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Constructing Spectral Siblings and Cousins

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Abstract

This paper investigates the construction of spectral siblings and spectral cousins—pairs of graphs whose characteristic polynomials differ by a constant or a linear function, respectively—through a series of graph operations. We establish sufficient conditions for generating families of such graphs by coalescing known siblings with specific structures.

1 Introduction

The relationship between graph energy and nullity in chemical graph theory is indeed a significant topic, particularly in understanding the thermodynamic stability of molecules represented by graphs. The larger (smaller)

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the energy of the graph, the stronger (weaker) the thermodynamic stability of the corresponding compound. On the other hand, the nullity of a graph is the algebraic multiplicity of number zero in its spectrum. Empirical and theoretical studies suggest an inverse correlation between graph energy and nullity. As nullity increases, the graph energy tends to decrease, indicating reduced stability. Conversely, graphs with low nullity (e.g., non-singular graphs) often exhibit higher energy, reflecting greater stability [1, 3, 5].

Let G be a simple graph with vertex set $V(G) = \{v_1, \cdots, v_n\}$ and edge set $E(G)$. The adjacency matrix $A(G) = [a_{ij}]$ of G is an $n \times n$ symmetric matrix defined by,

$$a_{ij} = \begin{cases} 1 & \text{if } v_i v_j \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

The characteristic polynomial of the graph G is defined as the characteristic polynomial of $A(G)$, *i.e.,*

$$\phi(G, x) = det(xI_n - A(G)),$$

where I_n is the identity matrix of order n. Let $\lambda_1, \cdots, \lambda_n$ be the eigenvalues of $A(G)$. The energy of G, introduced by Gutman in 1978 [8], is defined as

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|.$$

This concept was motivated by Hückel molecular orbital theory in chemistry. In particular, Günthard and Primas [13] showed that, under certain assumptions, the total π-electrons energy in conjugated hydrocarbons can be expressed as the sum of the absolute values of the eigenvalues of the molecular graph's adjacency matrix.

The nullity of a graph G, denoted by $\eta(G)$, is defined as the algebraic multiplicity of the eigenvalue zero in the spectrum of its adjacency matrix. Equivalently, $\eta(G)$ equals the number of eigenvalues of $A(G)$ that are zero. A graph G is called *non-singular* if $\eta(G) = 0$ and *singular*, if $\eta(G) > 0$.

In the study of graph energy, there is already a close relationship between the graph energy and the nullity. A related conjecture is proposed in [3, 5] as follows.

Conjecture 1. *[3, 5] Let G and G_0 be two structurally similar graphs with $\eta(G) < \eta(G_0)$. Then $E(G) > E(G_0)$.*

Due to the ambiguity of the definition of structurally similar graphs involved in the conjecture, earlier attempts [5, 10–12] to justify its validity were based on designing an approximate expression for the energy that contains the nullity term. Recently, Gutman [7] found that the effect of nullity on the energy can be straightforwardly evaluated by calculating the energy of two structurally similar graphs—known as siblings—whose characteristic polynomials differ by exactly a constant. Therefore, the definition of siblings and the related result are given as follows.

Definition 1. [7] Let G_1 be a non-singular simple graph and G_2 a singular simple graph. Then G_1 and G_2 are called siblings (more precisely, *spectral siblings*), if the difference of their characteristic polynomials, $\phi(G_1, x) - \phi(G_2, x)$, is independent of the variable x, *i.e.*, is a constant.

Theorem 1 ([7]). *If the graphs G_1 and G_2 are siblings, then the effect of nullity on the energy of G_1 is equal to $E(G_1) - E(G_2)$.*

Two pairs of siblings, $T_1(k)$, $T_2(k)$ and $T_3(k)$, $T_4(k)$, illustrated in Figure 1, were provided in [7]. A similar construction, in which the characteristic polynomials differ by a linear function, leads to the concept of spectral cousins.

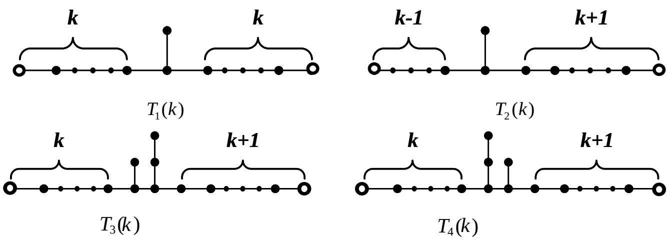

Figure 1. Two pairs of siblings.

Definition 2. Let G_1 be a non-singular simple graph and G_2 a singular simple graph. Then G_1 and G_2 are called *cousins* (more precisely, *spectral* *cousins*), if the difference of their characteristic polynomials, $\phi(G_1, x) - \phi(G_2, x)$, is a linear function of x.

In this paper, we introduce several graph operations to systematically construct spectral siblings and spectral cousins. In Section 2, we propose two graph operations for generating spectral siblings. Correspondingly, constructions for spectral cousins are presented in Section 3.

2 Constructing spectral siblings

In this section, we focus on the construction of spectral siblings. Specifically, we propose a recursive graph operation that generates a series of siblings from a given pair of spectral siblings. Before presenting the main result, we first introduce the following necessary lemmas.

For a vertex $v \in V(G)$, denote by $G - v$ the subgraph obtained from G by deleting the vertex v and all edges incident to it. For an edge $uv \in G$, let $G - uv$ and $G + uv$ denote the graphs resulting from deleting or adding the edge uv, respectively.

Lemma 1. *[15] Let uv be an edge of G. Then*

$$\phi(G) = \phi(G - uv) - \phi(G - u - v) - 2 \sum_{C \in \mathcal{C}(uv)} \phi(G - C), \tag{1}$$

where $\mathcal{C}(uv)$ is the set of cycles containing uv.

Lemma 2 (Sachs Theorem)**.** *[15] Let G be a graph with characteristic polynomial $\phi(G) = \sum\limits_{k=0}^{n} a_k x^{n-k}$. Then for $k \geq 1$,*

$$a_k = \sum_{S \in L_k} (-1)^{\omega(S)} 2^{c(S)}, \tag{2}$$

where L_k denotes the set of Sachs subgraphs of G with k vertices, i.e., the subgraphs in which every component is either a K_2 or a cycle, $\omega(S)$ is the number of connected components of S, and $c(S)$ is the number of cycles contained in S. In addition, $a_0 = 1$.

Let G and H be two graph with $v_1, v_2 \in V(G)$ and $u_1, u_2 \in V(H)$. Denote $G \circ H$ as the resulting graph by coalescing v_1, u_1 and v_2, u_2, respectively.

Theorem 2. *Let G_1, G_2 be spectral siblings and $G_1 \circ K_{1,3}$, $G_2 \circ K_{1,3}$ be the graphs obtained by coalescing G_1, G_2 with $K_{1,3}$ as described above. Let b be the pendant vertex of $K_{1,3}$ which is not coalesced. If $(G_1 \circ K_{1,3}) - b$ and $(G_2 \circ K_{1,3}) - b$ are isomorphic, then $G_1 \circ K_{1,3}$ and $G_2 \circ K_{1,3}$ are also spectral siblings.*

Proof. Let a be the vertex in $K_{1,3}$ adjacent to b. Then b is a pendent vertex in both $G_i \circ K_{1,3}$, $i = 1, 2$. By Lemma 1, the characteristic polynomials satisfy

$$\phi(G_1 \circ K_{1,3}, x) = x\phi(G_1 \circ K_{1,3} - b, x) - \phi(G_1, x),$$

$$\phi(G_2 \circ K_{1,3}, x) = x\phi(G_2 \circ K_{1,3} - b, x) - \phi(G_2, x).$$

Taking the difference of these two equations yields

$$\phi(G_1 \circ K_{1,3}, x) - \phi(G_2 \circ K_{1,3}, x) = \phi(G_1, x) - \phi(G_2, x). \tag{3}$$

Since G_1 and G_2 are siblings, the right-hand side is a constant, implying that $G_1 \circ K_{1,3}$ and $G_2 \circ K_{1,3}$ are also siblings.

It remains to verify that one graph is non-singular and the other is singular.

For $i = 1, 2$, let $\mathbf{r}_i, \mathbf{z}_i$ be the row vectors in $A(G_i \circ K_{1,3})$ corresponding to a and b, respectively. Thus the adjacency matrix of $G_i \circ K_{1,3}$ can be represented as

$$\begin{bmatrix} A(G_i) & \mathbf{r}_i^T & \mathbf{z}_i^T \\ \mathbf{r}_i & 0 & 1 \\ \mathbf{z}_i & 1 & 0 \end{bmatrix}.$$

By performing Gaussian elimination using the last row and column, the nonzero entries in $\mathbf{r}_i^\top$ and $\mathbf{r}_i$ can be eliminated. This operation preserves the nullity, so the singularity of $G_i \circ K_{1,3}$ is the same as that of G_i.

Therefore, $G_1 \circ K_{1,3}$ and $G_2 \circ K_{1,3}$ are spectral siblings. ∎

According to Theorem 2, the graphs $T_3'(k) = T_3(k) \circ K_{1,3}$ and $T_4'(k) =$

$T_4(k) \circ K_{1,3}$, shown in Figure 2, are siblings. Furthermore, by iteratively applying Theorem 2, an infinite family of spectral siblings can be constructed recursively. An example of such a construction starting from $T_1(2)$ and $T_2(2)$ is shown in Figure 3. In all figures, coalesced vertices are marked with hollow dots.

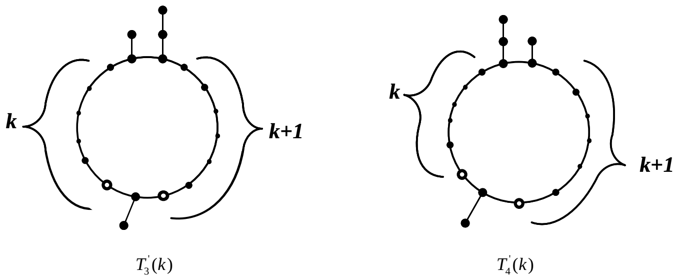

Figure 2. A pair of siblings, $T_3'(k)$ and $T_4'(k)$, constructed from $T_3(k)$ and $T_4(k)$.

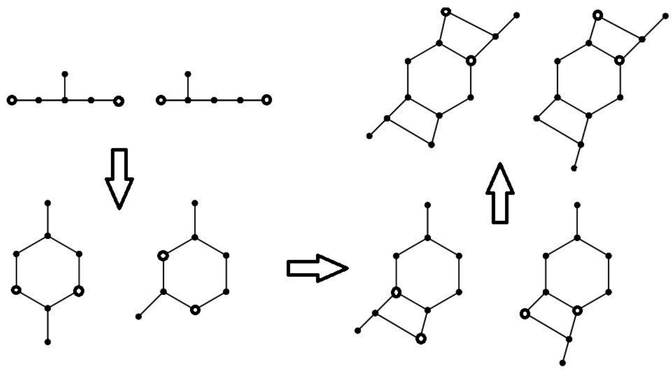

Figure 3. A series of siblings constructed from $T_1(2)$ and $T_2(2)$.

In what follows, we focus on the construction of spectral siblings based on the acyclic graphs. We begin by recalling a classical result.

Lemma 3. *A tree T is non-singular if and only if it has a unique perfect matching.*

This result extends naturally to forests. The following theorem provides a method for constructing spectral siblings by adding an edge within a pair of acyclic siblings.

Theorem 3. *Let G_1, G_2 be acyclic spectral siblings, and let $u_1, v_1 \in V(G_1)$ and $u_2, v_2 \in V(G_2)$. Define $G_1^+ = G_1 + u_1v_1$ and $G_2^+ = G_2 + u_2v_2$. Then G_1^+, G_2^+ are spectral siblings, if the following conditions hold:*

1. *u_i and v_i are non-adjacent in G_i, for $i = 1, 2$;*
2. *$G_1 - u_1 - v_1$ and $G_2 - u_2 - v_2$ are isomorphic;*
3. *$G_1^+ - C_1$ and $G_2^+ - C_2$ are isomorphic, where C_i is the cycle formed by adding edge u_iv_i in G_i, $i = 1, 2$.*

Proof. According to Lemma 1, for $i = 1, 2$, the characteristic polynomial of G_i^+ is given by

$$\phi(G_i^+, x) = \phi(G_i, x) - \phi(G_i^+ - u_i - v_i, x) - 2 \sum_{C_i \in \mathcal{C}(u_iv_i)} \phi(G_i^+ - C_i, x),$$

where $\mathcal{C}(u_iv_i)$ denotes the set of cycles containing the edge u_iv_i. Under the given conditions, G_1 and G_2 are siblings and $G_1^+ - u_1 - v_1$, $G_2^+ - u_2 - v_2$ as well as $G_1^+ - C_1$, $G_2^+ - C_2$ are isomophic. Therefore, G_1^+ and G_2^+ are siblings.

It remains to consider the singularity of G_i^+, $i = 1, 2$. Without loss of generality, assume $\eta(G_1) > 0$ and $\eta(G_2) = 0$. It is sufficient to show that G_1^+ is singular and G_2^+ is non-singular. In fact, we only need to prove that $\eta(G_1^+) > 0$, because if $\eta(G_2^+)$ also greater than zero, this would contradict the fact that the difference of their characteristic polynomials is a constant.

Since G_1 and G_2 are acyclic, by Lemma 3, G_1 has no perfect matching and G_2 has a unique perfect matching. Note that $|V(G_1)| = |V(G_2)|$ is even. We consider three cases based on the structure of G_i^+.

Case 1. Both G_1^+ and G_2^+ are acyclic. If $\eta(G_1^+) = 0$, by Lemma 3, then G_1^+ also has a perfect matching containing the edge u_1v_1, implying that $G_1 - u_1 - v_1$ has a perfect matching. However, since G_2 has a unique perfect matching not containing u_2v_2, the graph $G_2 - u_2 - v_2$ has no perfect matching. This contradicts condition (2). Hence, $\eta(G_1^+) > 0$ and $\eta(G_2^+) = 0$.

Case 2. Both G_1^+ and G_2^+ are unicyclic graphs. Then both G_1 and G_2 are trees. Let $\phi(G_i^+) = \sum\limits_{k=0}^{n} a_k^{(i)} x^{n-k}$, $i = 1, 2$. If $\eta(G_1^+) = 0$, by Lemma 2, $a_n^{(1)} = \sum\limits_{S \in L_n} (-1)^{\omega(S)} 2^{c(S)} \neq 0$. So G_1^+ has Sachs subgraphs.

Subcase 2.1. Suppose G_1^+ has a Sachs subgraph containing the cycle C_1. Let $P_{u_i v_i}$ be the unique path between u_i and v_i in graph G_i, $i = 1, 2$. Then $G_1 - P_{u_1 v_1}$ must have a perfect matching and $|V(G_1 - P_{u_1 v_1})|$ is even. This implies G_1 has a perfect matching, contradicting $\eta(G_1) > 0$.

Subcase 2.2. Suppose all Sachs subgraphs of G_1^+ are perfect matchings, containing the edge $u_1 v_1$. Then $G_1 - u_1 - v_1$ has a perfect matching and by condition (2), so does $G_2 - u_2 - v_2$. However, the perfect matching of G_2 includes at least one edge with one endpoint in $P_{u_2 v_2}$ and the other in $G_2 - V(P_{u_2 v_2})$. Otherwise, G_2^+ has a Sachs subgraph containing C_2. Since $G_1^+ - C_1$ and $G_2^+ - C_2$ are isomorphic, G_1^+ also has a Sachs subgraph containing C_1, a contradiction. Then the removal of u_2 and v_2 in G_2^+ disrupts the matching structure, leaving vertices in $P_{u_2 v_2} - u_2 - v_2$ inadequately covered in $G_2 - u_2 - v_2$, thereby preventing the existence of a perfect matching in $G_2 - u_2 - v_2$. Contradiction.

In both cases, $\eta(G_1^+) > 0$ and $\eta(G_2^+) = 0$, so G_1^+ and G_2^+ are siblings.

Case 3. Suppose G_1^+ is acyclic and G_2^+ is unicyclic. Then u_1 and v_1 must lie in different connected components in G_1, while u_2 and v_2 must lie in the same connected component in G_2. This structural discrepancy would manifest in the graphs $G_1 - u_1 - v_1$ and $G_2 - u_2 - v_2$, preventing them from being isomorphic, contradicting condition (2). Therefore, this scenario is impossible under the given conditions of the theorem.

Based on the analysis of the three cases above, the conclusion holds. ■

As established, $T_3(k)$ and $T_4(k)$ in Figure 2 are siblings. According to Theorem 3, $T_3^*(k)$ and $T_4^*(k)$, shown in Figure 4, are siblings. The endpoints of the newly added edges in both graphs are marked by hollow dots.

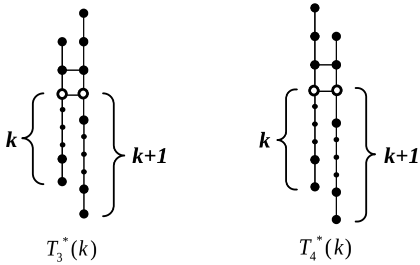

Figure 4. A pair of siblings, $T_3^*(k)$ and $T_4^*(k)$, constructed from $T_3(k)$ and $T_4(k)$.

3 Constructing spectral cousins

In this section, we explore the construction of spectral cousins. Let H be the graph shown in Figure 5, where u, v are the pendant vertices. We propose the following method for constructing spectral cousins.

Theorem 4. *Let G_1, G_2 be spectral siblings and $G_1 \circ H$, $G_2 \circ H$ be the graphs obtained by coalescing G_1, G_2 with H (shown in Figure 5), where $u, v \in H$ are the coalesced vertices. If $(G_1 \circ H) - a - b$ and $(G_2 \circ H) - a - b$ are isomorphic and $\eta(G_1) \geq 2$, then $G_1 \circ H$ and $G_2 \circ H$ are spectral cousins.*

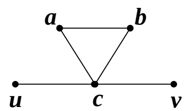

Figure 5. The graph H in Theorem 4

Proof. According to Lemma 1, the characteristic polynomials satisfy

$$\phi(G_1 \circ H, x) = \phi(G_1 \circ H - ab, x) - \phi(G_1 \circ H - a - b, x) - 2\phi(G_1, x),$$
$$\phi(G_2 \circ H, x) = \phi(G_2 \circ H - ab, x) - \phi(G_2 \circ H - a - b, x) - 2\phi(G_2, x).$$

Since $G_1 \circ H - a - b$ and $G_2 \circ H - a - b$ are isomorphic, their characteristic polynomials are identical. Thus,

$$\phi(G_1\circ H,x)-\phi(G_2\circ H,x)=\phi(G_1\circ H-ab,x)-\phi(G_2\circ H-ab,x)-2c, \quad (4)$$

where $c=\phi(G_1,x)-\phi(G_2,x)$ is a constant. Hence, it is sufficient to prove that $\phi(G_1\circ H-ab,x)-\phi(G_2\circ H-ab,x)$ is a linear function. In fact,

$$\phi(G_1\circ H-ab,x)=x\phi(G_1\circ H-b,x)-x\phi(G_1,x), \quad (5)$$

$$\phi(G_2\circ H-ab,x)=x\phi(G_2\circ H-b,x)-x\phi(G_2,x). \quad (6)$$

By Theorem 2, $G_1\circ H-b$ and $G_2\circ H-b$ are siblings. Therefore, $\phi(G_1\circ H,x)-\phi(G_2\circ H,x)$ is a linear function.

Next, we consider the singularity of $G_i\circ H$, $i=1,2$. From Equation (5) and (6), $G_1\circ H-ab$ and $G_2\circ H-ab$ are singular graph. Furthermore, by Cauchy interlacing Theorem [2], $G_1\circ H-a-b$ has at least one eigenvalue equal to zero, due to $\eta(G_1)\geq 2$. Therefore, the constant term of $\phi(G_1\circ H-a-b,x)$ is zero. Since $G_1\circ H-a-b$ and $G_2\circ H-a-b$ are isomorphic, $G_2\circ H-a-b$ is also singular. It indicats that, the singularity of $G_i\circ H$ aligns with that of G_i. That completes the proof. ■

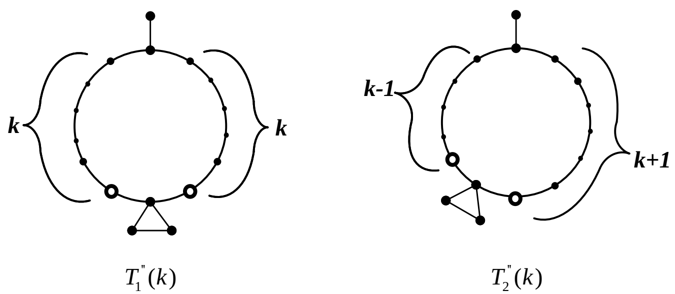

Figure 6. A pair of cousins, $T_1''(k)$ and $T_2''(k)$, constructed from $T_1(k)$ and $T_2(k)$.

As we know, $T_1(k)$ and $T_2(k)$ in Figure 1 are siblings. In addition, the nullities of $T_1(k)$ and $T_2(k)$ depend on the parity of k, *i.e.*,

- $\eta(T_1(k)) = 2$, $\eta(T_2(k)) = 0$, if k is odd;
- $\eta(T_1(k)) = 0$, $\eta(T_2(k)) = 2$, if k is even.

According to Theorem 4, $T_1^{''}(k)$ and $T_2^{''}(k)$, shown in Figure 6, are spectral cousins. The coalesced vertices are indicated by hollow dots.

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