Spectral determination of some chemical graphs

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Abstract. Let $T_k^n$ denote the caterpillar obtained by attaching $k$ pendant edges at two pendant vertices of the path $P_n$ and two pendant edges at the other vertices of $P_n$. It is proved that $T_k^n$ is determined by its signless Laplacian spectrum when $k = 2$ or 3, while $T_2^n$ by its Laplacian spectrum.

1. Introduction

All graphs are simple and undirected in this paper. Let $A(G)$ be the adjacency matrix of $G$, and $D(G)$ the diagonal matrix of vertex degrees. The matrices $D(G) - A(G)$ and $D(G) + A(G)$ are called the Laplacian matrix and the signless Laplacian matrix of $G$, respectively. The spectrum of $A(G)$, $D(G) - A(G)$ and $D(G) + A(G)$ are called the $A$-spectrum, the $L$-spectrum and the $Q$-spectrum of $G$, respectively. The eigenvalues of $D(G) - A(G)$ and $D(G) + A(G)$ are called the $L$-eigenvalues and the $Q$-eigenvalues of $G$, respectively. Since $D(G) - A(G)$ and $D(G) + A(G)$ are real symmetric and positive semi-definite, all their eigenvalues are nonnegative. The largest eigenvalues of $D(G) - A(G)$ and $D(G) + A(G)$ are called the $L$-index and the $Q$-index of $G$, respectively. It is well known that the smallest $L$-eigenvalue of a graph is 0. The characteristic polynomials of $D(G) - A(G)$ and $D(G) + A(G)$ are called the $L$-polynomial and the $Q$-polynomial of $G$, respectively. We say that $G$ is determined by its $L$-spectrum (resp. $Q$-spectrum) if there is no other non-isomorphic graph with the same $L$-spectrum (resp. $Q$-spectrum). Two graphs are said to be $A$-cospectral (resp. $L$-cospectral, $Q$-cospectral) if they have the same $A$-spectrum (resp. $L$-spectrum, $Q$-spectrum). As usual, $P_n$, $C_n$ and $K_n$ denote the path, the cycle and the complete graph of order $n$, respectively. Let $K_{m,n}$ denote the complete bipartite graph with parts of size $m$ and $n$.

The problem “which graphs are determined by their spectra?” originates from chemistry. Günthard and Primas [4] raised this question in the context of Hückel’s theory. Since this problem is generally very difficult, van Dam and Haemers [13] proposed a more modest problem, that is “Which trees are determined by their spectra?” Some results for spectral determination of starlike trees can be found in [2,5,6,9,10,14]. Some double starlike trees determined by their $L$-spectra are given in [7,8]. Some caterpillars determined by their $L$-spectra are given in [1,11,12].

The theory of graph spectra has many important applications in chemistry, especially in treating hydrocarbons. The molecular graph of a hydrocarbon is a tree with maximal degree 4. Let $T_k^n$ denote the
caterpillar obtained by attaching \( k \) pendant edges at two pendant vertices of \( P_n \) and two pendant edges at the other vertices of \( P_n \). For \( k \leq 3 \), \( T_k^n \) is the molecular graph of certain hydrocarbon. For instance, \( T_3^n \) is the molecular graph of a linear alkane (see Fig.1). In this paper, we prove that \( T_k^n \) is determined by its \( Q \)-spectrum when \( k = 2 \) or 3, while \( T_2^n \) by its \( L \)-spectrum. The graph \( T_2^n \) is shown in Fig.2.

Fig. 1. Some examples for graph \( T_3^n \)

\[ T_2^3 \text{ (Ethane)} \quad T_3^3 \text{ (Propane)} \quad T_4^3 \text{ (Butane)} \]

Fig. 2. The graph \( T_2^n \)

2. Preliminaries

In this section, we give some properties which play important role throughout this paper.

Lemma 2.1. [3] For a graph \( G \), the multiplicity of the \( Q \)-eigenvalue 0 of \( G \) is equal to the number of bipartite components of \( G \).

Lemma 2.2. [2] Let \( G \) be a connected graph of order \( n > 1 \), and the maximum degree of \( G \) is \( \Delta \). Let \( q(G) \) be the \( Q \)-index of \( G \). Then \( q(G) \geq \Delta + 1 \), with equality if and only if \( G \) is the star \( K_{1,n-1} \).

Lemma 2.3. [2] For a connected graph \( G \), let \( H \) be a proper subgraph of \( G \). Let \( q(G) \) and \( q(H) \) be the \( Q \)-indices of \( G \) and \( H \), respectively. Then \( q(H) < q(G) \).

Lemma 2.4. [3] Let \( G \) be a graph with \( n \) vertices, \( m \) edges, \( t \) triangles and degree sequence \( d_1, d_2, \ldots, d_n \). Assume that \( q_1, q_2, \ldots, q_n \) are the \( Q \)-eigenvalues of \( G \). Let \( T_k = \sum_{i=1}^n q_i^k \), then

\[
T_0 = n, T_1 = \sum_{i=1}^n d_i = 2m, T_2 = 2m + \sum_{i=1}^n d_i^2, T_3 = 6t + 3 \sum_{i=1}^n d_i^2 + \sum_{i=1}^n d_i^3.
\]
For a graph $G$, let $\phi_A(G, x)$ be the characteristic polynomial of the adjacency matrix of $G$, $\phi_Q(G, x)$ be the $Q$-polynomial of $G$.

**Lemma 2.5.** [3] Let $G$ be a graph of order $n$ and size $m$, $L(G)$ be the line graph of $G$. Then

$$\phi_A(L(G), x) = (x + 2)^m - n \phi_Q(G, x + 2).$$

A connected graph with $n$ vertices is said to be unicyclic if it has $n$ edges. If the girth of an unicyclic graph is odd (resp. even), then this unicyclic graph is said to be odd (resp. even) unicyclic.

**Lemma 2.6.** [2] For a connected graph $G$ with $m$ edges, let $L(G)$ be the line graph of $G$, $\phi_A(L(G), x)$ be the characteristic polynomial of the adjacency matrix of $L(G)$. The following statements hold:

(i) If $G$ is odd unicyclic, then $\phi_A(L(G), -2) = (-1)^m 4$.

(ii) If $G$ is a tree, then $\phi_A(L(G), -2) = (-1)^m (m + 1)$.

(iii) If $G$ is neither odd unicyclic nor a tree, then $\phi_A(L(G), -2) = 0$.

**Lemma 2.7.** [3] For any bipartite graph, the $Q$-polynomial coincides with the $L$-polynomial.

For a graph $G$ with $n$ vertices, let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of the adjacency matrix of $G$. For an integer $k \geq 0$, the number $\sum_{i=1}^n \lambda_i^k$ is called the $k$-th spectral moment of $G$, denoted by $S_k(G)$. Let $N_k(G)$ denote the number of subgraphs of $G$ isomorphic to a graph $F$.

Let $K_{1,n-1}$ be a star of order $n$, $U_n$ be the graph obtained from a cycle $C_{n-1}$ by attaching a pendant vertex to one vertex of $C_{n-1}$. Let $B_4, B_5$ be two graphs obtained from two triangles $T_1, T_2$ by identifying one edge of $T_1$ with one edge of $T_2$ and identifying one vertex of $T_1$ with one vertex of $T_2$, respectively (see Fig. 3).

![Fig. 3. Four graphs $U_4, U_5, B_4, B_5$](image)

**Lemma 2.8.** [15] For any graph $G$, we have

\[
\begin{align*}
S_3(G) &= 6N_{C_3}(G), \\
S_4(G) &= 2N_{P_5}(G) + 4N_{P_4}(G) + 8N_{C_4}(G), \\
S_5(G) &= 30N_{C_5}(G) + 10N_{U_4}(G) + 10N_{C_4}(G), \\
S_6(G) &= 2N_{P_5}(G) + 12N_{P_4}(G) + 24N_{C_4}(G) + 40N_{C_3}(G) + 6N_{P_3}(G) \\
&\quad + 12N_{K_{1,3}}(G) + 36N_{K_{1,2}}(G) + 24N_{K_{1,1}}(G) + 12N_{U_4}(G) + 12N_{C_4}(G).
\end{align*}
\]

In [11], Shen and Hou proved that the graph $T^2_n$ is determined by its $L$-spectrum.

**Theorem 2.9.** [11] Graph $T^2_n$ is determined by its $L$-spectrum.

### 3. The spectrum of the corona of two graphs

In order to get our main results, we will give an upper bound for the $L$-index of graph $T^2_n$ in this section.

Let $G$ be a graph with $n$ vertices, $H$ be a graph with $m$ vertices. The corona of $G$ and $H$, denoted by $G \circ H$, is the graph with $n + mn$ vertices obtained from $G$ and $n$ copies of $H$ by joining the $i$-th vertex of $G$ to each vertex in the $i$-th copy of $H(i = 1, \ldots, n)$. For a graph $F$, let $rF$ denote the union of $r$ disjoint copies of $F$. 
Let $\mu_i(G)$ (resp. $\eta_i(G)$) denote the $i$-th largest L-eigenvalue (resp. Q-eigenvalue) of a graph $G$. If $G$ has distinct L-eigenvalues $\xi_1, \xi_2, \ldots, \xi_n$ (resp. Q-eigenvalue $\eta_1, \eta_2, \ldots, \eta_m$) with multiplicities $k_1, k_2, \ldots, k_n$ (resp. $l_1, l_2, \ldots, l_m$) for the L-spectrum (resp. Q-spectrum) of $G$. Let $\phi_L(G, x)$ and $\phi_Q(G, x)$ be the L-polynomial and Q-polynomial of $G$, respectively. The following theorem is known in the literature, but to make the paper more self-contained we give here the proof.

**Theorem 3.1.** Let $G$ be a graph with $n$ vertices, $H$ a graph with $m$ vertices. The following statements hold:

(a) $\phi_L(G \circ H, x) = \phi_L(G, x^2)\phi_L(H, x - 1)^n$, i.e., the L-spectrum of $G \circ H$ is $\left((\mu_i(G) + m + 1) \pm \sqrt{(\mu_i(G) + m - 1)^2 + 4m}\right)/2$, $(i = 1, \ldots, m, j = 1, \ldots, n)$.

(b) If $H$ is an $r$-regular graph, then $\phi_Q(G \circ H, x) = \phi_Q(G, x^2)\phi_Q(H, x - 1)^n$, i.e., the Q-spectrum of $G \circ H$ is $\left((\mu_i(G) + m + 2r + 1) \pm \sqrt{(\mu_i(G) + m - 1)^2 + 4m}\right)/2$, $(i = 1, \ldots, m, j = 1, \ldots, n)$.

**Proof.** Let $L(G)$ and $L(H)$ be the Laplacian matrices of $G$ and $H$, respectively. The L-polynomial of $G \circ H$ is

$$
\begin{vmatrix}
(x-m)I_n - L(G) & J_1 & \cdots & J_n \\
J_1 & (x-1)I_m - L(H) \\
\vdots & \ddots & \ddots \\
J_n & \cdots & (x-1)I_m - L(H)
\end{vmatrix},
$$

where $J_k (k = 1, \ldots, n)$ is a $n \times m$ matrix in which each entry of the $k$-row is 1 and all other entries are 0. Since the row sum of $(x-1)I_m - L(H)$ is $x-1$, we have

$$
\phi_L(G \circ H, x) = \begin{vmatrix}
(x-m) - \frac{m}{x} & J_1 & \cdots & J_n \\
O & (x-1)I_m - L(H) \\
\vdots & \ddots & \ddots \\
O & \cdots & (x-1)I_m - L(H)
\end{vmatrix},
$$

Since the smallest L-eigenvalue of a graph is 0, we get

$$
\phi_L(G \circ H, x) = \prod_{j=1}^{n} [x^2 - (\mu_j(G) + m + 1)x + \mu_j(G)] \prod_{i=1}^{m-1} (x - \mu_i(H) - 1)^n.
$$

So the L-spectrum of $G \circ H$ is

$$
(\mu_i(H) + 1)^m, \left((\mu_i(G) + m + 1) \pm \sqrt{(\mu_i(G) + m - 1)^2 + 4m}\right)/2, (i = 1, \ldots, m, j = 1, \ldots, n).
$$

Hence part (a) holds.

If $H$ is an $r$-regular graph, then every row sum of the signless Laplacian matrix of $H$ is $2r$. Similar to the above arguments, we can get part (b). $\square$

**Corollary 3.2.** The L-index of graph $T^2_n$ is smaller than $\frac{7\sqrt{33}}{2}$. 

\[\text{Changjiang Bu et al. / Filomat 26:6 (2012), 1123–1131}\]
Lemma 4.1. Proof. Note that \( T_n^k = P_n \circ 2K_1 \). The \( L \)-spectra of \( P_n \) and \( 2K_1 \) are \( 2 + 2 \cos \frac{\pi i}{n} (i = 1, \ldots, n) \) and \( 0^{(2)} \), respectively. By Theorem 3.1, the \( L \)-spectrum of \( T_n^k \) is
\[
1^{(n)}, \mu_i + 3 \pm \sqrt{(\mu_i + 1)^2 + 8} \quad (i = 1, \ldots, n),
\]
where \( \mu_i = 2 + 2 \cos \frac{\pi i}{n} \). Since the \( L \)-index of \( T_n^k \) is \( \frac{\mu_i + 3 \pm \sqrt{(\mu_i + 1)^2 + 8}}{2} \), by \( \mu_1 < 4 \), we get \( \frac{\mu_i + 3 \pm \sqrt{(\mu_i + 1)^2 + 8}}{2} < \frac{7 + \sqrt{33}}{2} \). \( \square \)

Corollary 3.3. The \( Q \)-index of \( C_n \circ 2K_1 \) is \( \frac{7 + \sqrt{33}}{2} \).

Proof. The \( Q \)-spectra of \( C_n \) and \( 2K_1 \) are \( 2 + 2 \cos \frac{2\pi i}{n} (i = 1, \ldots, n) \) and \( 0^{(2)} \), respectively. By Theorem 3.1, the \( Q \)-spectrum of \( C_n \circ 2K_1 \) is
\[
1^{(n)}, q_i + 3 \pm \sqrt{(q_i + 1)^2 + 8} \quad (i = 1, \ldots, n),
\]
where \( q_i = 2 + 2 \cos \frac{2\pi i}{n} \). Clearly the \( Q \)-index of \( C_n \circ 2K_1 \) is \( \frac{7 + \sqrt{33}}{2} \). \( \square \)

4. Spectral determination of graph \( T_n^k \) and graph \( T_n^2 \)

In this section, we will prove that \( T_n^k \) is determined by its \( Q \)-spectrum when \( k = 2 \) or \( 3 \), while \( T_n^2 \) by its \( L \)-spectrum.

It is known that two \( Q \)-cospectral graphs have the same number of vertices and edges. This property also holds for \( A \)-spectrum and \( L \)-spectrum.

Lemma 4.1. Let \( G \) be a graph \( Q \)-cospectral with a tree \( T \) of order \( n \), then one of the following holds:
1. \( G \) is a tree;
2. \( G \) is the union of a tree with \( f \) vertices and \( c \) odd unicyclic graphs, and \( n = 4f \).

Proof. Since \( G \) is \( Q \)-cospectral with a tree of order \( n \), \( G \) is a graph of order \( n \) and size \( n - 1 \). If \( G \) is connected, then \( G \) is a tree. If \( G \) is disconnected, then \( G \) has at least one component which is a tree. From Lemma 2.1 we know that \( G \) has exactly one bipartite component, so \( G \) is the union of a tree and several odd unicyclic graphs. Suppose that \( G \) is the union of a tree of order \( f \) and \( c \) odd unicyclic graphs. By Lemma 2.5, the line graphs of \( G \) and \( T \) have the same \( A \)-spectrum. From Lemma 2.6 we can get \( n = 4f \). \( \square \)

For a graph \( G \) which is \( Q \)-cospectral with \( T_n^2 \), we will show in lemma below that \( G \) and \( T_n^2 \) have the same degree sequence.

Lemma 4.2. Let \( G \) be any graph \( Q \)-cospectral with \( T_n^2 \). Then \( G \) and \( T_n^2 \) have the same degree sequence and \( G \) has no triangles.

Proof. If \( G \) has an isolated vertex, by Lemma 4.1, there exists an integer \( c \) such that \( 3n = 4f \), a contradiction. Hence \( G \) has no isolated vertices.

Let \( a_i \) be the number of vertices of degree \( i \) in \( G \) (note, \( a_0 = 0 \)). Let \( \Delta(G) \) be the maximum degree of \( G \). Since \( T_n^2 \) is a tree, by Lemma 2.7, the \( Q \)-index of \( T_n^2 \) equals to its \( L \)-index. From Corollary 3.2 we know that the \( Q \)-index of \( T_n^2 \) is smaller than \( \frac{7 + \sqrt{33}}{2} \). By Lemma 2.2, we have \( \Delta(G) + 1 < \frac{7 + \sqrt{33}}{2} \), so \( \Delta(G) \leq 5 \). By Lemma 2.4, we have
\[
\sum_{i=1}^{5} a_i = 3n, \quad \sum_{i=1}^{5} ia_i = 2(3n - 1) = 6n - 2,
\]
\[
\sum_{i=1}^{5} i^2a_i = 2n + 3^2 \times 2 + 4^2(n - 2) = 18n - 14,
\]
\[ \sum_{i=1}^{n} t^3 a_i + 6t(G) = 2n + 3^3 \times 2 + 4^3(n - 2) = 66n - 74, \]

where \( t(G) \) is the number of triangles in \( G \). Solving the above equations, we have

\[ a_1 = 2n + t(G) + a_5, \quad a_2 = -3t(G) - 4a_5, \quad a_3 = 2 + 3t(G) + 6a_5, \quad a_4 = n - 2 - t(G) - 4a_5. \]

By \( a_2 = -3t(G) - 4a_5 \geq 0 \), we have \( a_2 = 4a_5 = t(G) = 0 \). So we get

\[ a_1 = 2n, \quad a_2 = 0, \quad a_3 = 2, \quad a_4 = n - 2, \]

i.e., \( G \) and \( T_n^2 \) have the same degree sequence. \( \Box \)

For a graph \( G \), let \( u \) and \( v \) be any two vertices of \( G \). We say that \( u, v \) is an adjacent vertex pair if \( u \) and \( v \) are adjacent. If the degrees of \( u \) and \( v \) are \( d(u) \) and \( d(v) \), we say that \( u, v \) is an adjacent vertex pair with degrees \( d(u) \) and \( d(v) \). Let \( (i, j) \) denote the number of adjacent vertex pairs with degrees \( i \) and \( j \) in \( G \).

**Lemma 4.3.** Let \( G \) be any graph Q-cospectral with \( T_n^2 \). Then

\[ (1, 3) = 4, \ (1, 4) = 2n - 4, \ (3, 3) = 0, \ (3, 4) = 2, \ (4, 4) = n - 3, \]

i.e., the line graph of \( G \) and the line graph of \( T_n^2 \) have the same degree sequence.

**Proof.** Let \( L(G) \) and \( L(T_n^2) \) be the line graphs of \( G \) and \( T_n^2 \), respectively. From Lemma 2.5 we know that \( L(G) \) and \( L(T_n^2) \) are A-cospectral. For two adjacent vertices \( v_1, v_2 \) of degrees \( d(v_1), d(v_2) \) in \( G \), the degree of the corresponding vertex \( v_1v_2 \) in \( L(G) \) is \( d(v_1) + d(v_2) - 2 \). We denote this correspond by

\[ \text{dend} \sim \text{dend} \rightarrow d(v_1) + d(v_2) - 2. \]

By Lemma 4.2, \( G \) and \( T_n^2 \) have the same degree sequence and \( G \) has no triangles. All possible correspondence for vertex degrees between \( G \) and \( L(G) \) are listed as follows.

\[ 1 \sim 3 \rightarrow 2, \ 1 \sim 4 \rightarrow 3, \ 3 \sim 3 \rightarrow 4, \ 3 \sim 4 \rightarrow 5, \ 4 \sim 4 \rightarrow 6. \]

Let \( a_i \) be the number of vertices of degree \( i \) in \( G \), then \( a_1 = 2n, a_2 = 0, a_3 = 2, a_4 = n - 2 \). By Lemma 2.8, we have \( N_{C_4}(L(G)) = N_{C_4}(L(T_n^2)) \). Lemma 4.1 implies that \( G \) cannot contain an even cycle. Since \( G \) has no triangles, we have \( N_{C_4}(L(G)) = N_{C_4}(L(T_n^2)) = (n - 2)N_{C_4}(K_4) \). Since \( L(G) \) and \( L(T_n^2) \) are A-cospectral, \( N_{C_4}(L(G)) = N_{C_4}(L(T_n^2)) \). For any graph \( H \) with vertex degrees \( d_1, d_2, \ldots, d_n \), we have

\[ N_{C_4}(H) = \sum_{i=1}^{n} \binom{d_i}{2}. \]

From the above equation and Lemma 2.8, we have

\[ \begin{align*}
N_{C_4}(L(G)) &= N_{C_4}(L(T_n^2)) = 4 + 3(2n - 4) + 10 \times 2 + 15(n - 3) = 21n - 33, \\
N_{C_4}(L(G)) &= (1, 3) + 3(1, 4) + 6(3, 3) + 10(3, 4) + 15(4, 4). \tag{1}
\end{align*} \]

Considering vertex degrees of \( G \), by \( a_3 = 2 \), we have \( 5 \leq (1, 3) + (3, 3) + (3, 4) \leq 6 \). It is easy to see that \( (1, 3) + (1, 4) = a_1 = 2n \). Note that \( G \) and \( T_n^2 \) both have \( 3n - 1 \) edges. Hence the following facts hold:

\[ \begin{align*}
(1, 3) + (1, 4) + (3, 3) + (3, 4) + (4, 4) &= 3n - 1, \\
(1, 3) + (1, 4) &= 2n, \tag{2}
5 \leq (1, 3) + (3, 3) + (3, 4) \leq 6.
\end{align*} \]
Let $x = (1, 3) + (3, 3) + (3, 4)$. From (1) and (2) we can get
$$7(1, 3) + 4(3, 4) = 9x - 18.$$  
If $x = 5$, then $(3, 3) = 1, (1, 3) + (3, 4) = 4$. By $7(1, 3) + 4(3, 4) = 27$, we have $(1, 3) = \frac{11}{3}$, a contradiction. Hence $x = 6, (3, 3) = 0, (1, 3) + (3, 4) = 6$. By $7(1, 3) + 4(3, 4) = 36$, we can get
$$(1, 3) = 4, (1, 4) = 2n - 4, (3, 3) = 0, (3, 4) = 2, (4, 4) = n - 3.$$  
In this case, $L(G)$ and $L(T_n^2)$ have the same degree sequence. \(\square\)

It is well known that the second smallest $L$-eigenvalue of a graph is larger than 0 if and only if this graph is connected. Hence if two graphs are $L$-cospectral, then they have the same number of components.

The coalescence of two graphs $M_1$ and $M_2$, denoted by $M_1 \cdot M_2$, is the graph obtained by identifying a vertex of $M_1$ with a vertex of $M_2$. For a subgraph $W$ of $K_{d_1} \cdot K_{d_2}$, if two cliques $K_{d_1}, K_{d_2}$ both have edges of $W$, i.e., the edges of $W$ are distributed in different cliques, we say that $W$ is a double $W$-subgraph of $K_{d_1} \cdot K_{d_2}$. Let $K_{d_1} \cdot K_{d_2}(W)$ denote the number of double $W$-subgraphs in $K_{d_1} \cdot K_{d_2}$.

For a subgraph $P$ of a graph $H$, if the edges of $P$ are distributed in three cliques of $H$, then $P$ is called a triple $P$-subgraph of $H$. Let $|H|^3$ be the number of triple $P$-subgraphs in $H$.

Now we will consider the $L$-spectral determination of graph $T_n^2$ shown in Fig.2. If $n = 1$, then $T_n^2 = P_3$. It is known that a path is determined by its $L$-spectrum (see [13]). It is also known that $T_n^2$ is determined by its $L$-spectrum (cf. [7, Theorem 3.1]). Hence $T_n^2$ is determined by its $L$-spectrum when $n \leq 2$.

**Theorem 4.4.** Graph $T_n^2$ is determined by its $L$-spectrum.

**Proof.** It is known that $T_n^2$ is determined by its $L$-spectrum when $n \leq 2$. So we only consider the case that $n > 2$. Let $G$ be any graph $L$-cospectral with $T_n^2$. Since $G$ and $T_n^2$ have the same number of components, $G$ is a tree. By Lemma 2.7, $G$ is $Q$-cospectral with $T_n^2$ and their $Q$-spectra coincide with their $L$-spectra. Let $L(G)$ and $L(T_n^2)$ be the line graphs of $G$ and $T_n^2$, respectively. From Lemma 2.5 we know that $L(G)$ and $L(T_n^2)$ are $A$-cospectral. Let $a_i$ be the number of vertices of degree $i$ in $G$. By Lemma 4.2, we have $a_1 = 2n, a_2 = 0, a_3 = 2, a_4 = n - 2$. By Lemma 4.3, we can get $(1, 3) = 4, (1, 4) = 2n - 4, (3, 3) = 0, (3, 4) = 2, (4, 4) = n - 3$. Hence $G$ has two vertices with degree 3, each vertex of degree 3 in $G$ has two pendant vertices and one vertex of degree 4 as its neighbors. Let $N_T(G)$ be the number of subgraphs of $G$ isomorphic to a graph $F$. Since $L(G)$ and $L(T_n^2)$ are $A$-cospectral, we have $N_{T_n^2}(L(G)) = N_T(L(T_n^2))$. By Lemma 2.8, we have $N_{C_1}(L(G)) = N_{C_1}(L(T_n^2))$. Note that $G$ is a tree. Lemma 4.2 implies that $N_{C_1}(L(G)) = N_{C_1}(L(T_n^2))$. By Lemma 2.8, we have $N_{P_1}(L(G)) = N_{P_1}(L(T_n^2))$. Let $U_4, U_5, B_4, B_5$ be the graphs shown in Fig.3. Since $G$ is a tree and $G$ and $T_n^2$ have the same degree sequence, by Lemma 4.3, we have $N_{K_{1,2}}(L(G)) = N_{K_{1,2}}(L(T_n^2)), N_{C_1}(L(G)) = N_{C_1}(L(T_n^2)) = 0, N_{B_3}(L(G)) = N_{B_3}(L(T_n^2)) = a_4N_{B_4}(K_4)$. Line graphs $L(G)$ and $L(T_n^2)$ can be regarded as the graphs obtained from several complete graphs by some coalescence operations. A vertex of degree $d \geq 3$ in $G$ corresponds to a clique $K_d$ of $L(G)$, two adjacent vertices with degrees $d_1, d_2 \geq 3$ in $G$ corresponds to the coalescence $K_{d_1} \cdot K_{d_2}$ in $L(G)$. By calculating, we have

$$N_{U_4}(L(G)) = N_{U_4}(L(T_n^2)) = a_4N_{U_4}(K_4) \cdot (4, 4)K_4 \cdot K_4 \cdot K_4 \cdot K_4 \cdot K_4 \cdot K_4 \cdot U_4,$$

$$N_{U_5}(L(G)) = N_{U_5}(L(T_n^2)) = (4, 4)K_4 \cdot K_4 \cdot K_4 \cdot K_4 \cdot K_4 \cdot K_4 \cdot (3, 4).$$

$$N_{B_3}(L(G)) = N_{B_3}(L(T_n^2)) = (4, 4)K_4 \cdot K_4 \cdot K_4 \cdot K_4 \cdot K_4 \cdot K_4 \cdot (3, 4).$$

By Lemma 2.8, we get $N_{C_1}(L(G)) = N_{C_1}(L(T_n^2))$. Hence the following facts hold:

$$\begin{align*}
N_{P_1}(L(G)) &= N_{P_1}(L(T_n^2)), N_{P_1}(L(G)) = N_{P_1}(L(T_n^2)), N_{C_1}(L(G)) = N_{C_1}(L(T_n^2)), \\
N_{C_1}(L(G)) &= N_{C_1}(L(T_n^2)), N_{K_{1,2}}(L(G)) = N_{K_{1,2}}(L(T_n^2)), N_{B_3}(L(G)) = N_{B_3}(L(T_n^2)), \\
N_{B_3}(L(G)) &= N_{B_3}(L(T_n^2)), N_{U_4}(L(G)) = N_{U_4}(L(T_n^2)), N_{C_1}(L(G)) = N_{C_1}(L(T_n^2)).
\end{align*}$$

From equations (3) and Lemma 2.8 we get $N_{P_1}(L(G)) = N_{P_1}(L(T_n^2))$. 

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By calculating, we have

\[ N_{P_i}(L(G)) = a_iN_{P_i}(K_4) + (4, 4)K_4 \cdot K_4(P_4) + (3, 4)K_4 \cdot K_3(P_4) + (L(G))_{P_i}^3, \]

\[ N_{P_i}(L(T_n^2)) = a_iN_{P_i}(K_4) + (4, 4)K_4 \cdot K_4(P_4) + (3, 4)K_4 \cdot K_3(P_4) + (L(T_n^2))_{P_i}^3. \]

Since \( N_{P_i}(L(G)) = N_{P_i}(L(T_n^2)) \), we have \((L(G))_{P_i}^3 = (L(T_n^2))_{P_i}^3)\). If there exist vertices of degree 4 outside the path between two vertices of degree 3 in \(G\), then \((L(G))_{P_i}^3 > (L(T_n^2))_{P_i}^3\), a contradiction. Hence all vertices of degree 4 in \(G\) belong to the path between two vertices of degree 3, i.e., \(G = T_n^2\).

Next we will consider the Q-spectral determination of graph \(T_n^2\).

**Theorem 4.5.** Graph \(T_n^2\) is determined by its Q-spectrum.

**Proof.** Let \(G\) be any graph Q-cospectral with \(T_n^2\). First, we show that the corona \(C_g \circ 2K_1\) cannot be a subgraph of \(G\) for any integer \(g \geq 3\). By Lemma 2.7 and Corollary 3.2, the Q-index of \(T_n^2\) is smaller than \(2 + \sqrt{32}\). If there exists an integer \(g\) such that \(C_g \circ 2K_1\) is a subgraph of \(G\), by Corollary 3.3 and Lemma 2.3, the Q-index of \(G\) is larger than or equal to \(2 + \sqrt{32}\), a contradiction. Hence \(C_g \circ 2K_1\) cannot be a subgraph of \(G\).

If \(G\) is connected, then \(G\) is a tree. By Lemma 2.7, \(G\) and \(T_n^2\) have the same L-spectrum. From Theorem 4.4 we can get \(G = T_n^2\).

If \(G\) is disconnected, by Lemma 4.1, \(G\) is the union of a tree and several odd unicyclic graphs. Suppose that \(G_1, \ldots, G_t\) are odd unicyclic components of \(G\), \(T\) is the component of \(G\) which is a tree. Let \(a_i\) be the number of vertices of degree \(i\) in \(G\). By Lemma 4.2, \(a_1 = 2n, a_2 = 0, a_3 = 2, a_4 = n - 2\). By Lemma 4.3, we can get \((1, 3) = 4, (1, 4) = 2n - 4, (3, 3) = 0, (3, 4) = 2, (4, 4) = n - 3\). Since \(C_g \circ 2K_1\) cannot be a subgraph of \(G\) for any integer \(g \geq 3\), we have \(c \leq 2\).

If \(c = 2\), then there are exactly one vertex of degree 3 in the unique cycle of \(G, (i = 1, 2)\). Hence \((3, 4) \geq 4\), a contradiction with \((3, 4) = 2\). If \(c = 1\), then there are at least one vertex of degree 3 in the unique cycle of \(G_1\). By \((3, 4) = 2, (1, 3) = 4\) we know that the star \(K_{1, 3}\) is a component of \(G\), i.e., \(T = K_{1, 3}\). From Lemma 4.1 we can get \(3n = 4 \times 4 = 16\), a contradiction.

Finally we will consider the Q-spectral determination of graph \(T_n^3\).

**Theorem 4.6.** Graph \(T_n^3\) is determined by its Q-spectrum.

**Proof.** From Lemma 2.3 we know that the Q-index of \(T_n^3\) is smaller than the Q-index of \(T_n^2\). By Lemma 2.7 and Corollary 3.2, the Q-index of \(T_n^3\) is smaller than \(2 + \sqrt{32}\). Hence the Q-index of \(T_n^3\) is smaller than \(2 + \sqrt{32}\).

Let \(G\) be any graph Q-cospectral with \(T_n^3\). If \(G\) has an isolated vertex, by Lemma 4.1, there exists an integer \(c\) such that \(3n + 2 = 4^c\), a contradiction. Hence \(G\) has no isolated vertices.

Now we show that the corona \(C_g \circ 2K_1\) cannot be a subgraph of \(G\) for any integer \(g \geq 3\). If there exists an integer \(g\) such that \(C_g \circ 2K_1\) is a subgraph of \(G\), by Corollary 3.3 and Lemma 2.3, the Q-index of \(G\) is larger than or equal to \(2 + \sqrt{32}\). But the Q-index of \(T_n^3\) is smaller than \(2 + \sqrt{32}\), a contradiction. Hence \(C_g \circ 2K_1\) cannot be a subgraph of \(G\) for any integer \(g \geq 3\).

If \(G\) is connected, then \(G\) is a tree. By Lemma 2.7, \(G\) and \(T_n^3\) have the same L-spectrum. From Theorem 2.9 we can get \(G = T_n^3\). Next we only consider the case that \(G\) is disconnected. Let \(a_i\) be the number of vertices of degree \(i\) in \(G\), \(\Delta(G)\) be the maximum degree of \(G\). Since \(G\) has no isolated vertices, we have \(a_0 = 0\). Since the Q-index of \(G\) is smaller than \(2 + \sqrt{32}\), by Lemma 2.2, we have \(\Delta(G) + 1 < 2 + \sqrt{32}\), so \(\Delta(G) \leq 5\). Let \(t(G)\) be the number of triangles in \(G\). By Lemma 2.4, we have

\[ \sum_{i=1}^{5} a_i = 3n + 2, \quad \sum_{i=1}^{5} a_2 = 2(3n + 1) = 6n + 2, \quad \sum_{i=1}^{5} a_3 = 2n + 2 + 4^2n = 18n + 2, \]

\[ \sum_{i=1}^{5} a_i + 6t(G) = 2n + 2 + 4^2n = 66n + 2. \]
Solving the above equations, we have

\[ a_1 = 2n + 2 + t(G) + a_5, \quad a_2 = -4a_5 - 3t(G), \quad a_3 = 6a_5 + 3t(G), \quad a_4 = n - t(G) - 4a_5. \]

Since \( a_2 \geq 0 \), we have \( a_5 = t(G) = 0 \). So we get \( a_1 = 2n + 2, \ a_2 = a_3 = 0, \ a_4 = n \). Since \( G \) is disconnected, by Lemma 4.1, \( G \) is the union of a tree and several odd unicyclic graphs. In this case, there exists an integer \( g \) such that \( C_g \circ 2K_1 \) is a subgraph of \( G \). But \( C_g \circ 2K_1 \) can not be a subgraph of \( G \) for any integer \( g \geq 3 \), a contradiction. \( \Box \)

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References