The characteristic polynomial of a graph containing loops

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Abstract

In this article, we focus on the characteristic polynomial of a graph containing loops without multiple edges. We present a relationship between the characteristic polynomial of a graph containing loops without multiple edges and the graph obtained by removing all the loops. In turn, we compute the characteristic polynomial of unitary addition Cayley graphs.

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1 Introduction

Let G be a graph with vertex set $\{v_1, v_2, \ldots, v_p\}$. The characteristic polynomial $\phi(G; x)$(or simply $\phi(G)$) of a graph G is the characteristic polynomial of its adjacency matrix. The adjacency matrix $A(G) = [a_{ij}]$ of a graph G is a square matrix of order $p \times p$ such that (i, j) entry of $A(G)$ is 1 if vertices v_i and v_j are adjacent; and 0 otherwise. The spectrum of an adjacency matrix is a list of its eigenvalues along with their multiplicities. The spectrum of a graph is a spectrum of its adjacency matrix.

The spectrum and the characteristic polynomial of a graph frequently appear in mathematical sciences, chemistry, and physics. As to graph theorists, the characteristic polynomial tells information about the structural properties of a graph. On the other hand, in chemistry, the characteristic equation is related to a secular equation formed from the chemical formula of organic molecules, the so-called unsaturated conjugated hydrocarbons. It is useful in predicting the relative stabilities of conjugated hydrocarbons.

A lone pair is another concept that is informative for a chemist. Lewis introduced it, and it forms the basis for an electronic theory of chemical bonds. The traditional representation of a lone pair by Lewis and Langmuir [14, 13] involved a pair of dotes located near an atom symbol. However, from the topological viewpoint, this is a rather poor image. There is no general convention on how lone pairs may be expressed in classical 2D models, therefore their presence is always ignored. Only in the Gillespie–Nyholm approach to molecular geometry [10, 8, 9] is a lone pair (a non bonding domain) studied as an object equivalent to a bonding domain involving an arrangement of both domain types around an atom.

Lone pairs describe the formation of donor-acceptor bonds as reflected in the concept of Lewis acids and bases [12]. Consider the chemical equation, $NH_3 + BH_3 = NH_3BH_3$ involving base ammonia, which has a lone pair, and an acid borane, which has a vacancy (the lack of electron pairs to form the stable octet configuration of a noble gas). The vacancy is hardly represented in molecular graphs or surfaces, although it is related to the depletion of the charge density. Reactions of this sort incorporate the same logical modeling paradox as do the recombination of two free radicals. A molecule with a well-defined graph and well-defined 2D surface is formed from ill-defined model structures. Hence, it is still an open question of how to extend the lone pair to molecular graphs.

The precise term molecular graph is ill-defined. For instance, the chemists frequently used these graphs to represent atoms and bonds in a chemical reaction [3, 5]. One may consider only heavy atoms (as in the so-called hydrogen-suppressed graphs) or the bonds representing only s-frameworks (graphs for p-systems). A single vertex may also represent a functional group. These graphs (and even molecular multigraphs with multiple edges) are incomplete in the sense of original Lewis dot formula that consists of all atoms and all valence electrons (represented by dots). Perhaps, the best image of a Lewis formula is the molecular pseudograph, a multigraph with loops representing lone pairs. Only this graph represents all valence electron pairs by edges (including non bonding lone pairs) and all atoms.

A clear model consisting of molecular pseudographs appeared in 1973 by Dugundji and Ugi [7]. They represent a molecule by a connection table (BE-matrix) that matches the adjacency matrix for multigraph with the number of valence electrons for each atom on the main diagonal. The loop appears while reconstructing a graph from the matrix because entries of the main diagonal denote the numbers of valence electrons necessary for a correct count of vertex degrees in a molecular pseudograph. Molecular pseudographs appeared in different fields of mathematical chemistry [2]. However, it is rarely used. Probably one of the reasons is that chemists frequently draw "lobes" of p-orbitals near the atoms in molecular graphs, and the loops may be confused with p-orbitals.

So, chemical terms and concepts (that may have imprecise definition in classical molecular models) needs to be translated into the language of pseudographs because the pseudographs coincide with Lewis formulas. Furthermore, every abstract pseudograph corresponds (if at all) to only a finite set of specific molecular pseudographs.

In Section 2, we discuss how a basic figure containing loops contributes to the coefficients of a characteristic polynomial of a graph. In Section 3, there are two main theorems along with other results; in one theorem the characteristic polynomial of a graph with loops is expressed in terms of the characteristic polynomials of its simple subgraphs, and the second theorem again relates the two characteristic polynomials. Sometimes, it helps in computing the characteristic polynomial of a graph without loops to work from the characteristic polynomial of the same graph containing loops. Consequently, we show that the characteristic polynomial of a unitary addition Cayley graph can be computed with the help of an anti-circulant graph.

2 Contribution of a loop to the basic figure

A basic figure $\mathcal{B}$ of a simple graph G is a subgraph of G whose each component is either a cycle or an edge. Given the characteristic polynomial of a simple graph, many authors have attempted to express the coefficients in terms of graphical structure. The value of the coefficients has been discovered independently by Sachs [16] and Spialter [20] as given in the following theorem:

Theorem 2.1. *The characteristic polynomial of a simple graph G is given by the following:*

$$\phi(G) = \sum_{\mathcal{B} \in \boldsymbol{B}(G)} (-1)^{k(\mathcal{B})} 2^{c(\mathcal{B})} x^{p-|V(\mathcal{B})|}, \tag{1}$$

where $\boldsymbol{B}(G)$ denotes the set of basic figures of a graph G, $k(\mathcal{B})$ and $c(\mathcal{B})$ denotes the number of components and cycles in a basic figure $\mathcal{B}$, respectively.

We deal with the case where the graph may contain loops. The diagonal entry (i, i) of an adjacency matrix of this graph is 1 if there is a loop at the vertex v_i, and 0 otherwise. In chemistry, such graphs are used to represent heteroconjugated molecules. In [21], the author shows that Sachs's formula (Theorem 2.1) for computing the characteristic polynomial of a simple graph can be extended as it is to compute the characteristic polynomial of a pseudograph (without multiple edges) associated with heteroconjugated molecules. The generalization involves the difference in the set of basic figures only, which would lead to a change in the number of components in a basic figure. In this case, a basic figure is a subgraph whose each component is either a cycle (containing 3 or more vertices) or a loop or an edge. Figure 1 and Table 1 show an example of a graph G with a loop and its basic figures. A basic figure without a loop of this graph is nothing but a basic figure of a graph without a loop.

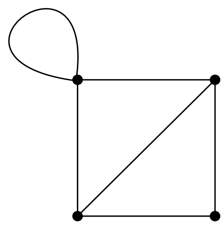

Figure 1: A graph G with a loop

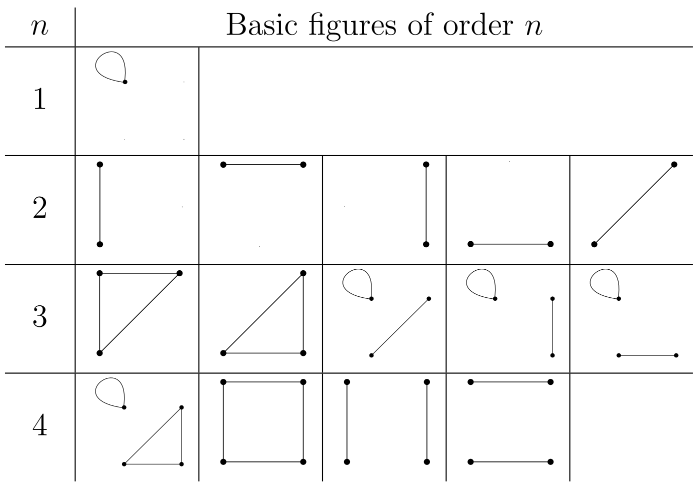

Table 1: Basic figures of different order of a graph G.

Let us look at the basic figures containing loops of a general graph G consisting of p vertices, q edges, and m loops (we do not count loops while counting edges). Define $\mathcal{L}$ to be the subset of the vertex set G containing those vertices which have a loop at it; and let $N(x)$ and $N[x]$ denote open and closed neighborhood of a vertex x, respectively.

A basic figure of order 1 containing a loop is just a single vertex with a loop. So it contributes $-m$ to the coefficient a_1. Similarly, a basic figure of order 2 that has a loop contains two loops at a time. It contributes $\binom{m}{2}$ to the coefficient a_2. A basic figure of order 3 containing a loop in any graph is either of the forms given in Figure 2. The basic figure in Figure 2(a) contributes $-\binom{m}{3}$ to the coefficient a_3, whereas the basic figure in Figure 2(b) contributes

$$mq - \sum_{x \in \mathcal{L}} |N(x)|. \tag{2}$$

Equation (2) is because, for any vertex x with a loop, we have to pick those edges from the set of edges of G, which are not incident to x. That is equal to subtracting the total number of neighbors of x from the total number of edges in G except for loops.

For a basic figure of order 4, we have three possibilities, as shown in Figure 3. The basic figure in Figure 3(a) contributes $\binom{m}{4}$ to the coefficient a_4. A

Figure 2: Possible basic figures of order 3 containing loop in any graph.

basic figure in 3(b) contributes

$$\begin{aligned}&\binom{m}{2}q - \sum_{\substack{x,y\in\mathcal{L}\\ xy\in E(G)}} \big(|N(x)|+|N(y)|-1\big) - \sum_{\substack{x,y\in\mathcal{L}\\ xy\notin E(G)}} \big(|N(x)|+|N(y)|\big)\\ &= \binom{m}{2}q + |E(G[\mathcal{L}])| - (m-1)\sum_{x\in\mathcal{L}} |N(x)|,\end{aligned}$$

where $\mathcal{L}$ and $N(x)$ are defined above, $E(G)$ is the set of edges of the graph G, and $G[\mathcal{L}]$ is the subgraph of G induced by $\mathcal{L}$. Here, first, we have to choose two vertices $x, y \in \mathcal{L}$ and then we have to select those edges which are neither incident to x nor to y. If x and y are not adjacent, then we need to subtract the total number of neighbors of x and y from the total number of edges in G except for loops. Otherwise, we need to subtract extra 1 (as in the second term) as the edge xy is counted twice while counting in terms of neighborhood. Next, a basic figure in Figure 3(c) contributes

$$\sum_{x\in\mathcal{L}} |\mathcal{C}_3^{\{x\}}|,$$

where $\mathcal{C}_n^{\{x\}}$ denotes the set of cycles of length n not containing x.

This analysis can be further generalized to a basic figure of a higher order. For $1 \le k \le m$, a basic figure of order k consisting of k loops contributes $(-1)^k\binom{m}{k}$ to the coefficient of x^{n-k}. A basic figure of order k consisting of $k-2$ loops and an edge contributes

$$\begin{aligned}&\binom{m}{k-2}q - \sum_{S_{k-2}\subseteq\mathcal{L}} \Big(\sum_{v_i\in S_{k-2}} \big(|N_G(v_i)|\big) - |E(G[S_{k-2}])|\Big)\\ &= \binom{m}{k-2}q + \binom{m-2}{k-4}|E(G[\mathcal{L}])| - \binom{m-1}{k-3}\sum_{v\in\mathcal{L}} |N_G(v)|,\end{aligned}$$

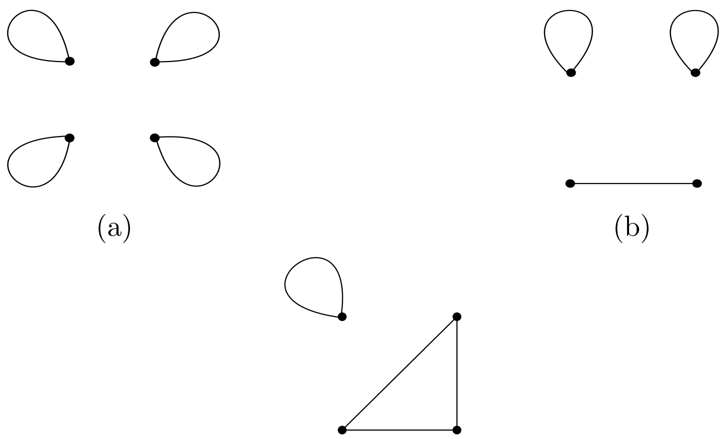

Figure 3: Possible basic figures of order 4 containing loop in any graph.

where the first summation runs over all $(k-2)$-element subsets of $\mathcal{L}$. Next, a basic figure of order k consisting of $k-n$ loops and a cycle C_n of order n contributes

$$\sum_{S_{k-n} \subseteq \mathcal{L}} \left| \mathcal{C}_n^{S_{k-n}} \right|,$$

where the summation is over all $(k-n)$-element subsets of $\mathcal{L}$ and $\mathcal{C}_n^{S_{k-n}}$ denotes the set of cycles of length n that do not contains elements of the set S_{k-n}.

3 Main Theorems

Consider a graph G containing n loops. The following theorem acts as a bridge between the characteristic polynomial of G and the characteristic polynomial of simple subgraphs of G.

Theorem 3.1. *If $l_1, l_2, \ldots, l_n$ represent loops at vertices $v_1, v_2, \ldots, v_n$, respectively in a graph G, then the relationship between the characteristic polynomials of G and $G - \{l_1, l_2, \ldots, l_n\}$ is given by the following:*

$$\phi(G) = \sum_{X \subseteq \mathcal{L}} (-1)^{|X|} \phi(G' - X), \tag{3}$$

where $\mathcal{L} = \{v_1, v_2, \ldots, v_n\}$ and $G' = G - \{l_1, l_2, \ldots, l_n\}$.

Proof. Let $\mathcal{B} \in \mathbf{B}(G)$ be a basic figure of G and let $\mathcal{L}(\mathcal{B})$ be a subset of $\mathcal{L}$ consisting of vertices that are in $\mathcal{B}$. Let $\mathcal{B}'$ be $\mathcal{B} - \mathcal{L}(\mathcal{B})$ viewed as a basic figure of $G' - \mathcal{L}(\mathcal{B})$, where $G' = G - \{l_1, l_2, \ldots, l_n\}$. Hence, we have $V(\mathcal{B}') = V(\mathcal{B}) - \mathcal{L}(\mathcal{B})$, $c(\mathcal{B}') = c(\mathcal{B})$, and $k(\mathcal{B}') = k(\mathcal{B}) - |\mathcal{L}(\mathcal{B})|$. It implies

$$\begin{aligned}|V(\mathcal{B}')| &= |V(\mathcal{B}) - \mathcal{L}(\mathcal{B})| \\ &= |V(\mathcal{B})| - |V(\mathcal{B}) \cap \mathcal{L}(\mathcal{B})| \\ &= |V(\mathcal{B})| - |\mathcal{L}(\mathcal{B})|\end{aligned}$$

and

$$(-1)^{k(\mathcal{B})} 2^{c(\mathcal{B})} = (-1)^{|\mathcal{L}(\mathcal{B})|} (-1)^{k(\mathcal{B}')} 2^{c(\mathcal{B}')}.$$

The proof of the theorem is now a computation,

$$\begin{aligned}\phi(G) &= \sum_{\mathcal{B} \in \mathbf{B}(G)} (-1)^{k(\mathcal{B})} 2^{c(\mathcal{B})} x^{p-|V(\mathcal{B})|} \\ &= \sum_{X \subseteq \mathcal{L}} \sum_{\substack{\mathcal{B} \in \mathbf{B}(G): \\ \mathcal{L}(\mathcal{B}) = X}} (-1)^{|\mathcal{L}(\mathcal{B})|} (-1)^{k(\mathcal{B}')} 2^{c(\mathcal{B}')} x^{p-|V(\mathcal{B}')|-|\mathcal{L}(\mathcal{B})|} \\ &= \sum_{X \subseteq \mathcal{L}} (-1)^{|X|} \sum_{\mathcal{B}' \in \mathbf{B}(G'-X)} (-1)^{k(\mathcal{B}')} 2^{c(\mathcal{B}')} x^{p-|V(\mathcal{B}')|-|X|} \\ &= \sum_{X \subseteq \mathcal{L}} (-1)^{|X|} \phi(G' - X).\end{aligned}$$

□

Corollary 3.2. *If l represents a loop at a vertex v in a graph G, then the characteristic polynomial $\phi(G)$ satisfies the following:*

$$\phi(G) = \phi(G - l) - \phi(G - v).$$

Corollary 3.3. *In the characteristic polynomial of G, the coefficient $a_i(G)$ of x^{p-i} is*

$$a_i(G) = \sum_{X \subseteq \mathcal{L}:\ |X| \le i} (-1)^{|X|} a_{i-|X|}(G' - X).$$

Proof. From Theorem 3.1, we have

$$\begin{aligned}\phi(G) &= \sum_{X \subseteq \mathcal{L}} (-1)^{|X|} \phi(G' - X) \\ &= \sum_{X \subseteq \mathcal{L}} (-1)^{|X|} \sum_{j=0}^{p-|X|} a_j(G' - X) x^{p-|X|-j}\end{aligned}$$

and now replacing the sum over j by a sum over i, where $i = j + |X|$,

$$= \sum_{X \subseteq \mathcal{L}} \sum_{i=|X|}^{p} x^{p-i} (-1)^{|X|} a_{i-|X|}(G' - X)$$

and reversing the order of summation, we have

$$= \sum_{i=0}^{p} x^{p-i} \sum_{\substack{X \subseteq \mathcal{L}: \\ |X| \leq i}} (-1)^{|X|} a_{i-|X|}(G' - X).$$

The corollary follows by extracting the coefficient of x^{p-i}. □

Here are a new set of formulas.

Theorem 3.4. *The characteristic polynomial of G satisfies*

$$\phi(G) = \sum_{\mathcal{B}' \in \boldsymbol{B}(G')} (-1)^{k(\mathcal{B}')} 2^{c(\mathcal{B}')} x^{p-|V(\mathcal{B}') \cup \mathcal{L}|} (x-1)^{|\mathcal{L} - V(\mathcal{B}')|}$$

and the coefficient of x^{p-i} is

$$a_i(G) = \sum_{\substack{\mathcal{B}' \in \boldsymbol{B}(G'): \\ |V(\mathcal{B}')| \leq i \leq |V(\mathcal{B}') \cup \mathcal{L}|}} (-1)^{k(\mathcal{B}') - |V(\mathcal{B}')| + i} 2^{c(\mathcal{B}')} \binom{|\mathcal{L} - V(\mathcal{B}')|}{|V(\mathcal{B}') \cup \mathcal{L}| - i}.$$

In particular,

$$\det A(G) = (-1)^p a_p(G) = \sum_{\substack{\mathcal{B}' \in \boldsymbol{B}(G'): \\ V(\mathcal{B}') \supseteq V(G) - \mathcal{L}}} (-1)^{k(\mathcal{B}') - |V(\mathcal{B}')|} 2^{c(\mathcal{B}')}.$$

Proof. The formulae are obtained by expanding the result in Theorem 3.1. We have

$$\begin{aligned} \phi(G) &= \sum_{X \subseteq \mathcal{L}} (-1)^{|X|} \phi(G' - X) \\ &= \sum_{X \subseteq \mathcal{L}} (-1)^{|X|} \sum_{\mathcal{B}' \in \mathbf{B}(G' - X)} (-1)^{k(\mathcal{B}')} 2^{c(\mathcal{B}')} x^{p-|V(\mathcal{B}')| - |X|} \end{aligned}$$

then interchanging the order of summation, we have

$$
\begin{aligned}
&= \sum_{\mathcal{B}'\in\mathbf{B}(G')} (-1)^{k(\mathcal{B}')}2^{c(\mathcal{B}')}x^{p-|V(\mathcal{B}')|} \sum_{X\subseteq\mathcal{L}-V(\mathcal{B}')} \Big(-\frac{1}{x}\Big)^{|X|} \\
&= \sum_{\mathcal{B}'\in\mathbf{B}(G')} (-1)^{k(\mathcal{B}')}2^{c(\mathcal{B}')}x^{p-|V(\mathcal{B}')|} \Big(\frac{x-1}{x}\Big)^{|\mathcal{L}-V(\mathcal{B}')|} \\
&= \sum_{\mathcal{B}'\in\mathbf{B}(G')} (-1)^{k(\mathcal{B}')}2^{c(\mathcal{B}')}x^{p-|V(\mathcal{B}')|-|\mathcal{L}-V(\mathcal{B}')|}(x-1)^{|\mathcal{L}-V(\mathcal{B}')|}
\end{aligned}
$$

and since $|V(\mathcal{B}')| + |\mathcal{L} - V(\mathcal{B}')| = |V(\mathcal{B}') \cup \mathcal{L}|$, this is

$$
\begin{aligned}
&= \sum_{\mathcal{B}'\in\mathbf{B}(G')} (-1)^{k(\mathcal{B}')}2^{c(\mathcal{B}')}x^{p-|V(\mathcal{B}')\cup\mathcal{L}|}(x-1)^{|\mathcal{L}-V(\mathcal{B}')|} \\
&= \sum_{\mathcal{B}'\in\mathbf{B}(G')} (-1)^{k(\mathcal{B}')}2^{c(\mathcal{B}')}x^{p-|V(\mathcal{B}')\cup\mathcal{L}|} \sum_{j=0}^{|\mathcal{L}-V(\mathcal{B}')|} x^j(-1)^{|\mathcal{L}-V(\mathcal{B}')|-j}\binom{|\mathcal{L}-V(\mathcal{B}')|}{j} \\
&= \sum_{\mathcal{B}'\in\mathbf{B}(G')} \sum_{j=0}^{|\mathcal{L}-V(\mathcal{B}')|} (-1)^{k(\mathcal{B}')+|\mathcal{L}-V(\mathcal{B}')|-j}2^{c(\mathcal{B}')}x^{p-|V(\mathcal{B}')\cup\mathcal{L}|+j}\binom{|\mathcal{L}-V(\mathcal{B}')|}{j}
\end{aligned}
$$

and replacing the sum over j by a sum over i, where $i = |V(\mathcal{B}') \cup \mathcal{L}| - j$, we have

$$
\begin{aligned}
&= \sum_{\mathcal{B}'\in\mathbf{B}(G')} \sum_{i=|V(\mathcal{B}')|}^{|V(\mathcal{B}')\cup\mathcal{L}|} (-1)^{k(\mathcal{B}')+|\mathcal{L}-V(\mathcal{B}')|-|V(\mathcal{B}')\cup\mathcal{L}|+i}2^{c(\mathcal{B}')}x^{p-i}\binom{|\mathcal{L}-V(\mathcal{B}')|}{|V(\mathcal{B}')\cup\mathcal{L}|-i} \\
&= \sum_{\mathcal{B}'\in\mathbf{B}(G')} \sum_{i=|V(\mathcal{B}')|}^{|V(\mathcal{B}')\cup\mathcal{L}|} (-1)^{k(\mathcal{B}')-|V(\mathcal{B}')|+i}2^{c(\mathcal{B}')}x^{p-i}\binom{|\mathcal{L}-V(\mathcal{B}')|}{|V(\mathcal{B}')\cup\mathcal{L}|-i}.
\end{aligned}
$$

Finally, reversing the order of summation again, we have i such that $0 \le i \le p$ and the basic figure $\mathcal{B}'$ must satisfy $|V(\mathcal{B}')| \le i \le |V(\mathcal{B}') \cup \mathcal{L}|$. It implies

$$
\phi(G) = \sum_{i=0}^{p} x^{p-i} \sum_{\substack{\mathcal{B}'\in\mathbf{B}(G'):\\ |V(\mathcal{B}')|\le i\le|V(\mathcal{B}')\cup\mathcal{L}|}} (-1)^{k(\mathcal{B}')-|V(\mathcal{B}')|+i}2^{c(\mathcal{B}')}\binom{|\mathcal{L}-V(\mathcal{B}')|}{|V(\mathcal{B}')\cup\mathcal{L}|-i},
$$

where the inner sum is the coefficient of x^{p-i}.

For $i = p$, the inner summation simplifies to

$$a_p = (-1)^p \sum_{\substack{\mathcal{B}' \in \mathbf{B}(G') \\ V(\mathcal{B}') \supseteq V(G) - \mathcal{L}}} (-1)^{k(\mathcal{B}') - |V(\mathcal{B}')|} 2^{c(\mathcal{B}')}$$

and the result follows. □

The result in Theorem 3.1 is useful when the characteristic polynomial of a graph without loops is known, and we wish to compute the characteristic polynomial of the same graph containing loops at some or on all vertices. The following theorem helps in computing the characteristic polynomial of a graph containing loops.

Theorem 3.5. *Let $v_1, v_2, \ldots, v_n$ be the vertices of a graph G and let $\mathcal{C}(v)^S$ denote the set of cycles containing a vertex v that do not contains elements of the set S. Then the relationship between the characteristic polynomial of G and $G - \{v_1, v_2, \ldots, v_n\}$ is given by the following:*

$$\phi(G) = x^n \phi(G - S_n) - \sum_{i=0}^{n-1} x^i \Big[\sum_{u \in N[v_{i+1}]} \phi(G - S_{i+1} - u) + 2 \sum_{C \in \mathcal{C}(v_{i+1})^{S_i}} \phi\big(G - S_i - V(C)\big) \Big], \quad (4)$$

where $S_0 = \{\}$ and for $i \geq 1$, $S_i = \{v_1, v_2, \ldots, v_i\}$.

Proof. We give a one-to-one correspondence between the basic figures of order r contributing to $\phi(G)$ and those contributing to one of the terms on the right. Let $\mathcal{B}$ be a basic figure of order r of a graph G contributing s to the coefficient a_r in $\phi(G)$. Consider the following cases:

1. If $v_1 \in \mathcal{B}$.
    (a) If $v_1 \in K_2 \subseteq \mathcal{B}$, let $\mathcal{B}'$ be $\mathcal{B} - V(K_2)$ viewed as a basic figure of $G - V(K_2)$. Here, $\mathcal{B}'$ contributes $-s$ to the coefficient a_r in $\phi(G - u - v_1)$, where $u \in N(v_1)$. Therefore, $\mathcal{B}'$ contributes s to the coefficient a_r in $-\phi(G - u - v_1)$ for all $u \in N(v_1)$.
    (b) If $v_1 \in C \subseteq \mathcal{B}$, let $\mathcal{B}'$ be $\mathcal{B} - V(C)$ viewed as a basic figure of $G - V(C)$. Here,

$$(-1)^{k(\mathcal{B}')} 2^{c(\mathcal{B}')} = -\frac{1}{2}(-1)^{k(\mathcal{B})} 2^{c(\mathcal{B})} = -\frac{s}{2}.$$

Therefore, $\mathcal{B}'$ contributes $-\frac{s}{2}$ to the coefficient a_r in $\phi(G-V(C))$. In turn, $\mathcal{B}'$ contributes s to the coefficient a_r in $-2\phi(G-V(C))$.

(c) If $v_1 \in \mathcal{B}$ with a loop at it, let $\mathcal{B}$ be $\mathcal{B} - \{v_1\}$ viewed as a basic figure of $G - v_1$. In this case, $\mathcal{B}'$ contributes $-s$ to the coefficient a_r in $\phi(G - v_1)$. Hence, it contributes s to the coefficient a_r in $-\phi(G - v_1)$.

Combining the above subcases, we have the contribution of $\mathcal{B}'$ in terms of the characteristic polynomials of $G - u - v_1$ and $G - V(C)$, where $u \in N[v_1]$.

2. If $v_1 \notin \mathcal{B}$ and $v_2 \in \mathcal{B}$.

(a) If $v_2 \in K_2 \subseteq \mathcal{B}$, let $\mathcal{B}'$ be $\mathcal{B} - V(K_2)$ viewed as a basic figure of $G - v_1 - V(K_2)$. Here, $\mathcal{B}'$ contributes $-s$ to the coefficient a_r in $x\phi(G - u - v_1 - v_2)$, where $u \in N(v_2)$. If $S_2 = \{v_1, v_2\}$, then $\mathcal{B}'$ contributes s to the coefficient a_r in $-x\phi(G - S_2 - u)$ for all $u \in N(v_2)$.

(b) If $v_2 \in C \subseteq \mathcal{B}$, let $\mathcal{B}'$ be $\mathcal{B} - V(C)$ viewed as a basic figure of $G - v_1 - V(C)$. Here,

$$(-1)^{k(\mathcal{B}')}2^{c(\mathcal{B}')} = -\frac{1}{2}(-1)^{k(\mathcal{B})}2^{c(\mathcal{B})} = -\frac{s}{2}.$$

Therefore, $\mathcal{B}'$ contributes $-\frac{s}{2}$ to the coefficient a_r in $x\phi(G - v_1 - V(C))$. In turn, $\mathcal{B}'$ contributes s to the coefficient a_r in $-2x\phi(G - S_1 - V(C))$, where $S_1 = \{v_1\}$.

(c) If $v_2 \in \mathcal{B}$ with a loop at it, let $\mathcal{B}$ be $\mathcal{B} - \{v_2\}$ viewed as a basic figure of $G - \{v_1, v_2\}$. In this case, $\mathcal{B}'$ contributes $-s$ to the coefficient a_r in $x\phi(G - S_2)$. Hence, it contributes s to the coefficient a_r in $-x\phi(G - S_2)$.

Here, we have the contribution of $\mathcal{B}'$ in terms of the characteristic polynomials of $G - S_2 - u$ and $G - S_1 - V(C)$, where $u \in N[v_2]$.

Now, for all i such that $3 \leq i \leq n$, define $S_i = \{v_1, v_2, \ldots, v_i\}$ and proceed likewise. The next case would be where the vertices v_1 and v_2 do not belong to $\mathcal{B}$ but $v_3 \in \mathcal{B}$; a similar analysis can be done. This process continues till none of the vertices $v_1, v_2, \ldots, v_n$ is present in $\mathcal{B}$. Let $\mathcal{B}'$ be the same basic figure viewed as a subgraph of $G - S_n$, then $\mathcal{B}'$ contributes s to the coefficient a_r in $x^n\phi(G - S_n)$. The result follows by combing all cases. □

One can also prove the above theorem by using the principle of mathematical induction on n. If we want to remove one vertex, the following corollary coincides with a result in article [18].

Corollary 3.6. *Let v be a vertex of a graph G and let $\mathcal{C}(v)$ denotes the set of cycles containing v. The characteristic polynomial $\phi(G)$ satisfies the following:*

$$\phi(G) = x\phi(G - S_1) - \sum_{u \in N[v]} \phi(G - S_1 - u) - 2 \sum_{C \in \mathcal{C}(v)} \phi(G - V(C)),$$

where $S_1 = \{v_1\}$.

The following theorem is stating another relationship between the characteristic polynomial of graphs G and G'. This time the theorem is useful when the characteristic polynomial of G is known, and we need to compute the characteristic polynomial of G'.

Theorem 3.7. *If $l_1, l_2, \ldots, l_n$ represent loops at vertices $v_1, v_2, \ldots, v_n$, respectively in a graph G, then the relationship between the characteristic polynomial of G and $G - \{l_1, l_2, \ldots, l_n\}$ is given by the following:*

$$\phi(G') = \phi(G) + \sum_{i=1}^{n} \phi(G - \{l_1, l_2, \ldots, l_{i-1}\} - v_i), \tag{5}$$

where $G' = G - \{l_1, l_2, \ldots, l_n\}$.

Proof. We prove the result using the principle of mathematical induction on the number of loops. Consider the graph G containing loops $l_1, l_2, \ldots, l_n$ at vertices $v_1, v_2, \ldots, v_n$, respectively. For the case $n = 1$, on the left-hand side, we have $\phi(G')$, where $G' = G - l_1$; and expanding the summation term in equation (5), we have a right-hand side as $\phi(G) + \phi(G - v_1)$. So, we need to prove that $\phi(G - l_1)$ is equal to $\phi(G) + \phi(G - v_1)$, which is true by using Corollary 3.2. This case describes the relationship between the characteristic polynomial of a graph G and a graph obtained upon removing one loop from G. Let us assume the result is true for $n = k - 1$; we have

$$\phi(G'_{k-1}) = \phi(G) + \sum_{i=1}^{k-1} \phi(G - \{l_1, l_2, \ldots, l_{i-1}\} - v_i), \tag{6}$$

where $G'_{k-1} = G - \{l_1, l_2, \ldots, l_{k-1}\}$ and we prove the result for $n = k$. Consider the graph G'_k which is $G - \{l_1, l_2, \ldots, l_k\}$ and can be written in terms of G'_{k-1} as follows:

$$G'_k = G - \{l_1, l_2, \ldots, l_{k-1}\} - l_k = G'_{k-1} - l_k.$$

Hence, we can obtain the graph G'_k from the graph G'_{k-1} by removing the loop l_k. So we can apply the case where one loop is being removed. We have

$$\phi(G'_k) = \phi(G'_{k-1} - l_k) = \phi(G'_{k-1}) - \phi(G'_{k-1} - v_k). \tag{7}$$

From equations 6 and 7, we have

$$\begin{aligned}
\phi(G'_k) &= \phi(G'_{k-1}) + \phi(G'_{k-1} - v_k) \\
&= \phi(G) + \sum_{i=1}^{k-1} \phi(G - \{l_1, l_2, \dots, l_{i-1}\} - v_i) + \phi(G'_{k-1} - v_k) \\
&= \phi(G) + \sum_{i=1}^{k-1} \phi(G - \{l_1, l_2, \dots, l_{i-1}\} - v_i) + \phi(G - \{l_1, l_2, \dots, l_{k-1}\} - v_k) \\
&= \phi(G) + \sum_{i=1}^{k} \phi(G - \{l_1, l_2, \dots, l_{i-1}\} - v_i).
\end{aligned}$$

Hence, the result is true for $n = k$. By the principle of mathematical induction, the result is true for n, where n is a natural number. □

In the above theorem, to obtain the characteristic polynomial of G', we keep on removing loops from G one at a time until we get G'. We use the relation between the characteristic polynomials of a graph and a graph obtained upon removing one loop.

Example 3.8. We wish to find the characteristic polynomial of the graph G shown in Figure 4.

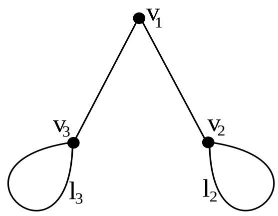

Figure 4: A graph G

Using Theorem 3.1, the characteristic polynomial of the given graph G satisfies the following:

$$\begin{aligned}\phi(G) &= \phi(G') - \phi(G' - v_2) - \phi(G' - v_3) + \phi(G' - \{v_2, v_3\}) \\ &= \phi(P_3) - \phi(P_2) - \phi(P_2) + \phi(P_1) \\ &= \phi(P_3) - 2\phi(P_2) + \phi(P_1) \\ &= x^3 - 2x - 2(x^2 - 1) + x \\ &= x^3 - 2x^2 - x + 2,\end{aligned}$$

where P_n denotes the path graph on n vertices.

Example 3.9. We wish to find the characteristic polynomial of the graph G' obtained on removing loops from the graph G shown in Figure 4. Using Theorem 3.7, the characteristic polynomial of G' satisfies the following:

$$\begin{aligned}\phi(G') &= \phi(G) + \phi(G - v_2) + \phi(G - l_2 - v_3) \\ &= x^3 - 2x^2 - x + 2 + x^2 - x - 1 + x^2 - 1 \\ &= x^3 - 2x.\end{aligned}$$

For a positive integer n, the unitary addition Cayley graph G_n is a simple graph whose vertex set is $\mathbb{Z}_n = \{0, 1, \ldots, n-1\}$, the ring of integers modulo n and in which two vertices x and y are adjacent if and only if $x + y \in U(n)$, where $U(n)$ denotes the set of units of the ring Z_n. The adjacency matrix associated with G_n is an $n \times n$ matrix $A(G_n) = [a_{ij}]$ such that $a_{ii} = 0$ and for $i \neq j$,

$$a_{ij} = \begin{cases} 1 & \text{if } i + j - 2 \in U(n), \\ 0 & \text{if } i + j - 2 \notin U(n). \end{cases}$$

Consider an anti-circulant matrix A_n of order n with first row as $a_0, a_1, \ldots, a_{n-1}$.

$$A_n = \begin{bmatrix} a_0 & a_1 & a_2 & \cdots & a_{n-1} \\ a_1 & a_2 & a_3 & \cdots & a_0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n-1} & a_0 & a_1 & \cdots & a_{n-2} \end{bmatrix}$$

with

$$a_j = \begin{cases} 1 & \text{if } \gcd(j, n) = 1, \\ 0 & \text{if } \gcd(j, n) > 1, \end{cases}$$

where $\gcd(a, b)$ denotes the greatest common divisor of numbers a and b.

Consider the graph $X(A_n)$ associated with the matrix A_n. We have the following theorem.

Theorem 3.10. *Let n be a positive integer. For even values of n, the unitary addition Cayley graph G_n is isomorphic to $X(A_n)$. For odd values of n, unitary addition Cayley graph G_n is isomorphic to the graph obtained from $X(A_n)$ on removing all loops.*

Proof. We prove the result by using adjacency matrices for both the graphs. First note that in a matrix A_n, the (i, j) entry is $a_{(i-1+j-1) \bmod n}$. For $i \neq j$, irrespective of n,

$$\begin{aligned} a_{ij} = 1 &\iff i + j - 2 \in U(n) \\ &\iff \gcd(i + j - 2, n) = 1 \\ &\iff \gcd(i - 1 + j - 1, n) = 1 \\ &\iff a_{i-1+j-1} = 1 \end{aligned}$$

For $i = j$, $a_{ij} = 0$ in $A(G_n)$. However, $a_{ij} = 1$ in A_n whenever $\gcd(i - 1 + j - 1, n) = 1$. For even values of n, $\gcd(2i - 2, n) \neq 1$, hence $a_{ij} = 0$ in A_n. Therefore, the unitary addition Cayley graph G_n is isomorphic to $X(A_n)$. For odd values of n, $\gcd(2i - 2, n) = 1$ is possible. Since these entries represent a loop in a graph, therefore G_n is isomorphic to the graph obtained from $X(A_n)$ on removing all loops. □

Finding the exact eigenvalues of unitary addition Cayley graphs is still an open problem. The authors in [15] tried to obtain bounds on these values. With the help of the above result, the characteristic polynomial of a unitary addition Cayley graph can be computed, and hence, one can find the eigenvalues as zeros of this polynomial.

4 Signed Unitary Addition Cayley Graph

In this section, we study unitary addition Cayley graphs in the realm of signed graphs using the algebraic approach. From [1], we know that any balanced signed graph and its underlying graph share the same spectrum. Here, therefore, we characterized for which values of n, S_n, and its negation are balanced.

A *signature* σ on a graph G is a mapping that assigns to each edge of G either a positive or a negative sign. The graph G equipped with a signature σ is called a *signed graph* [11], denoted by $S := (G, \sigma)$, where $G = (V, E)$ is an underlying graph and $\sigma \colon E \longrightarrow \{+, -\}$ is the signature that labels each edge of G either by '+' or '$-$'. The edge which receives the positive (respectively, negative) sign is called a *positive* (respectively, *negative*) *edge*. A signed graph is an *all-positive* (respectively, *all-negative*) if all its edges are positive (respectively, negative); further, it is said to be *homogeneous* if it is either an all-positive or an all-negative and *heterogeneous* otherwise. The *negation* $\eta(S)$ of a signed graph S is another signed graph obtained from S by negating the sign of every edge in S.

One of the fundamental concepts in the theory of signed graphs is that of balance. Harary [11] introduced the idea of balanced signed graphs for the analysis of social networks, in which a positive edge stands for a friendly connection, and a negative edge represents a hostile connection. A signed graph S is balanced if every cycle in S has an even number of negative edges.

The following is the characterization of balance for an arbitrary signed graph given by Harary in the year 1953.

Theorem 4.1 ([11]). *A signed graph is balanced if and only if its vertex set can be partitioned into two subsets, one of them may be empty, such that any edge joining two vertices within the same subset is positive, while an edge joining two vertices in different subsets are negative.*

However, if it is not possible to partition the given signed graph according to Harary criterion, a related but alternative theory of clustering was presented by Davis in the year 1967.

Theorem 4.2 ([6]). *A signed graph S is clusterable if and only if S contains no cycle having exactly one negative edge.*

A *marking* μ on a graph G is a mapping that assigns to each vertex of G either a positive or a negative sign. A *marked graph* [4] is an ordered pair $G_\mu := (G, \mu)$, where $G = (V, E)$ is an underlying graph and $\mu \colon V(G) \longrightarrow \{+, -\}$ is the labeling that labels each vertex of G either '+' or '$-$'.

The definition of the new notion is as follows:

Definition 4.3. A signed unitary addition Cayley graph is an ordered pair $S_n := (G_n, \sigma)$, where G_n is the unitary addition Cayley graph with $\mathbb{Z}_n$ as vertex set and for an edge v_iv_j of S_n, σ is defined as

$$\sigma(v_iv_j) = \begin{cases} + & \text{if } v_i \in U(n) \text{ and } v_j \in U(n), \\ - & \text{otherwise.} \end{cases}$$

With this definition, the edges incident to a vertex v ($v \notin U(n)$) are negative for any positive integer n. The signed unitary addition Cayley graphs S_4 and S_5 are shown in Figure 5.

(a) S_4

(b) S_5

Figure 5: Signed Unitary Addition Cayley Graphs

The following results from different articles are quoted, which we need to prove our results.

Theorem 4.4 ([19]). *For any positive integer n, the unitary addition Cayley graph G_n is bipartite if and only if either n is even or $n = 3$.*

Following is another characterization for a balanced signed graph in terms of marking of the vertices.

Theorem 4.5 ([17]). *A signed graph $S = (G, \sigma)$ is balanced if and only if there exists a marking μ of its vertices such that for each edge v_1v_2 in S, $\sigma(v_1v_2) = \mu(v_1)\mu(v_2)$ holds.*

Theorem 4.6. *For any positive integer n, S_n is always clusterable.*

Proof. We prove the result by using contradiction. Assume S_n is not clusterable for any positive integer n. According to the Theorem 4.2, there exists a cycle C containing exactly one negative edge. Let v_iv_j be a negative edge in C. By Definition 4.3, vertices v_i and v_j when viewed as elements of $\mathbb{Z}_n$, does not belong to $U(n)$ together. There are two possibilities; either one of the v_i and v_j belongs to $U(n)$, or none of them belongs to $U(n)$. For the first case, without loss of generality, let us assume $v_i \in U(n)$ and $v_j \notin U(n)$. Again by Definition 4.3, all edges incident to v_j are negative. In turn, cycle C must contain two negative edges, which are incident to vertex v_j. Therefore, there exists no cycle in S_n containing exactly one negative edge. Hence, S_n is clusterable, which contradicts our assumption. For the second case, if both

v_i and v_j does not belong to $U(n)$, then again using the same argument, we get a contradiction. □

Lemma 4.7. *For any positive integer n and an integer i between 0 and n, $i \in U(n)$ if and only if $n - i \in U(n)$.*

Proof. Let n be any positive integer. We prove the result by contradiction. For the necessity part, suppose $i \in U(n)$. We need to show $n - i \in U(n)$. Assume $n - i \notin U(n)$, that is, $\gcd(n - i, n) \neq 1$. Let $\gcd(n - i, n) = k$ with $k > 1$. It implies that k divides both $n - i$ and n. In turn, there exist α and β such that $n - i = \alpha k$ and $n = \beta k$. Substituting the value of n from second equation to first equation, we have $\beta k - i = \alpha k$, which implies that $i = \gamma k$, where $\gamma = \beta - \alpha$. It implies that $\gcd(i, n)$ is at least k. It contradicts our hypothesis. Therefore, $n - i \in U(n)$.

For the sufficiency, suppose $n - i \in U(n)$, and we need to show $i \in U(n)$. Again assume $i \notin U(n)$, that is, $\gcd(i, n) \neq 1$. Let $\gcd(i, n) = k$ with $k > 1$. It implies that k divides both i and n. There exist α and β such that $i = \alpha k$ and $n = \beta k$. In this case, $n - i = \beta k - \alpha k$, which implies that $n - i = \gamma k$, where $\gamma = \beta - \alpha$. Now, $\gcd(n - i, n) \neq 1$ as k divides both $n - i$ and n, which contradicts the fact that $n - i \in U(n)$. Therefore, $i \in U(n)$. □

Lemma 4.8. *For any even positive integer n, S_n is always an all-negative signed graph.*

Proof. Note that for any even positive integer n, $U(n)$ contains all odd integers between 0 and n, and a sum of two odd integers is always even. Therefore, the sum does not belong to $U(n)$. Hence, the elements of $U(n)$ when viewed as vertices of S_n are non-adjacent. By Definition 4.3, edges in S_n are negative and hence the result is true. □

Lemma 4.9. *For a positive integer n, if $n = p^a$, where p is a prime number and a is a positive integer, then S_n is balanced.*

Proof. We prove the result with the help of a marking of vertices of the graph S_{p^a}. Assign a marking μ such that $\mu(v)$ is positive if v belongs to $U(p^a)$, and is negative otherwise. Consider an edge $v_i v_j$. If it is positive, then by Definition 4.3, v_i and v_j belong to the set $U(p^a)$, and hence it satisfy the condition $\sigma(v_i v_j) = \mu(v_i)\mu(v_j)$. If it is negative, then only one of the v_i and v_j belongs to $U(p^a)$. Without loss of generality, assume $v_i \in U(p^a)$ and $v_j \notin U(p^a)$. In this case, v_i receives positive sign and v_j receives negative sign. Therefore, $\sigma(v_i v_j) = \mu(v_i)\mu(v_j)$ is true. The case where the edge $v_i v_j$

is negative, and both end vertices do not belong to $U(p^a)$ does not exist. As if vertices v_i and v_j does not belong to $U(p^a)$, then there exist α and β such that $v_i = \alpha p$ and $v_j = \beta p$. It implies that the sum $v_i + v_j = \gamma p$, where $\gamma = \alpha + \beta$. In turn $v_i + v_j \notin U(p^a)$. That is, the vertices v_i and v_j are not adjacent in unitary addition Cayley graph G_{p^a}. Consequently, whenever there is an edge v_iv_j, it satisfies the marking criteria given in Theorem 4.5, and therefore the result follows. □

Theorem 4.10. *For a positive integer n, S_n is balanced if and only if either n is even or is a prime power.*

Proof. For the necessity part, suppose S_n is balanced and $n = p_1^{a_1} p_2^{a_2} \cdots p_k^{a_k}$, where $p_1, p_2, \ldots, p_k$ are distinct prime numbers in increasing order and $a_1, a_2, \ldots, a_n$ are positive integers. If $p_1 = 2$, then the result is true. Assume $p_1 \neq 2$. To get the desired result, we show that $k = 1$. Assume $k > 1$. We contradict the hypothesis by showing that either an all-negative cycle $1 - p_1 - p_2 - 1$ or an all-negative cycle $1 - p_1 - (n - p_2) - 1$ or both are present in S_n. First, note that the numbers 1, p_1 and p_2 are distinct, and also $n - p_2$ is never equal to 1 or p_1.

Since $p_1 \neq 2$, $p_1 + 1 < p_i$ for all i such that $2 \leq i \leq k$. Therefore, $p_1 + 1$ is not a multiple of p_i for any i such that $1 \leq i \leq k$. It implies $p_1 + 1 \in U(n)$, and hence vertices 1 and p_1 are adjacent. Next, we show that the vertex p_1 is adjacent to vertices p_2 and $n - p_2$. Note that for all i such that $3 \leq i \leq k$ the inequality $p_1 < p_2 < p_i$ holds. In turn, we have $p_1 + p_2 < 2p_2 < p_i + p_2$. Next, adding p_i on both the sides of inequality $p_2 < p_i$, we have $p_i + p_2 < 2p_i$. Therefore, for all i such that $3 \leq i \leq k$, $p_1 + p_2 < 2p_i$. Also, since the sum $p_1 + p_2$ is even, $p_1 + p_2 \neq p_i$. Consequently, the sum $p_1 + p_2$ is not a multiple of p_i for any i such that $3 \leq i \leq k$. Further, the sum $p_1 + p_2$ is not a multiple of p_1 and p_2. As if for some α, $p_1 + p_2 = \alpha p_1$, then $p_2 = \beta p_1$, where $\beta = \alpha - 1$. It contradicts the fact that p_1 and p_2 are prime numbers. Again for the same reason, sum $p_1 + p_2$ is not a multiple of p_2. Therefore, $p_1 + p_2 \in U(n)$ and the vertices p_1 and p_2 are adjacent. On the same lines, we can show that the sum $p_2 - p_1$ is not a multiple of p_i for any i such that $1 \leq i \leq k$ and hence $p_2 - p_1 \in U(n)$. By Lemma 4.7, we have $n - (p_2 - p_1) \in U(n)$. It implies that $n - p_2 + p_1 \in U(n)$ and hence the vertices $n - p_2$ and p_1 are adjacent.

Next, we claim it is not possible that the vertex 1 is neither adjacent to p_2 nor adjacent to $n - p_2$. If it is true, then $p_2 + 1 \notin U(n)$ and $n - p_2 + 1 \notin U(n)$. First, $p_2 + 1$ must be a multiple of p_i for some i such that $1 \leq i \leq k$. Clearly, $p_2 + 1 < p_i$ for all i such that $3 \leq i \leq k$ and also $p_2 + 1$ can never be a multiple of p_2. Therefore, the only possible value of i such that $p_2 + 1$ is a multiple of p_i is 1; consequently, there exist α such that

$$p_2 + 1 = \alpha p_1 \tag{8}$$

Next, $n - p_2 + 1 \notin U(n)$ implies $n - (p_2 - 1) \notin U(n)$. By Lemma 4.7, $p_2 - 1 \notin U(n)$. Therefore, $p_2 - 1$ must be a multiple of p_i for some i such that $1 \leq i \leq k$. Again, the only possible value of i is 1. Hence, there exists β such that

$$\begin{aligned}
& p_2 - 1 = \beta p_1 \\
\Longrightarrow\ & \alpha p_1 - 1 - 1 = \beta p_1 \qquad \text{[using equation (8)]} \\
\Longrightarrow\ & \alpha p_1 - 2 = \beta p_1 \\
\Longrightarrow\ & \alpha p_1 - \beta p_1 = 2 \\
\Longrightarrow\ & (\alpha - \beta) p_1 = 2.
\end{aligned}$$

Since p_2 is a prime number, $p_2 + 1$ and $p_2 - 1$ are positive integers in decreasing order. Since p_1 is also a prime number, from the right-hand side of equation (8) and the equation succeeding it, we have $\alpha - \beta > 0$. In turn, we get a contradiction as the last implication mentioned-above is not possible. Therefore, the vertex 1 must be adjacent to at least one of the vertices p_2 or $n - p_2$.

Next, we know that $\gcd(1, n) = 1$, $\gcd(p_1, n) \neq 1$ and $\gcd(p_2, n) \neq 1$. Hence, $1 \in U(n)$ but the elements p_1 and p_2 does not belong to $U(n)$. Using Lemma 4.7, $n - p_2 \notin U(n)$. By the definition of signed unitary addition Cayley graph, the edges $1p_1$, $1p_2$, p_1p_2, $1(n-p_2)$ and $p_1(n-p_2)$, if exist, are negative edges. Therefore, the result follows.

For the sufficiency part, if n is even, then by Theorem 4.4 and Lemma 4.8, S_n is an all-negative bipartite graph. Therefore, it is balanced. If n is a prime power, then by Lemma 4.9, S_n is balanced. □

Theorem 4.11. *For a positive integer n, $\eta(S_n)$ is balanced if and only if either n is even or $n = 3$.*

Proof. For the necessity part, suppose $\eta(S_n)$ is balanced. If n is even, it is done. If it is not even, we need to show that it is equal to 3. Assume n is an odd number greater than 3. We contradict the hypothesis by showing that $\eta(S_n)$ contains a cycle $0 - 1 - (n-2) - 0$ with exactly one negative edge. Note that the numbers 0, 1, and $n - 2$ are distinct if and only if $n > 3$. Since n is odd, $2 \in U(n)$. By Lemma 4.7, $n - 2 \in U(n)$. Therefore, the vertex 0 is adjacent to $n - 2$. Next, $1 \in U(n)$ implies 0 and 1 are also adjacent. Also, again by Lemma 4.7, $n-1 \in U(n)$ which implies $(n-2)+1 \in U(n)$. Hence, 1 is adjacent to $n-2$. Now, since $0 \notin U(n)$, edges 01 and $0(n-2)$ are negative edges in S_n. Moreover, an edge $1(n-2)$ is a positive edge. Therefore, in $\eta(S_n)$, the cycle on 0, 1, and $n-2$ contains one negative edge making $\eta(S_n)$ unbalanced, which contradicts. Therefore, $n = 3$.

For the sufficiency part, if n is even, then by Lemma 4.8, S_n is an all-negative graph. Therefore, $\eta(S_n)$ is an all-positive graph; it is balanced. For $n = 3$, S_n is a tree, which implies that $\eta(S_n)$ is balanced. □

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References

[1] B. D. Acharya, *Spectral criterion for cycle balance in networks*, Journal of Graph Theory, 4 (1980), 1–11.

[2] E. Babaev and R. Hefferlin, *The concepts of periodicity and hyperperiodicity: from atoms to molecules*, in: D. Rouvray, ed., Concepts in Chemistry: A Contemporary Challenge, Research Studies Press, London, 1996, pp. 24–81.

[3] A. T. Balaban, *Chemical Applications of Graph Theory*, Academic Press, 1976.

[4] L. W. Beineke and F. Harary, *Consistent graphs with signed points*, Rivista di matematica per le scienze economiche e sociali, 1 (1978), 81–88.

[5] D. Bonchev, *Chemical Graph Theory: Introduction and Fundamentals*, vol. 1, CRC Press, 1991.

[6] J. A. Davis, *Clustering and structural balance in graphs*, Human Relations, 20 (1967), 181–187.

[7] J. Dugundji and I. Ugi, *An algebraic model of constitutional chemistry as a basis for chemical computer programs*, in Computers in Chemistry, Springer, 1973, pp. 19–64.

[8] R. Gillespie and I. Hargittai, *The VSEPR Model of Molecular Geometry*, Allyn and Bacon, Newton, Mass., 1991.

[9] R. Gillespie and R. Nyholm, *Inorganic stereochemistry*, Quarterly Reviews, Chemical Society, 11 (1957), 339–380.

[10] R. J. Gillespie, *Molecular Geometry*, Van Nostrand Reinhold, 1972.

[11] F. Harary, *On the notion of balance of a signed graph*, Michigan Mathematical Journal, 2 (1953), 143–146.

[12] W. B. Jensen, *The Lewis acid-base concepts: an overview*, Krieger Publishing, 1979.

[13] I. Langmuir, *The arrangement of electrons in atoms and molecules*, J. Amer. Chem. Soc., 41 (1919), 868–934; *Isomorphism, isosterism and covalence*, J. Amer. Chem. Soc., 41 (1919), 1543–1559.

[14] G. N. Lewis, *Valence and the Structure of Atoms and Molecules*, The Chemical Catalog Company, 1923; Dover Publications, New York, 1966.

[15] N. Palanivel and A. Chithra, *Energy and Laplacian energy of unitary addition Cayley graphs*, Filomat, 33 (2019), 3599–3613.

[16] H. Sachs, *Beziehungen zwischen den in einem graphen enthaltenen kreisen und seinem charakteristischen polynom*, Publ. Math. Debrecen, 11 (1964), 119–134.

[17] E. Sampathkumar, *Point signed and line signed graphs*, Nat. Acad. Sci. Letters, 7 (1984), 91–93.

[18] A. J. Schwenk, *Computing the characteristic polynomial of a graph*, in: Graphs and Combinatorics, Springer, 1974, pp. 153–172.

[19] D. Sinha, P. Garg, and A. Singh, *Some properties of unitary addition cayley graphs*, Notes on Number Theory and Discrete Mathematics, 17 (2011), 49–59.

[20] L. Spialter, *The atom connectivity matrix (ACM) and its characteristic polynomial (ACMCP)*, Journal of Chemical Documentation, 4 (1964), 261–269.

[21] N. Trinajstić, *Computing the characteristic polynomial of a conjugated system using the Sachs theorem*, Croatica Chemica Acta, 49 (1977), 593–633.