Graph Invertibility and Median Eigenvalues

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Abstract

Let \((G, w)\) be a weighted graph with a weight-function \(w : E(G) \to \mathbb{R}\setminus\{0\}\). A weighted graph \((G, w)\) is invertible to a new weighted graph if its adjacency matrix is invertible. A graph inverse has combinatorial interest and can be applied to bound median eigenvalues of a graph such as have physical meanings in Quantum Chemistry. In this paper, we characterize the inverse of a weighted graph based on its Sachs subgraphs that are spanning subgraphs with only \(K_2\) or cycles (or loops) as components. The characterization can be used to find the inverse of a weighted graph based on its structures instead of its adjacency matrix. If a graph has its spectra split about the origin, i.e., half of eigenvalues are positive and half of them are negative, then its median eigenvalues can be bounded by estimating the largest and smallest eigenvalues of its inverse. We characterize graphs with a unique Sachs subgraph and prove that these graphs have their spectra split about the origin if they have a perfect matching. As applications, we show that the median eigenvalues of stellated graphs of trees and corona graphs belong to different halves of the interval \([-1, 1]\).

1 Introduction

In this paper, graphs may contain loops but no multiple edges. Let \(G\) be a graph with vertex set \(V(G)\) and edge set \(E(G)\). Its adjacency matrix \(A\) is defined as the \(ij\)-entry \((A)_{ij} = 1\) if \(ij \in E(G)\) and \((A)_{ij} = 0\) otherwise. Assume that \(\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n\) where \(n = |V(G)|\), are the eigenvalues of \(A\) (also the eigenvalues of \(G\)). In Quantum Chemistry, the eigenvalues of a molecular graph have physical meanings. For example, the sum of absolute value of eigenvalues of a graph \(G\), also called the energy of \(G\) \([10]\), is often equal to the total Hückel \(\pi\)-electron energy of the molecule represented by \(G\). Also many physico-chemical parameters of molecules are determined by or are dependent upon the HOMO-LUMO gap \([5, 9]\), which is often given as the difference between the median eigenvalues, \(\lambda_H - \lambda_L\), where \(H = \lfloor (n+1)/2 \rfloor\) and \(L = \lceil (n+1)/2 \rceil\).

Throughout the more traditional chemical literature, there has been extensive effort to deal with the HOMO-LUMO gap mostly in an explicit consideration of individual molecules case by case.

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A few mathematical methods have been developed especially in the last decade to characterize the HOMO-LUMO gaps of graphs in a general manner \[7, 12, 14, 15, 20, 21, 22, 30\]. Recently, Mohar introduced a graph partition method to bound the HOMO-LUMO gaps for subcubic graphs \[20, 21, 22\]. However, not all graphs have these nice partition properties and a desired partition is hard to find, even for plane subcubic graphs \[20\].

It is well-known that the eigenvalues of a bipartite graph are symmetric about the origin. If the adjacency matrix \(A\) of a bipartite graph \(G\) is invertible, then the reciprocal of the maximum eigenvalue of \(A^{-1}\) is equal to the \(\lambda_H\) of \(G\) and the reciprocal of the least eigenvalue of \(A^{-1}\) is equal to \(\lambda_L\). Based on this fact, the invertibility of adjacency matrices of trees had been discussed in order to evaluate their HOMO-LUMO gaps \[7, 12\], and later the method has been extended to bipartite graphs with a unique perfect matching \[14, 25\]. Besides the chemical interests, the invertibility of adjacency matrices of graphs is of independent interest as indicated in \[7, 19\]. For examples, the invertibility of adjacency matrices of graphs has connections to other interesting combinatorial topics such as Möbius inversion of partially ordered sets (see the treatment in Chapter 2 of Lovász \[17\]) \[7, 25\] and Motzkin numbers \[3, 19\].

Here, the aim of this paper is to extend this idea to graphs with more general settings. Note that, the eigenvalues of non-bipartite graphs are not symmetric about the origin. But, our methodology works when the eigenvalues of a graph evenly split about the origin, i.e., half of them are positive and half of them are negative. Another purpose of this paper is to discuss the invertibility of graphs. It is very clear when a matrix is invertible. But the inverse of an adjacency matrix of a graph is not necessarily an adjacency matrix of another graph. In fact, if the adjacency matrix \(A\) of a graph \(G\) is invertible and \(A^{-1}\) is an adjacency matrix of another simple graph, then \(G\) has to be the graph \(nk\) \[11\]. Godsil \[7\] defined an inverse of a bipartite graph \(G\) with a unique perfect matching to be a graph, denoted by \(G^{-1}\) with adjacency matrix diagonally similar to the inverse of adjacency matrix of \(G\), i.e., the adjacency matrix of \(G^{-1}\) is \(D\lambda^{-1}D\) for some diagonal matrix \(D\) with entries 1 or \(-1\) on its diagonal, where \(\lambda\) is the adjacency matrix of \(G\) (see also \[14\]). This definition uniquely defines the inverse of a graph. But the invertible graphs are still quite limited. In order to make a more encompassing definition of the inverse of a graph, McLeman and McNicholas \[19\] defined that a graph \(G_1\) is an inverse of a graph \(G_2\) if \(\lambda\) is an eigenvalue of \(G_1\) if and only if \(1/\lambda\) is an eigenvalue of \(G_2\). But the inverses of a graph defined by McLeman and McNicholas are not always unique because there exist cospectral invertible graphs (see Figure \[1\] cf. \[8\]). Based on these two different definitions, the invertibility of bipartite graphs with unique perfect matching has been discussed in \[7, 14, 19, 25\]. However, their methods can not be easily used for non-bipartite graphs. In these papers, the authors seek to deal with signs in the computation of the inverse of the adjacency matrix of the original graph. In order to avoid the special treatment of signs, we here modify the definition of graph inverse to weighted graphs, with signs allowed on the weights. The modified definition can uniquely and broadly define the inverse for graphs.

A weighted graph \((G, w)\) is a graph with a weight function \(w : E(G) \to \mathbb{R}\setminus\{0\}\). The adjacency matrix of a weighted graph, denoted by \(\mathbb{A}\), is defined as

\[
(\mathbb{A})_{ij} := \begin{cases} 
w(ij) & \text{if } ij \in E(G); \\
0 & \text{otherwise}
\end{cases}
\]
where loops, with \( w(ii) \neq 0 \), are allowed. A weighted graph \((G, w)\) is invertible if its adjacency matrix has an inverse that is also an adjacency matrix of a weighted graph.

A graph can be treated as a weighted graph with the constant weight function \( w : E(G) \to 1 \). Another important family of weighted graphs is signed graphs. A signed graph \((G, \sigma)\) is a weighted graph with a weight function \( \sigma : E(G) \to \{-1, +1\} \), where \( \sigma \) is called the signature of \( G \) (see [27]). Two signatures of a graph \( G \) are equivalent to each other if one can be obtained from the other by changing the signatures of all edges in an edge-cut of \( G \). A signed graph is balanced if it is equivalent to a graph. In Godsil’s definition, a bipartite graph with a unique perfect matching is invertible if its inverse is a balanced signed graph. Signed graphs have extensive applications in combinatorics and matroid theory [28]. For more details and interesting problems on signed graphs, one may refer to the survey of Zaslavsky [29].

A Sachs subgraph is a spanning subgraph with only \( K_2 \) or cycles (including loops) as components. In this paper, we investigate the invertibility of weighted graphs and characterize their inverses based on Sachs subgraphs. A characterization of graphs with a unique Sachs subgraph is obtained. For signed graphs with a unique Sachs subgraph, we show that their spectra split about the origin if they have a perfect matching. As applications, we show that the median eigenvalues of stellated graphs of trees and corona graphs belong to the interval \([-1, 1]\).

## 2 Inverses of weighted graphs

Let \((G, w)\) be a weighted graph. The following is a straight-forward proposition that establishes the equivalent relation between the invertibility of weighted graphs and the invertibility of real symmetric matrices.

**Proposition 2.1.** Let \((G, w)\) be a weighted graph with adjacency matrix \( A \). Then \((G, w)\) is invertible if and only if \( \det(A) \neq 0 \), and the inverse of an invertible weighted graph \((G, w)\) is unique.

**Proof.** Let \((G, w)\) be a weighted graph. Then \( \det(A) \neq 0 \) if and only if then \( A \) has an inverse \( A^{-1} \). Note that \((A^{-1})^T = (A^T)^{-1} = A^{-1} \). Hence \( A^{-1} \) is a symmetric matrix, which is corresponding to a weighted graph. Note that, \( A^{-1} \) is unique. So the the inverse of \((G, w)\) is unique. The proposition follows. \( \square \)

The adjacency matrix \( A \) of a weighted graph \((G, w)\) is a linear transformation from the vector space \( \mathbb{R}^n \) to itself. If \((G, w)\) is invertible, then \( A \) is full rank. In other words, all column vectors \( b_i \),
of $A$ for $i \in V(G)$ form a basis of $\mathbb{R}^n$.

Throughout the paper, we always use $(A)_{ij}$ to denote the $(i, j)$-entry of the matrix $A$, and $A_{(ij)}$ to denote the submatrix of $A$ by deleting the $i$-th row and the $j$-th column.

A subgraph $H$ of a graph $G$ is spanning if $V(H) = V(G)$. A weighted graph $(H, w_H)$ is a subgraph of $(G, w)$, if $H$ is a subgraph of $G$ and $w_H(e) = w(e)$ for any $e \in E(H) \subseteq E(G)$. The weight of a subgraph $H$ is defined as $w(H) = \prod_{e \in E(H)} w(e)$. A spanning subgraph $S$ is called a Sachs subgraph of $G$ if every component of $S$ is either $K_2$ or a cycle (including loops). For a Sachs subgraph $S$, denote the set of all cycles of $S$ by $C$, the set of all loops of $S$ by $L$ and the set of all $K_2$'s of $S$ by $M$ which is a matching of $G$. So a Sachs subgraph consists of three parts: cycles, loops and a matching. In the rest of the paper, we also denote a Sachs subgraph as $S = C \cup M \cup L$. The determinant of adjacency matrix of a graph can be represented by its Sachs subgraphs as follows.

**Theorem 2.2** (Harary, [10]). Let $G$ be a simple graph and $A$ the adjacency matrix. Then

$$
det(A) = \sum_S 2^{|C|} (-1)^{|C| + |E(S)|},$$

where $S = C \cup M$ is a Sachs subgraph.

The following result extends Theorem 2.2 to weighted graphs $(G, w)$ which may contain loops.

**Theorem 2.3.** Let $(G, w)$ be a weighted graph and $A$ the adjacency matrix. Then

$$
det(A) = \sum_S 2^{|C|} w(C \cup L) w^2(M) (-1)^{|C| + |L| + |E(S)|},$$

where $S = C \cup M \cup L$ is a Sachs subgraph.

**Proof.** By the definition of determinant,

$$
det(A) = \sum_{\pi} \text{sgn}(\pi) \prod_{i \in V(G)} (A)_{i\pi(i)},$$

where $\pi$ is a permutation on $V(G) = \{1, 2, \ldots, n\}$. A permutation $\pi$ on $V(G)$ contributing to $\det(A)$ corresponds to a Sachs subgraph $S$: a cycle of $\pi$ with length $k \notin \{1, 2\}$ corresponds to a cycle of $G$ with length $k$, a cycle of $\pi$ of length 1 (fixing a vertex) corresponds to a loop of $G$, and a cycle of length 2 corresponds to an edge (or $K_2$). Hence,

$$
\text{sgn}(\pi) \prod_{i \in V(G)} (A)_{i\pi(i)} = (-1)^{|C| + |E(C)| + |M|} \prod_{C \in C} w(C) \prod_{(i) \in \pi} (A)_{ii} \prod_{(ij) \in \pi} (A)_{ij} (A)_{ji} = (-1)^{|C| + |L| + |E(S)|} w(C) w(L) w^2(M).
$$

But a Sachs subgraph $S = C \cup M \cup L$ corresponds to $2^{|C|}$ permutations because for each cycle $C = i_1 i_2 \cdots i_k$ ($k \geq 3$), there are two different corresponding cyclic permutations $(i_1 i_2 \cdots i_k)$ and $(i_k i_1 i_2 \cdots i_{k-1})$. So,

$$
det(A) = \sum_{\pi} \text{sgn}(\pi) \prod_{i \in V(G)} (A)_{i\pi(i)} = \sum_S 2^{|C|} w(C \cup L) w^2(M) (-1)^{|C| + |L| + |E(S)|}.
$$

This completes the proof.
For some special weighted graphs, the formula in Theorem 2.3 can be simplified. For example, via the following corollary.

**Corollary 2.4.** Let \((G, \sigma)\) be a signed simple graph with a unique Sachs subgraph. If \(G\) has a perfect matching \(M\), then \(\det(\mathcal{A}) = (-1)^{|M|}\), where \(\mathcal{A}\) is the adjacency matrix of \((G, \sigma)\).

**Proof.** Note that, a perfect matching is a Sachs subgraph. Since \((G, \sigma)\) is simple and has a unique Sachs subgraph, it follows that the unique Sachs subgraph of \(G\) is the perfect matching \(M\). By Theorem 2.3 and the fact that \(C = \emptyset\) and \(L = \emptyset\),

\[
\det(\mathcal{A}) = \sum_S 2^{|C|} \sigma(C \cup L) \sigma^2(M)(-1)^{|C|+|L|+|E(S)|}
\]

\[
= (-1)^{|M|} \sigma^2(M).
\]

Note that \(\sigma : E(G) \to \{-1, 1\}\). So \(\sigma^2(M) = 1\). Further, \(\det(\mathcal{A}) = (-1)^{|M|}\).

Let \((G, w)\) be an invertible weighted graph. The next result characterizes the inverse of \((G, w)\).

**Theorem 2.5.** Let \((G, w)\) be a weighted graph with adjacency matrix \(\mathcal{A}\), and

\[
P_{ij} = \{P| P\text{ is a path joining } i \text{ and } j \neq i \text{ such that } G - V(P) \text{ has a Sachs subgraph } S\}\.
\]

If \((G, w)\) has an inverse \((G^{-1}, w^{-1})\), then

\[
w^{-1}(ij) = \begin{cases} \frac{1}{\det(\mathcal{A})} \sum_{P \in P_{ij}} \left( w(P) \left( \sum_S w(C \cup L) w^2(M) 2^{|C|} (-1)^{|C|+|L|+|E(S)\cup E(P)|} \right) \right) & \text{if } i \neq j; \\
\frac{1}{\det(\mathcal{A})} \det(\mathcal{A}_{(ii)}) & \text{otherwise}
\end{cases}
\]

where \(S = C \cup M \cup L\) is a Sachs subgraph of \(G - V(P)\).

**Proof.** Since \((G, w)\) is invertible, \(\mathcal{A}^{-1}\) exists and is an adjacency matrix of \((G^{-1}, w^{-1})\). According to the definition of the inverse of a weighted graph, \(w^{-1}(ij) = (\mathcal{A}^{-1})_{ij}\).

By Proposition 2.1 and Cramer’s rule,

\[
(\mathcal{A}^{-1})_{ij} = (\mathcal{A}^{-1})_{ji} = \frac{c_{ij}}{\det(\mathcal{A})}
\]

where \(c_{ij} = (-1)^{i+j} \det(\mathcal{A}_{(ij)})\). Let \(M_{i,j}\) be the matrix obtained from \(\mathcal{A}\) by replacing the \((i, j)\)-entry by 1 and all other entries in the \(i\)-th row and \(j\)-th column by 0. Then by Laplace expansion, \(c_{ij} = \det(M_{i,j})\)

If \(i = j\), then \(\det(M_{i,i}) = \det(\mathcal{A}_{(ii)})\). So \(w^{-1}(ii) = \det(\mathcal{A}_{(ii)})/\det(\mathcal{A})\). So in the following, assume that \(i \neq j\).

Since all \((i, k)\)-entries \((k \neq j)\) of \(M_{i,j}\) are equal to 0 and its \((i, j)\)-entry is 1, only permutations taking \(i\) to \(j\) contribute to the the determinant of \(M_{i,j}\). Let \(\Pi_{i \to j}\) be the family of all permutations on \(V(G) = \{1, 2, \ldots, n\}\) taking \(i\) to \(j\). Denote the cycle of \(\pi\) permuting \(i\) to \(j\) by \(\pi_{ij}\). For convenience, \(\pi_{ij}\) is also used to denote the set of vertices which corresponds to the elements in the permutation.
cycle \( \pi_{ij} \), for example, \( V(G) \setminus \pi_{ij} \) denotes the set of vertices in \( V(G) \) but not in \( \pi_{ij} \). Denote the permutation of \( \pi \) restricted on \( V(G) \setminus \pi_{ij} \) by \( \pi \setminus \pi_{ij} \). Then

\[
\det(M_{i,j}) = \sum_{\pi \in \Pi} \text{sgn}(\pi) \prod_{k \in V(G) \setminus \pi_{ij}} w(k\pi(k))
\]

This completes the proof.

In the above theorem, \( \det(A_{(ii)}) \) can be represented by a formula in terms of all Sachs subgraphs of the subgraph \( (G - i, w) \) obtained from \( (G, w) \) by deleting the vertex \( i \) and any incident loop and edges as given in Theorem 2.3. A weighted graph \( (G, w) \) is simply invertible or has a simple inverse if its inverse is a weighted simple graph (i.e., without loops). The following proposition is a direct corollary of Proposition 2.1 and Theorem 2.5.

**Proposition 2.6.** A weighted graph \( (G, w) \) is simply invertible if and only if for every vertex \( i \), \( (G - i, w) \) is not invertible.

The following proposition shows that an invertible simple weighted bipartite graph is always simply invertible.

**Proposition 2.7.** Every invertible simple weighted bipartite graph is simply invertible.

**Proof.** Let \( (G, w) \) be an invertible weighted graph such that \( G \) is simple and bipartite. Then \( \det(A) \neq 0 \) where \( A \) is the adjacency matrix of \( (G, w) \). So \( (G, w) \) has at least one Sachs subgraph \( S = C \cup M \cup L \). Further, \( L = \emptyset \) because \( G \) is simple. So a simple bipartite graph with a Sachs subgraph has even number of vertices. For every vertex \( i \in V(G) \), \( (G - i, w) \) has no Sachs subgraph because \( G - i \) is bipartite and has odd number of vertices. So \( (G - i, w) \) is not invertible. It follows from Proposition 2.6 that \( (G, w) \) is simply invertible.

The inverses of simple bipartite graphs with a unique Sachs subgraph (i.e., a unique perfect matching) have been discussed in [14, 19, 25]. In the next section, we consider the inverse of signed graphs with a unique Sachs subgraph and extend results in [14, 19, 25] for non-bipartite graphs.

### 3 Signed graphs with a unique Sachs subgraph

Let \( (G, \sigma) \) be a signed graph. If \( (G, \sigma) \) has a unique Sachs subgraph, then the determinant of its adjacency matrix is not zero by Theorem 2.3. By Proposition 2.1, a signed graph with a unique Sachs subgraph is always invertible. In this section, we study properties of the inverse of signed graphs \( (G, \sigma) \).
Before proceeding to our results, we need some definitions. Let $G$ be a graph and $M$ a matching $G$. A cycle of $G$ is $M$-alternating if the edges of $G$ alternate between $M$ and $E(G) \setminus M$. So an $M$-alternating cycle is always of even size. A path $P$ (or a cycle $C$) of $G$ is $M$-alternating if all vertices of $P$ (or $C$) are covered by $M$ and the edges of $P$ (or $C$) alternate between $M$ and $E(G) \setminus M$.

Let $G$ have a Sachs subgraph $S = C \cup M \cup L$. If $C$ contains a cycle of even size, then the edges of the cycle can be partitioned into two disjoint matchings. Replacing the cycle in $S$ by any one of these two matchings generates another Sachs subgraph of $G$. If $S$ is a unique Sachs subgraph of $G$, then every cycle in $C$ is of odd size. This fact we use repeatedly in the proof of the following result which characterizes all simple graphs with a unique Sachs subgraph. A family $\mathcal{D}$ of cycles is independent if there is no edge joining vertices from two different cycles in $\mathcal{D}$.

**Theorem 3.1.** A simple graph $G$ has a unique Sachs subgraph if and only if $G$ can be reduced to a family of independent odd cycles by repeatedly deleting pendant edges together with their end-vertices.

*Proof. Sufficiency:* Let $G$ be a simple graph which can be reduced to a family of independent odd cycles by repeating the deletion of pendant edges together with their end-vertices. Let $M$ be the set of all edges of $G$ deleted in the process and $C$ be the set of remaining odd cycles. Clearly, $C \cup M$ is a Sachs subgraph. On the other hand, for any Sachs subgraph $S$ of $G$, $M \subseteq S$. Since $C$ is the set of independent odd cycles, $C \subseteq S$. So $S = C \cup M$. Hence $G$ has a unique Sachs subgraph.

*Necessary:* Assume that $G$ has a unique Sachs subgraph $S = C \cup M \cup L$. Then $L = \emptyset$ because $G$ is simple. If $G$ consists of a family of independent odd cycles, then we are done. Without loss of generality, we may assume that $G$ is connected but not an odd cycle. First, we establish the following:

**Claim:** $G$ has a pendant edge.

*Proof of Claim:* Suppose on the contrary that $G$ does not have a pendant edge.

First, suppose that $C = \emptyset$. Then $S$ is a perfect matching of $G$. Choose a longest $S$-alternating path $P$ (edges of $P$ alternate between $S$ and $E(G) \setminus S$). Let $x$ and $y$ be the end-vertices of $P$ and $xx', yy' \in E(P) \cap S$. Since $P$ is a longest path and $G$ has no pendant edges, both $x$ and $y$ have respective neighbors $x^+$ and $y^+$ in $V(P) \setminus \{x', y'\}$. Let $C_x := xx'P x^+ x$ be the cycle traveling from $x$ to $x^+$ through the path $P$ then returning to $x$ through the edge $x^+ x$. Similarly, $C_y := yy'P y^+ y$. If $C_x$ has even size, then the symmetric difference $E(C_x) \oplus S$ is another perfect matching of $G$, a contradiction to $G$ having a unique Sachs subgraph. Hence $C_x$ is of odd size. So is $C_y$.

If $C_x \cap C_y = \emptyset$, then $P - V(C_x \cup C_y)$ has an even number of vertices and hence has a perfect matching $M'$ (see Figure 2 Left). So $(S \setminus E(P)) \cup \{C_x, C_y\} \cup M'$ is another Sachs subgraph of $G$, a contradiction. So, $C_x \cap C_y \neq \emptyset$ (see Figure 2 Right). Let $C := xP y^+ yP x^+ x$. Since both $C_x$ and...
$C_y$ have odd sizes, it follows that $C$ is an $M$-alternating cycle of $G$. Hence the symmetric difference
$E(C) \oplus S$ is another perfect matching of $G$, contradicting that $G$ has a unique Sachs subgraph.

So in the following, assume that $C \neq \emptyset$. Note that every cycle of $C$ has odd sizes. Let $C \in C$. Recall that $S = C \cup M$. Let $x$ be a vertex of $C$ and $P$ be a longest path starting at $x$ such that the edges of $P$ are alternating between $E(G) \setminus M$ and $M$.

![Figure 3](image)
The unique Sachs subgraph $S$ contains a cycle $C$.

If another end vertex $y$ of $P$ is not covered by the matching $M$, then $y$ is contained in a cycle $C'$ of $C$. If $C' \neq C$, then the graph consisting of $C, C'$ and the path $P$ has a perfect matching, denoted by $M'$ (see Figure 3, Left). So $G$ has another Sachs subgraph obtained from $S$ by replacing $C, C'$ and the edges in $P' \cap M$ by $M'$, a contradiction. So assume that $C = C'$, then $x, y \in V(C)$. Since $C$ is of odd size, there is a path $P'$ of $C$ connecting $x$ and $y$ with an odd number of vertices. Then $P' \cup P$ is an odd cycle and $C - V(P')$ is a path with an even number of vertices. So $G$ has another Sachs subgraph consisting of $S \setminus (\{C\} \cup E(P))$, the cycle $P' \cup P$ and a perfect matching of $C - V(P')$, again a contradiction.

So assume that $y$ is covered by the matching $M$ (see Figure 3, Right). Since $G$ has no pendant edges, $y$ has another neighbor $y'$ in $P$. By the same argument as above, the cycle $C' := y'Pyy'$ consisting of the segment of $P$ from $y'$ to $y$ and the edge $yy'$ is of odd size. Let $G' = C \cup P$. Then $G' - V(C')$ has a perfect matching, denoted by $M'$. So $G$ has another Sachs subgraph obtained from $S$ by replacing $C$ and $P \cap M$ by $C'$ and $M'$, a contradiction. This contradiction completes the proof of our Claim. \[ \square \]

Now by our Claim, $G$ has a pendant edge $e$. Deleting the edge $e$ together with its end vertices generates a subgraph $G_1$ of $G$ which still has a unique Sachs subgraph. Applying the claim on $G_1$, then either $G_1$ also contains a pendant edge or else $G_1$ is a family of independent odd cycles. If the former holds, delete the pendant edge together with its end-vertices. We continue this process until there is no pendant edge left. Then the remaining graph consists of independent odd cycles. This completes the proof. \[ \square \]

If $G$ is a bipartite graph with a unique Sachs subgraph, then $G$ does not contain odd cycles and hence contains a pendant edge by Theorem 3.1. So we have the following corollary.

**Corollary 3.2** ([25], cf. [18]). A bipartite graph with a unique perfect matching has a pendant edge.

For signed graphs with a unique Sachs subgraph, the simply invertible property implies that the inverse weight function is integral (also call integral inverse) as described in the following theorem, which also generalizes and extends Theorem 2.1 in [19] for bipartite graphs with a unique perfect matching.
Theorem 3.3. Let \((G, \sigma)\) be a simple signed graph with a unique Sachs subgraph \(S\). Then:

1. \((G, \sigma)\) has an integral inverse if and only if \(S\) is a perfect matching;
2. if \((G, \sigma)\) has a simple inverse, then \(S\) is a perfect matching.

Proof. Let \(S = C \cup M \cup L\) be the unique Sachs subgraph of \((G, \sigma)\). Since \((G, w)\) is simple, \(L = \emptyset\).

Then by Theorem 2.3 it follows that

\[
\det(A) = \sigma(C)\sigma^2(M)2^{|C|}(-1)^{|C|+|E(S)|} = \sigma(C)2^{|C|}(-1)^{|C|+|E(S)|}.
\]

Note that every cycle in \(C\) is of odd size.

(1) First, assume that \(S\) is a perfect matching. Then \(C = \emptyset\) and hence \(\det(A) = (-1)^{|M|}\). By Theorem 2.5 \((G, \sigma)\) has an integral inverse.

For the other direction, assume that \((G, \sigma)\) has an integral inverse. Suppose on the contrary that \(C \neq \emptyset\). Let \(C\) be a cycle of \(C\). Then \(C\) is of odd size. Note that, for any vertex \(i \in V(C)\), \(C\) has a maximum matching \(M_C\) which covers all vertices of \(C\) except \(i\). By Theorem 3.1 the graph \(G - i\), obtained from \(G\) by deleting the vertex \(i\), still has a unique Sachs subgraph \(S'\). Note that \(S\) contains one more cycle (the cycle \(C\)) than \(S'\). By Theorem 2.5 \(|(A^{-1})_{ii}| = 1/2\), which contradicts that \((G, \sigma)\) has an integral inverse.

(2) It suffices to show that \(C = \emptyset\). If not, let \(C \in \mathcal{C}\). Then \(C\) is an odd cycle. Let \(i\) be a vertex of \(C\). By a similar argument as above, we have \((A^{-1})_{ii} \neq 0\). So the inverse of \((G, \sigma)\) is not simple, a contradiction. This completes the proof.

Remark. The other direction of (2) in the above theorem does not always hold. For example, the graph \(G\) in Figure 4: \(G - w\) is invertible because \(G - w\) has a unique Sachs subgraph.

![Figure 4](image)

Figure 4: The graph \(G\) with a unique perfect matching but without simple inverse.

In the following, we consider two important families of graphs, one is called stellated graphs [13, 26] and the other is called corona graphs [19]. Let \(G\) be a graph. The stellated graph of \(G\), denoted by \(st(G)\), is the line graph of the subdivision of \(G\) obtained from \(G\) by subdividing every edge once (see Figure 5). The stellated graph of \(G\) is also called inflated graph [4] or para-line graph of \(G\) [24]. A graph \(G\) is called a stellated graph if \(G = st(H)\) for some graph \(H\). The spectrum of stellated graphs (or para-line graphs) have been studied in [24]. For chemical applications of the stellated graphs of trees, refer to [13].

Lemma 3.4. Let \(G\) be a connected simple graph with at least one edge. Then its stellated graph \(st(G)\) has a perfect matching, and \(st(G)\) has a unique perfect matching if and only if \(G\) is a tree.
Proof. Let $G$ be a connected simple graph with at least one edge, and $\text{st}(G)$ the stellated graph of $G$. For a vertex $v$ of $G$, assume its degree is $d(v)$. Let $E_v = \{e_1, e_2, ..., e_{d(v)}\}$ be the set of edges incident with $v$. Then $\text{st}(G)$ can be treated as a graph obtained from $G$ by replacing every vertex $v$ by a clique consisting of $v_1, v_2, ..., v_{d(v)}$ such that for an edge $uv \in E(G)$, joining $v_i$ and $v_j$ if $uv = e_i \in E_v$ and $uv = e_j' \in E_u$. So $M = \{v_iu_j | v_iu_j \in E(\text{st}(G)) \text{ and } uv \in E(G)\}$ is a perfect matching of $\text{st}(G)$ (for example thick edges in $\text{st}(K_{1,4})$ in Figure 4).

On the other hand, $G$ is obtained from $\text{st}(G)$ by contracting these maximal clique to a vertex of $G$. Let $M$ be a perfect matching of $\text{st}(G)$. Note that an $M$-alternating cycle of $\text{st}(G)$ corresponds to a cycle of $G$. So $\text{st}(G)$ has a unique perfect matching $M$ if and only if $\text{st}(G)$ has no $M$-alternating cycles. Hence $G$ has no cycles. So $G$ is a tree.

By Lemma 3.4, a stellated graph without isolated vertices always has a perfect matching. So if a stellated graph has a unique Sachs subgraph, then it has a unique perfect matching. On the other hand, if a stellated graph has a unique perfect matching, then it is a stellated graph of a tree and hence has a unique Sachs subgraph. Let $T$ be a tree. For any two vertices of $T$, there is exactly one path joining them. For any two vertices $i$ and $j$ of $\text{st}(T)$, there is at most one $M$-alternating path $P$ joining $i$ and $j$ because $P/(E(P) \setminus M)$ is a path in $T$. If $i$ and $j$ are joined by an $M$-alternating path $P_{ij}$, let $\tau(i, j) := |E(P_{ij}) \setminus M|$. Now, we proceed to consider the inverse of signed stellated graphs with a unique Sachs subgraph (equivalently, a unique perfect matching).

Figure 6: The stellated graph $K_{1,4}$ (left) and its inverse (right): dashed edges has weight $-1$, solid edges have weight 1, and thick edges form a perfect matching.
Theorem 3.5. Let \((G, \sigma)\) be a signed stellated graph with a unique perfect matching \(M\). Then \((G, \sigma)\) has an inverse \((G^{-1}, \sigma^{-1})\) which is a signed graph such that, for any two vertices \(i\) and \(j\),

1. \(ij \in E(G^{-1})\) if and only if there is an \(M\)-alternating path \(P_{ij}\) joining \(i\) and \(j\) in \((G, \sigma)\); and
2. \(\sigma^{-1}(ij) = (-1)^{\tau(i,j)}\sigma(P_{ij})\).

Proof. Let \((G, \sigma)\) be a signed stellated graph with a unique perfect matching. By the above argument, \(M\) is the unique Sachs subgraph of \((G, \sigma)\). Let \(A\) be the adjacency matrix of \((G, \sigma)\). Then by Corollary 2.4 \(\det(A) = (-1)^{|M|}\). Hence \((G, \sigma)\) has inverse \((G^{-1}, \sigma^{-1})\).

By Lemma 3.4 \(G\) is the stellated graph of a tree \(T\). So every cycle \(C\) of \(G\) is contained in a maximal clique corresponding to a vertex of \(T\). Note that \(G - V(C)\) has at least \(|C|\) components each without a perfect matching. Hence, for any vertex \(i\) of \(G\), a Sachs subgraph of \(G - i\) contains no cycles and hence is a perfect matching. However, \(G - i\) has an odd number of vertices. Hence \(G - i\) has no Sachs subgraph. So \((G^{-1}, \sigma^{-1})\) is simple.

Let \(P\) be a path joining two vertices \(i\) and \(j\). Then \(G - V(P)\) has a Sachs subgraph if and only if \(P\) is an \(M\)-alternating path. By Theorem 2.5 \((A^{-1})_{ij} \neq 0\) if and only if there is an \(M\)-alternating path joining \(i\) and \(j\). It follows immediately that \(i\) and \(j\) are adjacent in \(G^{-1}\) if and only if there is an \(M\)-alternating path \(P_{ij}\) joining them.

Note that, for any two vertices \(i\) and \(j\) of \(G\), there is at most one \(M\)-alternating path \(P_{ij}\) joining \(i\) and \(j\). So if \(ij \in E(G^{-1})\), by Theorem 2.5 \(\sigma^{-1}(ij) = (A^{-1})_{ij} = \sigma(P_{ij})(-1)^{\tau(i,j)}\). This completes the proof.

The corona of a graph \(H\) is a graph \(G\) obtained from \(H\) by adding a neighbor of degree 1 to each vertex of \(H\) \([25]\). A graph \(G\) is a corona graph if it is the corona of some graph. A corona graph has an even number of vertices and half of them have degree 1. So a corona graph has a unique Sachs subgraph that is a perfect matching. The inverse of a bipartite corona graph has been discussed in \([1, 19, 25]\). A weighted graph \((G, w)\) is self-invertible if it has an inverse \((G^{-1}, w^{-1})\) such that \(G^{-1}\) is isomorphic to \(G\). Note that, their weight-functions \(w\) and \(w^{-1}\) may be different. Based on Godsil’s definition of inverse, Simion and Cao \([25]\) show that if \(G\) is a bipartite graph with a unique perfect matching \(M\) such that \(G/M\) is bipartite, then \(G\) is self-invertible if and only if \(G\) is isomorphic to a bipartite corona graph (see also \([1]\)). The self-invertibility of a corona bipartite graphs is also verified for McLeman-McNicholas’s definition \([19]\). This result is partially generalized to non-bipartite signed graphs as follows.

Theorem 3.6. Let \((G, \sigma)\) be a simple signed corona graph. Then \((G, \sigma)\) is self-invertible.

Proof. Let \(V(G) = \{v_1, v_2, ..., v_n, u_1, u_2, ..., u_m\}\) such that \(d_G(u_i) = 1\) and \(v_iu_i \in E(G)\). Then \(G\) has a unique Sachs subgraph which is a perfect matching \(M = \{v_iu_i|0 \leq i \leq n\}\). Let \(A\) be the adjacency matrix of \((G, \sigma)\). Then \(\det(A) = (-1)^{|M|}\) by Corollary 2.4 \(G\) has inverse \((G^{-1}, \sigma^{-1})\).

Let \(P_{xy}\) be a path joining two vertices \(x\) and \(y\) of \(G\). Since \(G\) is a simple corona graph, \(G - V(P_{xy})\) has a Sachs subgraph if and only if, for each \(v_i \in V(P_{xy})\), we have \(u_i \in V(P_{xy})\). It follows immediately that \(xy = u_iv_i\text{, or } x = u_i\text{, } y = u_j\) and \(P_{xy} = u_iv_iv_ju_j\) for some \(i\) and \(j\). By Theorem 2.5...
for any two vertices $x, y \in V(G^{-1})$, it follows that $\sigma^{-1}(xy) = (A^{-1})_{xy} = \sigma(P_{xy})(-1)^{r(x,y)}$. Hence,

$$\sigma^{-1}(xy) = \begin{cases} 
\sigma(xy) & \text{if } xy = u_iv_i; \\
-\sigma(P_{u_iu_j}) & \text{if } xy = u_iu_j \text{ where } P_{u_iu_j} = u_iv_ju_j; \\
0 & \text{otherwise.}
\end{cases}$$

So $(G^{-1}, \sigma^{-1})$ is a simple signed graph. In $G^{-1}$, $d_{G^{-1}}(v_i) = 1$, $v_iu_i \in E(G)$, and $u_iu_j \in E(G^{-1})$ if and only if $v_iv_j \in E(G)$. So the mapping $\phi : V(G) \to V(G^{-1})$ that $\phi(u_i) = v_i$ and $\phi(v_i) = u_i$ is an isomorphism between $G$ and $G^{-1}$. Hence $(G, \sigma)$ is self-invertible.

\[\Box\]

4 Eigenvalues

Let $(G, w)$ be a weighted graph with $n$ vertices. Assume that $\lambda_1(G, w) \geq \lambda_2(G, w) \geq \cdots \lambda_n(G, w)$ are all eigenvalues of $(G, w)$. The spectrum of $(G, w)$ is the family of all eigenvalues. The spectrum of $(G, w)$ splits about the origin if it has half positive eigenvalues and half negative eigenvalues. Let $H = [(n+1)/2]$ and $L = [(n+1)/2]$. The median eigenvalues are $\lambda_H(G, w)$ and $\lambda_L(G, w)$. If the spectrum of $(G, w)$ splits about the origin, then $\lambda_H(G, w) > 0 > \lambda_L(G, w)$. Many graphs representing stable molecules have a spectrum split about the origin. In [13], it has been shown that the spectrum of the stellated graph of a tree splits about the origin.

**Proposition 4.1.** Let $(G, w)$ be an invertible graph and $(G^{-1}, w^{-1})$ be its inverse. If the spectrum of $(G, w)$ splits about the origin, so does the spectrum of $(G^{-1}, w^{-1})$ and $\lambda_H(G, w) = 1/\lambda_1(G^{-1}, w^{-1})$ and $\lambda_L(G, w) = 1/\lambda_n(G^{-1}, w^{-1})$.

**Proof.** Since $(G, w)$ is invertible, its adjacency matrix $A$ has inverse $A^{-1}$ which is the adjacency matrix of $(G^{-1}, w^{-1})$. Note that, $\lambda$ is an eigenvalue of $A$ if and only if $1/\lambda$ is an eigenvalue of $A^{-1}$. Since the spectrum of $(G, w)$ splits about the origin, then the proposition follows. \[\Box\]

For non-weighted graphs $G$, it is well-known that $G$ is bipartite if and only if the spectrum of $G$ is symmetric about the origin. But for a weighted graph, one direction is necessarily but not the other.

**Proposition 4.2.** Let $(G, w)$ be a weighted simple bipartite graph. Then the spectrum of $(G, w)$ is symmetric about the origin.

**Proof.** Since $(G, w)$ is a weighted simple bipartite graph, then its adjacency matrix $A = \begin{bmatrix} 0 & B \\ B^T & 0 \end{bmatrix}$.

Let $\lambda$ be an eigenvalue of $A$, and $x = \begin{bmatrix} u \\ v \end{bmatrix}$ an eigenvector of $\lambda$. It is easily seen that $-\lambda$ is an eigenvalue of $A$ with eigenvector $\begin{bmatrix} u \\ -v \end{bmatrix}$. \[\Box\]

**Remark.** The other direction of the above proposition holds if $w$ is a positive function. If $w$ is not positive, then it is not always true. For example, the weighted graph $(G, w)$ in Figure 7 with $w(e) = 1$ if $e$ is an edge of the triangle 1231 and $-1$ otherwise: if $\lambda$ is an eigenvalue of $(G, w)$
with eigenvector \( \mathbf{x} = [x_1, x_2, x_3, x_4, x_5]^\top \), then \( -\lambda \) is also an eigenvalue of \((G, w)\) with eigenvector \( \mathbf{x}' = [x_5, x_4, x_3, x_2, x_1]^\top \).

**Theorem 4.3.** Let \((G, \sigma)\) be a signed graph with a perfect matching \( M \). If for any weight-function \( w : E(G) \to I = [-1, 1] \) such that \( w(e) \in \{-1, 1\} \) for every \( e \in M \), \((G, w)\) is invertible, then the spectrum of \((G, \sigma)\) splits about the origin.

**Proof.** Let \((G, w)\) be a weighted graph and \( w : E(G) \to [-1, 1] \) be a weight-function such that \( w(e) \in \{-1, 1\} \) for \( e \in M \). Let \( A \) be the adjacency matrix of \((G, w)\).

Since \((G, w)\) is invertible, so is \( A \). Hence \( \det(A) \neq 0 \). Let \( A_0 \) be the adjacency matrix of \((G, w_0)\) such that \( w_0(e) = 0 \) if \( e \in E(G) \setminus M \) and \( w_0(e) \in \{-1, 1\} \) if \( e \in M \). Then \( A_0 \) is the adjacency matrix of \( M \), an invertible bipartite graph, whose spectrum is symmetric about the origin and not equal to \( 0 \) by Proposition 4.2.

Let \( \lambda(w) \) be an eigenvalue of \( A \) and \( \mathbf{x} \) be an eigenvector of \( \lambda(w) \). Then

\[
\lambda(w) = \frac{\langle A\mathbf{x}, \mathbf{x} \rangle}{\langle \mathbf{x}, \mathbf{x} \rangle}.
\]

Hence \( \lambda(w) \) is a function of \( w \), which is continuous on \([-1, 1]\). Since \( \det(A) \neq 0 \), it follows that \( \langle A\mathbf{x}, \mathbf{x} \rangle \neq 0 \). Hence \( \lambda(w) \neq 0 \). So for any \( w : E(G) \to [-1, 1] \), \( \lambda(w) \) has the same sign. Let \( \sigma(e) \to \{-1, 1\} \) for any \( e \in E(G) \). Then \( \lambda(\sigma)\lambda(w_0) > 0 \). Hence the spectrum of \((G, \sigma)\) splits about the origin. \( \square \)

**Theorem 4.4.** Let \((G, \sigma)\) be a signed graph with a unique Sachs subgraph. If \( G \) has a perfect matching \( M \), then the spectrum of \((G, \sigma)\) splits about the origin.

**Proof.** Consider \((G, w)\) where \( w : E(G) \to [-1, 1] \) such that \( w : M \to \{-1, 1\} \). Since \( G \) has a unique Sachs subgraph which is a perfect matching \( M \), by Corollary 2.4, we have

\[
\det(A) = (-1)^{|M|}.
\]

Hence \((G, w)\) is invertible. By the above theorem, the spectrum of \((G, w)\) splits about the origin. So does the spectrum of \((G, \sigma)\). \( \square \)

Since both a stellated graph without isolated vertices and a corona graph have a perfect matching, the following results are direct corollaries of Theorem 4.4.

**Corollary 4.5.** Let \( G \) be a stellated graph with a unique Sachs subgraph. Then the spectrum of \( G \) splits about the origin if \( G \) does not contain an isolated vertex.

**Corollary 4.6.** The spectrum of a corona graph splits about the origin.
5 Median eigenvalues

Let $G$ be a graph and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, the eigenvalues of $G$. The difference of median eigenvalues $\Delta = \lambda_H - \lambda_L$ in chemistry is called the HOMO-LUMO gap of the neutral pi-network molecule corresponding the graph $G$, so that $\Delta$ is also called the HOMO-LUMO gap of $G$ \[5\]. A graph $G$ is a special signed graph $(G, \sigma)$ such that $\sigma : E(G) \to \{1\}$. So all results above can be applied to graphs as special cases.

Let $A$ be the adjacency matrix of $G$. Define $x : V(G) \to \mathbb{R}$ such that $x(i) = x_i$, and let $x = (x_1, x_2, ..., x_n)^T \in \mathbb{R}^n$ where. Then by Rayleigh-Ritz quotient,

$$\lambda_1(G, \sigma) = \max_{x \in \mathbb{R}^n} \frac{\langle Ax, x \rangle}{\langle x, x \rangle} = \max_{x \in \mathbb{R}^n} \frac{\sum (A_{ij} x_i x_j)}{\|x\|},$$

and

$$\lambda_n(G, \sigma) = \min_{x \in \mathbb{R}^n} \frac{\langle Ax, x \rangle}{\langle x, x \rangle} = \min_{x \in \mathbb{R}^n} \frac{\sum (A_{ij} x_i x_j)}{\|x\|}.$$

**Theorem 5.1.** Let $G$ be a stellated graph of a tree with at least two vertices. Then $-1 \leq \lambda_L(G) < 0 < \lambda_H(G) \leq 1$.

**Proof.** Let $G$ be a stellated graph of a tree $T$. By Lemma 3.3 then $G$ has a unique perfect matching $M$. Hence $G$ has an inverse which is a signed graph $(G^{-1}, \sigma)$ by Theorem 3.5. By Corollary 3.4 we have $\lambda_L(G) < 0 < \lambda_H(G)$. In order to show $\lambda_H(G) \leq 1$ and $\lambda_L(G) > -1$, it suffices to show that $\lambda_1(G^{-1}, \sigma) \geq 1$ and $\lambda_n(G^{-1}, \sigma) < -1$ by Proposition 4.1.

Assume that $T$ has $k$ leaves with degree sequences as $1 = d_1 = \cdots = d_k < d_{k+1} \leq \cdots \leq d_t \leq d_s$. Then in $G$, each vertex $v_\ell$ of $T$ with degree $d_\ell$ is replaced by a clique with size $d_\ell$, denoted by $K_{d_\ell}$.

Let $i$ and $j$ be two vertices of $G$. By Theorem 3.5, $ij \in E(G^{-1})$ if and only if there is an $M$-alternating path $P_{ij}$ joining them, and $\sigma(ij) = (-1)^{|E(P_{ij})\setminus M|}$. If $ij \in M$, then $\sigma(ij) = 1$ that implies that $M$ is also a perfect matching of $G^{-1}$. If $i$ and $j$ satisfies that $i'j', j'i' \in M$ and $i'j' \in E(K_{d_{i'}})$ for some $\ell$, then $i'j'i'$ is the only one $M$-alternating path of $G$ joining $i'$ and $j'$. Hence $ij \in E(G^{-1})$ and $\sigma(ij) = (-1)^{|E(P)\setminus M|} = -1$. Hence, $G^{-1}$ has a clique $K_{d_{i'}}$ corresponding to $K_{d_{i'}}$ consisting of vertices in $N(V(K_{d_{i'}}))$ and every edge in $K_{d_{i'}}$ has weight $-1$. For example, see Figure 8, two cliques of order 4 illustrated in dashed lines.

First, we show that $\lambda_1(G^{-1}, \sigma) \geq 1$. Let $Q$ be the graph obtained from $(G^{-1}, \sigma)$ by contradicting all edges of $M$ which have positive signature. For any ordering of the vertices of $Q$: $q_1, q_2, \cdots, q_t$, let $E(q_\alpha) := \{q_\gamma q_\alpha \mid q_\gamma q_\alpha \in E(Q) \text{ and } \gamma < \alpha\}$. Assign a weight $x(q_\alpha) \in \{-1, 1\}$ to each vertex $q_\alpha$ such that

$$\sum_{q_\gamma q_\alpha \in E(q_\alpha)} x(q_\gamma) \sigma(q_\gamma q_\alpha) x(q_\alpha) \geq 0.$$

The weight-function always exists because we can adjust the sign of $x(q_\alpha)$ to change the above inequality. Hence, $Q$ has a weight-function $x : V(Q) \to \{-1, 1\}$ such that

$$\sum_{q_\gamma q_\alpha \in E(Q)} x(q_\gamma) \sigma(q_\gamma q_\alpha) x(q_\alpha) \geq 0.$$
Figure 8: A stellated graph of a tree (left: thick lines form a perfect matching) and its inverse (right: dashed lines have weight $-1$ and others have weight $1$).

Let $i, j \in V(G^{-1})$ and $ij \in M$. Assume that $ij$ is contracted to a vertex $q_\alpha$ in $Q$. Now, extend the weight-function $x$ to $V(G^{-1})$ such that $x(i) = x(j) = x(q_\alpha)$, and define the vector $x : V(G^{-1}) \to \{-1, 1\}^n$ such that $x_i = x(i)$. Let $\mathcal{A}$ be the adjacency matrix of $(G^{-1}, \sigma)$. Note that $E(G^{-1}) = E(Q) \cup M$. Then it follows that

$$
\langle \mathcal{A}x, x \rangle = 2 \sum_{ij \in E(G^{-1})} (\mathcal{A})_{ij}x_ix_j = 2 \sum_{ij \in E(Q)} (\mathcal{A})_{ij}x_ix_j + 2 \sum_{ij \in M} (\mathcal{A})_{ij}x_ix_j
$$

$$
= 2 \sum_{ij \in E(Q)} x_i\sigma(ij)x_j + 2 \sum_{ij \in M} x_i\sigma(ij)x_j
$$

$$
\geq 2|M|.
$$

Further,

$$
\lambda_1(G^{-1}, \sigma) \geq \frac{2 \sum_{ij \in E(G^{-1})} (\mathcal{A})_{ij}x_ix_j}{\|x\|} \geq \frac{2|M|}{|V(G)|} = 1.
$$

In the following, we concentrate on the upper bound for $\lambda_n(G^{-1}, \sigma)$. Let $E_P$ be the set of all pendant edges (incident with a degree-1 vertex). Then $E_P \subseteq M$. So for any edge $ij \in E_P$, $\sigma(ij) = 1$. Let $R$ be the graph obtained from $G^{-1}$ by contracting all edges in $E_P$ and all cliques $K_{d_\ell}$ for $k + 1 \leq \ell \leq n$. By a similar argument as above, $R$ has a weight-function $x : V(R) \to \{-1, 1\}$ such that

$$
\sum_{r_\gamma, r_\alpha \in E(R)} x(r_\gamma)\sigma(r_\gamma r_\alpha)x(r_\alpha) \leq 0,
$$

where $r_\gamma, r_\alpha$ are vertices of $R$. Now, define the vector $x$ such that $x_i = x(r_\alpha)$ if $i \in V(K'_{d_\ell})$, and then $x_j = -x_i$ if $ij \in E_P$ and $i \in V(K'_{d_\ell})$. Note that $E(G^{-1}) = E(R) \cup (\bigcup E(K'_{d_\ell})) \cup E_P$. So

$$
\langle \mathcal{A}x, x \rangle = 2 \sum_{ij \in E(G^{-1})} (\mathcal{A})_{ij}x_ix_j \quad \text{(1)}
$$

$$
= 2 \sum_{ij \in E(R)} \sigma(ij)x_ix_j + 2 \sum_{d_{k+1} \leq \alpha \leq d_\ell} \sum_{ij \in E(K'_{d_\ell})} \sigma(ij)x_ix_j + 2 \sum_{ij \in E_P} \sigma(ij)x_ix_j \quad \text{(2)}
$$

$$
\leq 2 \sum_{d_{k+1} \leq \alpha \leq d_\ell} \sum_{ij \in E(K'_{d_\ell})} (-1) - 2|E_P| \quad \text{(3)}
$$

$$
= -2 \sum_{k+1 \leq \ell \leq t} \frac{d_\ell}{2} - 2|E_P|. \quad \text{(4)}
$$
Hence,
\[
\lambda_n(G^{-1}, \sigma) \leq 2 \frac{\sum_{ij \in E(G^{-1})} \langle A \rangle_{ij} x_i x_j}{\| x \|} \leq \frac{-2 \sum_{k+1 \leq t \leq \ell} (\frac{d_t}{2}) - 2 |E_P|}{|V(G)|}.
\]
(5)

Since a vertex of \(G^{-1}\) is either a pendent vertex or contained in \(K_\alpha\) for some \(\alpha\), it follows that \(2 \sum_{k \leq t \leq \ell} (\frac{d_t}{2}) + 2 |E_P| \geq |V(G^{-1})|\) and equality holds if and only if \(G\) is \(K_2\). So \(\lambda_n(G^{-1}, \sigma) \leq -1\). This completes the proof. \(\square\)

**Remark.** For some specific trees, a better bound for HOMO-LUMO gap of their stellated graphs could be obtained by the method used in the above proof. For example, the alkanes, trees with only degree-1 vertices and degree-4 vertices. If \(G\) is a stellated graph of an alkane, then \(d_{k+1} = \cdots = d_t = 4\) and hence \((\frac{d_t}{2}) = 6\). On the other hand, by degree condition, it is easily deduced that \(k = (2|V(G)| - 2)/3\) and \(t - k = (|V(G)| + 2)/3\). So, by Inequality (5), \(\lambda_n(G^{-1}, \sigma) \leq -2(6(t - k) + 2k)/|V(G)| < -10/3\). Hence the HOMO-LUMO gap for stellated graphs of alkanes is at most 1.3.

**Theorem 5.2.** Let \(G\) be a connected corona graph. Then \(-1 \leq \lambda_L(G) < 0 < \lambda_H(G) \leq 1\).

**Proof.** Let \(G\) be the corona of a connected graph \(H\). Then \(G\) has a unique Sachs subgraph which is a perfect matching \(M\). By Theorem 3.1, \(G\) has an inverse \((G^{-1}, \sigma)\) and \(G\) is isomorphic to \(G^{-1}\).

For an edge \(ij \in E(G^{-1})\), \(\sigma(ij) = -1\) if \(ij \notin M\) and \(\sigma(ij) = 1\) if \(ij \in M\). Since \(G^{-1}\) is also a corona graph, every edge \(ij \in M\) is incident with a vertex of degree-1.

Let \(A\) be the adjacency matrix of \((G^{-1}, \sigma)\). A similar argument as the proof of Theorem 4.1 shows that \(\lambda_1(G^{-1}, \sigma) \geq 1\).

For the upper bound of \(\lambda_n(G^{-1}, \sigma)\), let \(x\) be the vector such that \(x_i = 1\) if \(i \in V(H)\) and \(x_i = -1\) if \(i \in V(G) \setminus V(H)\). Note that all vertices in \(V(G) \setminus V(H)\) has degree 1. Hence
\[
\lambda_n(G^{-1}, \sigma) \leq \frac{\langle A x, x \rangle}{\| x \|} = \frac{2 \sum_{ij} \sigma(ij) x_i x_j}{|V(G)|} = \frac{-2 |E(G)|}{|V(G)|} \leq -1.
\]
(6)
The last inequality in (6) holds if and only if \(G\) is a \(K_2\). (Otherwise it will be \(-3/2\).)

By Proposition 4.1 and Corollary 4.6 we have \(\lambda_H(G) = 1/\lambda_1(G^{-1}, \sigma) \leq 1\) and \(\lambda_L(G) = 1/\lambda(G^{-1}, \sigma) \geq -1\). This completes the proof. \(\square\)

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