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Spectral determination of some chemical graphs

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Abstract. Let T_n^k 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_n^k is determined by its signless Laplacian spectrum when $k = 2$ or 3, while T_n^2 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_n^k denote the

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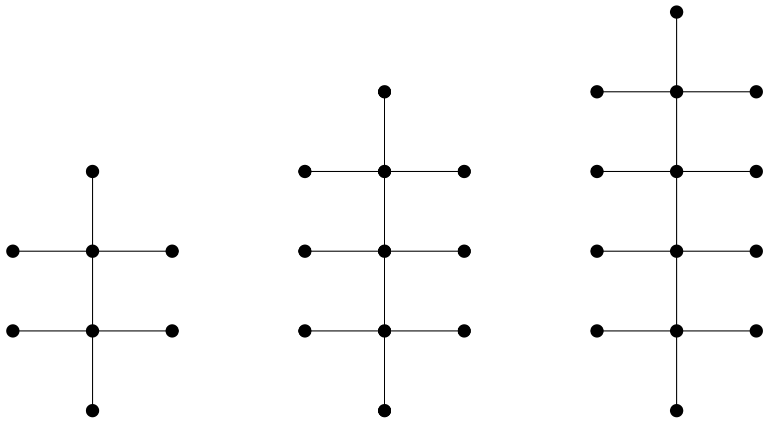
caterpillar obtained by attaching k pendant edges at two pendant vertices of P_n and two pendant edges at the other vertices of P_n. For $k \leq 3$, T_n^k is the molecular graph of certain hydrocarbon. For instance, T_n^3 is the molecular graph of a linear alkane (see Fig.1). In this paper, we prove that T_n^k is determined by its Q-spectrum when $k = 2$ or 3, while T_n^2 by its L-spectrum. The graph T_n^2 is shown in Fig.2.



T_2^3 (Ethane) T_3^3 (Propane) T_4^3 (Butane)

Fig. 1. Some examples for graph T_n^3

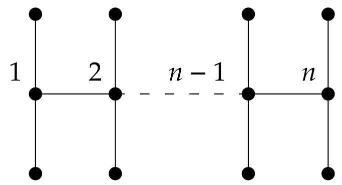


Fig. 2. The graph T_n^2

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 Δ. 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 $N_F(G)$ 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).

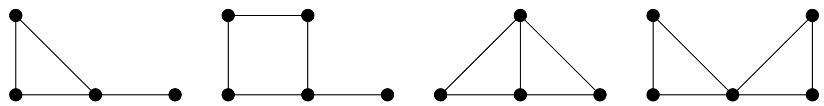


Fig. 3. Four graphs U_4, U_5, B_4, B_5

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

$$\begin{aligned} S_3(G) &= 6N_{C_3}(G), \\ S_4(G) &= 2N_{P_2}(G) + 4N_{P_3}(G) + 8N_{C_4}(G), \\ S_5(G) &= 30N_{C_3}(G) + 10N_{U_4}(G) + 10N_{C_5}(G), \\ S_6(G) &= 2N_{P_2}(G) + 12N_{P_3}(G) + 24N_{C_3}(G) + 40N_{C_4}(G) + 6N_{P_4}(G) \\ &+ 12N_{K_{1,3}}(G) + 36N_{B_4}(G) + 24N_{B_5}(G) + 12N_{U_5}(G) + 12N_{C_6}(G). \end{aligned}$$

In [11], Shen and Hou proved that the graph T_n^3 is determined by its L-spectrum.

Theorem 2.9. [11] *Graph T_n^3 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_n^2 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. $q_i(G)$) denote the i-th largest L-eigenvalue (resp. Q-eigenvalue) of a graph G. If G has distinct L-eigenvalues $\xi_1, \xi_2, \ldots, \xi_m$ (resp. Q-eigenvalue $\eta_1, \eta_2, \ldots, \eta_m$) with multiplicities $k_1, k_2, \ldots, k_m$, we shall write $\xi_1^{(k_1)}, \xi_2^{(k_2)}, \ldots, \xi_m^{(k_m)}$ (resp. $\eta_1^{(k_1)}, \eta_2^{(k_2)}, \ldots, \eta_m^{(k_m)}$) 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 selfcontained we give here the proof.

Theorem 3.1. *Let G be a graph with n vertices, H be a graph with m vertices. The following statements hold:*
(a) $\phi_L(G \circ H, x) = \phi_L(G, \frac{x^2-(m+1)x}{x-1})[\phi_L(H, x-1)]^n$, i.e., the L-spectrum of $G \circ H$ is

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

(b) If H is an r-regular graph, then $\phi_Q(G \circ H, x) = \phi_Q(G, \frac{x^2-(m+2r+1)x+2mr}{x-2r-1})[\phi_Q(H, x-1)]^n$, i.e., the Q-spectrum of $G \circ H$ is

$$(q_i(H)+1)^{(n)},\ \frac{(q_j(G)+m+2r+1) \pm \sqrt{(q_j(G)+m-2r-1)^2+4m}}{2}\ (i = 2, \ldots, m, j = 1, \ldots, n).$$

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

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

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

$$\begin{aligned} \phi_L(G \circ H, x) &= \begin{vmatrix} (x-m-\frac{m}{x-1})I_n - L(G) & J_1 & \cdots & J_n \\ O & (x-1)I_m - L(H) & & \\ \vdots & & \ddots & \\ O & & & (x-1)I_m - L(H) \end{vmatrix} \\ &= \phi_L(G, \frac{x^2-(m+1)x}{x-1})[\phi_L(H, x-1)]^n. \end{aligned}$$

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

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

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). □

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

Proof. Note that $T_n^2 = P_n \circ 2K_1$. 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^2 is

$$1^{(n)}, \frac{\mu_i + 3 \pm \sqrt{(\mu_i+1)^2+8}}{2} \ (i=1,\ldots,n),$$

where $\mu_i = 2+2\cos\frac{\pi i}{n}$. Since the L-index of T_n^2 is $\frac{\mu_1+3\pm\sqrt{(\mu_1+1)^2+8}}{2}$, by $\mu_1 < 4$, we get $\frac{\mu_1+3\pm\sqrt{(\mu_1+1)^2+8}}{2} < \frac{7+\sqrt{33}}{2}$. □

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

$$1^{(n)}, \frac{q_i + 3 \pm \sqrt{(q_i+1)^2+8}}{2} \ (i=1,\ldots,n),$$

where $q_i = 2+2\cos\frac{2\pi i}{n}$. Clearly the Q-index of $C_n \circ 2K_1$ is $\frac{7+\sqrt{33}}{2}$. □

4. Spectral determination of graph T_n^2 and graph T_n^3

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 $n = 4^c f$.

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 $n = 4^c f$. □

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 $3n = 4^c$, 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 $\Delta(G) \le 5$. By Lemma 2.4, we have

$$\sum_{i=1}^{5} a_i = 3n, \ \sum_{i=1}^{5} i a_i = 2(3n-1) = 6n-2,$$

$$\sum_{i=1}^{5} i^2 a_i = 2n + 3^2 \times 2 + 4^2(n-2) = 18n - 14,$$

$$\sum_{i=1}^{5} i^3 a_i + 6t(G) = 2n + 3^3 \times 2 + 4^3(n-2) = 66n - 74,$$

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

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

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

$$a_1 = 2n,\ a_2 = 0,\ a_3 = 2,\ a_4 = n - 2,$$

i.e., G and T_n^2 have the same degree sequence. □

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

$$d(v_1) \sim d(v_2) \to d(v_1) + d(v_2) - 2.$$

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 follow.

$$1 \sim 3 \to 2,\ 1 \sim 4 \to 3,\ 3 \sim 3 \to 4,\ 3 \sim 4 \to 5,\ 4 \sim 4 \to 6.$$

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 $N_{C_3}(L(G)) = N_{C_3}(L(T_n^2))$. 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, $N_{P_2}(L(G)) = N_{P_2}(L(T_n^2))$. For any graph H with vertex degrees $d_1, d_2, \ldots, d_n$, we have

$$N_{P_3}(H) = \sum_{i=1}^{n} \binom{d_i}{2}.$$

From the above equation and Lemma 2.8, we have

$$\begin{cases} N_{P_3}(L(G)) = N_{P_3}(L(T_n^2)) = 4 + 3(2n-4) + 10 \times 2 + 15(n-3) = 21n - 33, \\ N_{P_3}(L(G)) = (1,3) + 3(1,4) + 6(3,3) + 10(3,4) + 15(4,4). \end{cases} \quad (1)$$

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:

$$\begin{cases} (1,3) + (1,4) + (3,3) + (3,4) + (4,4) = 3n - 1, \\ (1,3) + (1,4) = 2n, \\ 5 \leq (1,3) + (3,3) + (3,4) \leq 6. \end{cases} \quad (2)$$

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. □

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 $K_{d_1} \cdot K_{d_2} (d_1, d_2 \geq 3)$, 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_4 is called a *triple P-subgraph* of H. Let $(H)_P^3$ 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_2^2 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 $N_F(G)$ 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 $N_{P_2}(L(G)) = N_{P_2}(L(T_n^2))$. By Lemma 2.8, we have $N_{C_3}(L(G)) = N_{C_3}(L(T_n^2))$. Note that G is a tree. Lemma 4.2 implies that $N_{C_4}(L(G)) = N_{C_4}(L(T_n^2))$. By Lemma 2.8, we have $N_{P_3}(L(G)) = N_{P_3}(L(T_n^2))$. 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 $N_{K_{1,3}}(L(G)) = N_{K_{1,3}}(L(T_n^2)), N_{C_6}(L(G)) = N_{C_6}(L(T_n^2)) = 0, N_{B_4}(L(G)) = N_{B_4}(L(T_n^2)) = a_4 N_{B_4}(K_4)$. 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

$$N_{U_4}(L(G)) = N_{U_4}(L(T_n^2)) = a_4 N_{U_4}(K_4) + (4,4)K_4 \cdot K_4(U_4) + (3,4)K_4 \cdot K_3(U_4),$$

$$N_{U_5}(L(G)) = N_{U_5}(L(T_n^2)) = (4,4)K_4 \cdot K_4(U_5) + (3,4)K_4 \cdot K_3(U_5),$$

$$N_{B_5}(L(G)) = N_{B_5}(L(T_n^2)) = (4,4)K_4 \cdot K_4(B_5) + (3,4)K_4 \cdot K_3(B_5).$$

By Lemma 2.8, we get $N_{C_5}(L(G)) = N_{C_5}(L(T_n^2))$. Hence the following facts hold:

$$\begin{cases} N_{P_2}(L(G)) = N_{P_2}(L(T_n^2)), N_{P_3}(L(G)) = N_{P_3}(L(T_n^2)), N_{C_3}(L(G)) = N_{C_3}(L(T_n^2)), \\ N_{C_4}(L(G)) = N_{C_4}(L(T_n^2)), N_{K_{1,3}}(L(G)) = N_{K_{1,3}}(L(T_n^2)), N_{B_4}(L(G)) = N_{B_4}(L(T_n^2)), \\ N_{B_5}(L(G)) = N_{B_5}(L(T_n^2)), N_{U_5}(L(G)) = N_{U_5}(L(T_n^2)), N_{C_6}(L(G)) = N_{C_6}(L(T_n^2)). \end{cases} \quad (3)$$

From equations (3) and Lemma 2.8 we get $N_{P_4}(L(G)) = N_{P_4}(L(T_n^2))$.

By calculating, we have

$$N_{P_4}(L(G)) = a_4N_{P_4}(K_4) + (4,4)K_4 \cdot K_4(P_4) + (3,4)K_4 \cdot K_3(P_4) + (L(G))^3_{P_4},$$

$$N_{P_4}(L(T_n^2)) = a_4N_{P_4}(K_4) + (4,4)K_4 \cdot K_4(P_4) + (3,4)K_4 \cdot K_3(P_4) + (L(T_n^2))^3_{P_4}.$$

Since $N_{P_4}(L(G)) = N_{P_4}(L(T_n^2))$, we have $(L(G))^3_{P_4} = (L(T_n^2))^3_{P_4}$. If there exist vertices of degree 4 outside the path between two vertices of degree 3 in G, then $(L(G))^3_{P_4} > (L(T_n^2))^3_{P_4}$, 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 $C_g \circ 2K_1$ can not 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 $\frac{7+\sqrt{33}}{2}$. 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 $\frac{7+\sqrt{33}}{2}$, a contradiction. Hence $C_g \circ 2K_1$ can not 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 $G_1, \ldots, G_c$ 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 $C_g \circ 2K_1$ can not 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 $G_i (i = 1,2)$. 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-2}^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^2 is smaller than $\frac{7+\sqrt{33}}{2}$. Hence the Q-index of T_n^3 is smaller than $\frac{7+\sqrt{33}}{2}$.

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 $C_g \circ 2K_1$ can not 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 $\frac{7+\sqrt{33}}{2}$. But the Q-index of T_n^3 is smaller than $\frac{7+\sqrt{33}}{2}$, a contradiction. Hence $C_g \circ 2K_1$ can not 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 $\frac{7+\sqrt{33}}{2}$, by Lemma 2.2, we have $\Delta(G) + 1 < \frac{7+\sqrt{33}}{2}$, so $\Delta(G) \leq 5$. Let $t(G)$ be the number of triangles in G. By Lemma 2.4, we have

$$\sum_{i=1}^{5} a_i = 3n+2, \ \sum_{i=1}^{5} ia_i = 2(3n+1) = 6n+2, \ \sum_{i=1}^{5} i^2a_i = 2n+2+4^2n = 18n+2,$$

$$\sum_{i=1}^{5} i^3a_i + 6t(G) = 2n+2+4^3n = 66n+2.$$

Solving the above equations, we have

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

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. □

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