if $(s_1, s_2) \in \{(4, 3), ((6, 2), (3, 5)\}$.

Then, by using some properties (Theorems 3.2–3.8) of $\Pi_i(i = 1, 2)$ and the invariants above one give all possible cospectral graphs of F. Note that $\Pi_2(H) = \Pi_2(F) = -2$, for $(s_1, s_2) \notin \{(4, 3), (6, 2), (3, 5)\}$, we have

$$H \in \{G_{11} \cup G_{12} | G_{11}, G_{12} \in \mathcal{G}_1\} \cup \{G_2 | G_2 \in \mathcal{G}_2\} \cup \{G_4 \cup P_{n_i} | G_4 \in \mathcal{G}_4, n_i \geq 2\}.$$

Finally, using the properties of the eigenvalues (Lemmas 9–11), by considering coefficients of the characteristic polynomial (Lemmas 5 and 8), one can determine the cospectral graphs of F.

From Lemmas 9 and 10, it is not hard to see that $\lambda_1(F) > \lambda_1(G_1)$ for all $G_1 \in \mathcal{G}_1$. By Lemma 5 , we have $b_6(G_4 \cup P_{n_i}) \geq b_6(F) + 1$ for all $G_4 \in \mathcal{G}_4, n_i \geq 2$ and $b_6(H) = b_6(F)$ for $H \in \{G_2 | G_2 \in \mathcal{G}_2\}$ if and only if $H = F(t_1, t_2)$, where $t_1 + t_2 = s_1 + s_2$. Hence, H must be $F(t_1, t_2)$ with $t_1 + t_2 = s_1 + s_2$. Let $t_1 > s_1$ and $t_2 < s_2$, by Lemmas 9 and 10, and it follows that $\lambda_1(F(s_1, s_2)) > \lambda_1(F(s_1, t_2)) > \lambda_1(F(t_1, t_2))$, which implies $H = F(s_1, s_2)$.

When $(s_1, s_2) \in \{(4, 3), ((6, 2), (3, 5)\}$, by direct computation, we have that $F(s_1, s_2)$ is DS. Therefore, we obtain the following result.

Theorem 10. *Let $s_1 \geq 2$ and $s_2 \geq 2$. Then, $F(s_1, s_2)$ is determined by its adjacency spectrum.*

5. Conclusions

In this paper, at first, we gave two invariants $\Pi_1(G)$ and $\Pi_2(G)$ of G, obtained their properties and all connected graphs with $\Pi_1(G) \in \{1, 0, -1, -2, -3\}$ and $\Pi_2(G) \in \{0, -1, -2, -3\}$. We then gave a method to characterize the graphs determined by their adjacency spectrum. To date, one can find the necessary and sufficient conditions for all G with $\Pi_2(G) \in \{0, -1\}$ to be determined by their adjacency spectrum, seeing [5–7,10,17]. For each graph G with $\Pi_2(G) = -2$, we find some DS graphs in the families $\mathcal{G}_4$ and $\mathcal{G}_5$ from [15,16,23–26] and some DS graphs in the family $\mathcal{T}_2$ from [9]. In this paper, we obtained two classes of DS graphs in the family $\mathcal{G}_2$ and $\mathcal{T}_3$. However, no other DS graphs in the family $\mathcal{G}_i$ were found, where $6 \leq i \leq 14$ and $i \neq 10$. A natural follow up would be to characterize DS graphs in the families $\mathcal{G}_i$, where $6 \leq i \leq 14$ and $i \notin \{10, 11\}$. A more interesting avenue would be that of constructing a database of cospectral graphs by the above method and computation.

Author Contributions: J.Y. and H.Z. contributed equally to conceptualization, methodology, validation, formal analysis, writing-review and editing; writing-original draft S.X. All authors read and approved the final manuscript.

Funding: This research was funded by NSFC 11801296, 11961055, the Qinghai Province Natural Science Funds 2019-ZJ-7012 and the 111 Project (D20035).

Data Availability Statement: Not applicable.

Acknowledgments: The authors are very grateful to anonymous referees and editors for their constructive suggestions and insightful comments, which have considerably improved the presentation of this paper.

Conflicts of Interest: The authors declare no conflict of interest.

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