symmetry

MDPI

Article

On Laplacian Eigenvalues of Wheel Graphs

Manal Alotaibi [1,*], Ahmad Alghamdi [2] and Hanan Alolaiyan [1]

[1] Department of Mthematics, College of Science, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia; holayan@ksu.edu.sa

[2] Department of Mathematical Sciences, Faculty of Applied Sciences, Umm Al-Qura University, P.O. Box 14035, Makkah 21955, Saudi Arabia; amghamdi@uqu.edu.sa

* Correspondence: alomanal@ksu.edu.sa

Abstract: Consider G to be a simple graph with n vertices and m edges, and $L(G)$ to be a Laplacian matrix with Laplacian eigenvalues of $\mu_1, \mu_2, \ldots, \mu_n = zero$. Write $S_k(G) = \sum_{i=1}^{k} \mu_i$ as the sum of the k-largest Laplacian eigenvalues of G, where $k \in \{1, 2, \ldots, n\}$. The motivation of this study is to solve a conjecture in algebraic graph theory for a special type of graph called a wheel graph. Brouwer's conjecture states that $S_k(G) \leq m + \binom{k+1}{2}$, where $k = 1, 2, \ldots, n$. This paper proves Brouwer's conjecture for wheel graphs. It also provides an upper bound for the sum of the largest Laplacian eigenvalues for the wheel graph W_{n+1}, which provides a better approximation for this upper bound using Brouwer's conjecture and the Grone–Merris–Bai inequality. We study the symmetry of wheel graphs and recall an example of the symmetry group of W_{n+1}, $n \geq 3$. We obtain our results using majorization methods and illustrate our findings in tables, diagrams, and curves.

Keywords: Laplacian eigenvalues; wheel graph; Grone–Merris–Bai theorem; Brouwer's conjecture; symmetry of wheel graphs; automorphism group of graphs

Citation: Alotaibi, M.; Alghamdi, A.; Alolaiyan, H. On Laplacian Eigenvalues of Wheel Graphs. *Symmetry* **2023**, *15*, 1737. https://doi.org/10.3390/sym15091737

Academic Editors: Abel Cabrera Martínez and Alejandro Estrada-Moreno

Received: 8 August 2023
Revised: 1 September 2023
Accepted: 6 September 2023
Published: 11 September 2023

1. Introduction

Denote as G a simple graph with a vertex set $V(G)$ and an edge set $E(G)$. The Laplacian matrix of G can be written as $L(G) = D(G) - A(G)$, where $D(G)$ is the degree matrix. Here, the degree matrix $D = [d_{ij}]$ of G is defined by

$$d_{ij} = \begin{cases} 0 & \text{for } i \neq j \\ d_i & \text{for } i = j, \end{cases}$$

where d_i is the degree of the vertex i. $A(G)$ is the adjacency matrix of G, where G is a graph with $V(G) = \{v_1, v_2, \ldots, v_n\}$, $E(G) = \{e_1, e_2, \ldots, e_m\}$, and without parallel edges. The adjacency matrix is the $n \times n$ symmetric binary matrix $A(G) = [a_{ij}]$, which is defined over the ring of integers such that

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

as in [1]. The characteristic polynomial of the Laplacian matrix is called the Laplacian polynomial. The second smallest root of the Laplacian polynomial of the graph G (counting multiple values separately) is known as the algebraic connectivity of G. The largest is known as the Laplacian spectral. Let $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_n = zero$ be the Laplacian eigenvalues of G, where $n = |V(G)|$.

Definition 1 ([2])**.** *For a graph G with n vertices, $S_k(G) = \sum_{i=1}^{k} \mu_i$, $k = 1, 2, \ldots, n$ is the sum of the k largest Laplacian eigenvalues of G and $d_i^* = |\{v \in V(G) : d_v \geq i\}|$, where $i = 1, 2, \ldots, n$. d_v is the degree of a vertex v in G.*

Obviously, $d_1^* \geq d_2^* \geq \ldots \geq d_n^*$. For the graph G with n vertices, the Grone–Merris–Bai conjecture [3] states that

$$S_k(G) \leq \sum_{i=1}^{k} d_i^*, \tag{2}$$

where $1 \leq k \leq n$. This conjecture was proven by Bai [3].

Let $m = |E(G)| = e(G)$ for the graph G. Then, we have the following conjecture [4].

Conjecture 1. *Let G be a graph with n vertices. Then,*

$$S_k(G) \leq m + \binom{k+1}{2} \tag{3}$$

for all $1 \leq k \leq n$.

The inequality 3 above holds for split graphs. In particular, it holds for threshold graphs [5]. The conjecture holds for regular graphs [6]. For the case where $k = 1$, Conjecture 1 is derived from the inequality $\mu_1(G) \leq n$ (see [4]). In [7], the authors found that for any tree and when k is equal to 2 for all graphs, Conjecture 1 is true.

Definition 2 ([8])**.** *The wheel graph W_{n+1} is created by joining a single vertex K_1, to each vertex on the cycle C_n. In other words, $W_{n+1} = K_1 \vee C_n$.*

Remark 1. *We thank the reviewer for providing the Laplacian eigenvalues for the wheel graph in an easy way by referring us to [9,10], which contain the following results:*

The Laplacian eigenvalues for the cycle graph C_n are $\{2 - 2\cos(\frac{2\pi j}{n}) : j = 0, 1, \ldots, n-1\}$, and the Laplacian eigenvalue for the isolated vertex K_1 is {0}. Then, the Laplacian eigenvalues for W_{n+1} (using the results in [4,8]) are

$$\sigma(W_{n+1}) = \sigma(C_n \vee K_1) = \{0,\ 3 - 2\cos(\frac{2\pi j}{n}) \text{ where } j \in \{1, \ldots, n-1\},\ n+1\}.$$

The sum of the spectrum of the wheel graph is the sum of the degrees of the vertices of the graphs, which is

$$S_{n+1}(W_{n+1}) = S_n(W_{n+1}) = \sum_{i=1}^{n} \mu_i = \sum_{i=1}^{n+1} d_i = n + 3n = 4n,$$

hence, $S_k(W_{n+1}) \leq 4n$, *for all* $k = 1, 2, \ldots, n+1$.

This paper is organized as follows. This section contains five subsections, including a literature review of studies on wheel graphs and overviews of molecular science and graph theory, the symmetry of wheel graphs, the automorphism group of graphs, and the determining set. We have tried to represent information in wheel graphs that are related to our work. Section 2 contains our approach to tackling this problem. In particular, we explain the notion of majorization. Section 3 contains our main results, including Brouwer's conjecture, which is valid for wheel graphs, and we provide a better approximation for this upper bound using Brouwer's conjecture and the Grone–Merris–Bai inequality. Then, we describe an application to international airports that gives us the wheel graph W_{11} and apply Brouwer's conjecture. We conclude this work with a discussion and conclusions in Sections 4 and 5.

1.1. Literature Review of Studies of Wheel Graphs

In 1995, Balasubramanian [11] found the Laplacian of fullerenes $C_{42} - C_{90}$ (see Section 1.2) using high-precision computational algorithms. In [12], the same author computed the

Laplacians of fullerenes as the generators of the number of spanning trees, which find applications in the computation of the magnetic properties of fullerenes. In 2001, the authors of [13] investigated cyclicity in four types of polycyclic graphs, including five-vertex graphs with a five-cycle, Schlegel graphs depicting platonic solids, buckminsterfullerene isomers, and C_{70} isomers, using the distance-related and resistance distance-related indices. In 2013, Wang et al. [14] determined whether $R(G)$ is the graph obtained from G by adding a new vertex corresponding to each edge of G and by joining each new vertex to the end vertices of the corresponding edge. $Q(G)$ is the graph created from G by joining a new vertex to every edge of G and by joining the edges of those pairs of new vertices that lie on adjacent edges of G. The Laplacian polynomials of $R(G)$ and $Q(G)$ of a regular graph G were derived, along with a formula and the lower bounds of the Kirchhoff index of these graphs. In 2023, Balasubramanian [15] obtained the characteristic polynomials and a number of spectral-based indices such as the Riemann–Zeta functional indices and spectral entropies of n-dimensional hypercubes using recursive Hadamard transforms. In [16], the same author used the Hadamard symmetry and recursive dynamic computational techniques to obtain a large number of degree- and distance-based topological indices, graph and Laplacian spectra and the corresponding polynomials, and entropies and the matching polynomials of n-dimensional hypercubes.

Regarding wheel graphs, in 2009, Zhang et al. [17] proved that, except for W_7, W_{n+1} can be determined by its Laplacian spectrum. They provided a graph that is cospectral with the wheel graph W_7. In 2015, Wen et al. [18] proved that all wind-wheel graphs are determined using both their Laplacian and signless Laplacian spectra. In 2020, Chu et al. [19] computed energies of multi-step wheel networks $W_{n,m}$ and closed forms of signless Laplacian and Laplacian spectra. These wheel networks are useful in networking and communication, as every node is one hoop neighbor to another. In 2021, Daoqiang et al. [20] studied the subtree number index of wheel graphs and other types of graphs. In 2022, Kuswardi et al. [21] investigated the chromatic number of the amalgamation of wheel graphs. In June 2023, Wei et al. [22] studied the complexity of wheel graphs with multiple edges and vertices. In July 2023, Greeni et al. [23] explained the embedding of a complete bipartite graph into a wheel-related graph. In May 2023, Selig et al. [24] showed us some combinatorial aspects of sandpile models of wheel and fan graphs.

1.2. Molecular Science and Graph Theory

Let us discuss some applications of graph theory to molecular science.

Fullerenes are molecules of carbon atoms that form large hollow shapes. Fullerenes are made of carbon atoms that join together to form hollow hexagonal rings. Fullerenes can be seen as graphs, where vertices represent atoms and edges represent the bonds between atoms. In fact, a fullerene graph is 3-connected and 3-regular with only pentagonal and hexagonal faces. One can observe that the number of pentagonal faces is always 12. This is because of Euler's formula. We highlight that this application will be studied in future work.

Another application that we can mention here in this regard is nanomaterial structures. One can develop models of nanomaterials using graph theory. This is a modern approach and a new strategy compared to traditional methods. Graph theory can be used as a unifying approach for the structural description of many materials and nanomaterials. This application is important in the study of networks and nanostructures. In fact, the structural analysis of nanoscale network materials using graph theory is now a very active area of research. One of our plans is to study and investigate this approach in the future (see [25–27]).

1.3. Symmetry of Wheel Graphs

In this section, we discuss the symmetry of wheel graphs. In particular, we study the results in the paper written by Tully in October 2021 [28].

There is a type of stochastic process with a property of discrete time called a random walk. In this process, a particle starts from one vertex, called the origin, and at each successive epoch, it moves from its current position to an adjacent vertex. Assume that $i \neq j = 0, 1, 2, \ldots, n$ and the transit time from i to j is the random time (number of steps) to get from v_i to v_j. Let ${}_{ij}T$ represent the transit time from i to j.

Using the structural symmetry of the W_n graph, we have:

- (Hub to periphery): ${}_{01}T = {}_{02}T = {}_{03}T = \ldots = {}_{0n}T$.
- (Periphery to hub): ${}_{10}T = {}_{20}T = {}_{30}T = \ldots = {}_{n0}T$.
- (Periphery to periphery): ${}_{ij}T = {}_{ji}T = {}_{j+ki+k}T = {}_{i+kj+k}T$ for all k integers and for all $i \neq j$ and $i, j = 1, 2, \ldots, n$, where the addition of node labels is interpreted as a modulo n operation (however, v_n is the counter-clockwise neighbor of v_1 on the periphery and $v_0 = H$ is the hub).

Hence, the time taken to loop back to the starting vertex can be defined as ${}_{00}T = 1 + {}_{10}T$; and for $i = 1, 2, \ldots, n$, [28] it can be defined as

$$
{}_{ii}T = {}_{11}T = \begin{cases} 1 + {}_{21}T & \text{with probability } 2/3, \\ 1 + {}_{01}T & \text{with probability } 1/3. \end{cases}
$$

The authors studied the transition time ${}_{ij}T$ from v_i to v_j and discussed the mean and the standard deviations of ${}_{ij}T$.

1.4. Automorphism Group of Graphs

Definition 3 ([29])**.** *The symmetry group of a graph G or its automorphism group consists of permutations of the vertices of G that preserve the adjacency matrix $A(G)$ of the graph, which is defined in (1).*

Remark 2. *Definition 3 is equivalent to saying that the symmetry group of G consists of permutations whose permutation matrices P satisfy*

$$
PA = AP.
$$

Theorem 1 ([30])**.** *The collection of symmetries of a graph G form a group with composition. This group is denoted as $Aut(G)$.*

Example 1 ([31])**.** *The wheel graph W_{n+1} with $n \geq 4$ has a symmetry group that is isomorphic to the symmetry of the cycle graph C_n, i.e., $Aut(W_{n+1}) \cong D_n$, where D_n is the dihedral group of order $2n$.*

1.5. Determining Set

Definition 4 ([32])**.** *For a simple graph G, the determining set is a non-empty subset, say T, in which for any two elements r and s in the symmetry group of G, if they are the same in the vertices of T, they are the same on the vertices of G. In other words, T is the determining set for the case where r and s are two automorphisms with $r(t) = s(t)$ for all t in T and $r = s$.*

The minimum size of such a set of vertices is the determining number of the graph.

Theorem 2 ([31])**.** *The determining number of the wheel graph W_{n+1}, $n \geq 3$ is 2.*

For recent results of the automorphism group of a graph, the reader is referred to [33–35].

2. Methodology

Research on graph theory is a very active area of research. In fact, it is an applied science that has a concrete relationship with pure and discrete mathematics.

Our methodology and strategies in this work are standard. Our approach is to use the previous literature in this field to build and investigate new problems. We focus on a specific type of graph, which is known as a wheel graph.

Linear algebra and matrix theory are very important tools for this work. Spectrum theory has proven to be a powerful tool for visualizing and understanding graph theory.

Another method that we have already used is order and majorization. The concept of majorization can be seen in [8]. It many applications in graph theory. For two non-increasing real sequences $\mathbf{x}$ and $\mathbf{y}$ of length n, we say that $\mathbf{x}$ is majorized by $\mathbf{y}$ (denote as $\mathbf{x} \preceq \mathbf{y}$) if $\sum_{i=1}^{k} x_i \leq \sum_{i=1}^{k} x_i$ for all $k \leq n$, and $\sum_{i=1}^{n} x_i \leq \sum_{i=1}^{n} y_i$.

3. Main Results

This section investigates whether Brouwer's conjecture holds for the wheel graph and determines an upper bound for the sum of the k-largest Laplacian eigenvalues of a wheel graph.

We denote the collection of all Laplacian spectra for a graph G by $\sigma(G)$.

Our main aim is to show that Brouwer's conjecture holds for the wheel graph, where $n \geq 3$, i.e.,

$$S_k(W_{n+1}) \leq 2n + \frac{k(k+1)}{2},$$

for all $k = 1, 2, \ldots, n+1$, and $n \geq 3$.

To achieve this, we present the cases where $n = 3, 4, 5$.

- Case I: At $n = 3$, observe that W_4 in Figure 1 is a regular graph. Therefore, according to [6], the Brouwer's conjecture holds for W_4.

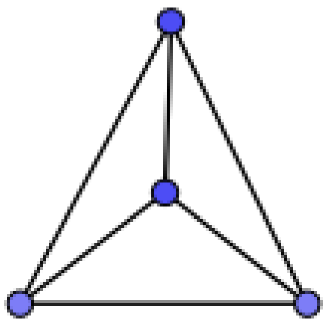

Figure 1. The wheel graph W_4.

- Case II: At $n = 4$, Figure 2, the Laplacian eigenvalues for W_5 are $\{4+1, 3 - 2\cos\frac{2\pi j}{4}$, where $j \in \{1,2,3\}, 0\} = \{5,5,3,3,0\}$. From Table 1 , we have

$$S_k(W_5) \leq e(W_5) + \binom{k+1}{2} = 8 + \frac{k(k+1)}{2}.$$

Table 1. $S_k(W_5)$ and $e(W_5) + \frac{k(k+1)}{2}$.

k	$S_k(W_5)$	$e(W_5) + \binom{k+1}{2}$
1	5	9
2	10	11
3	13	14
4	16	18
5	16	23

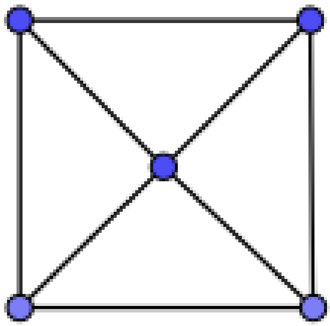

Figure 2. The wheel graph W_5.

Therefore, Brouwer's conjecture holds for W_5 for all $k = 1, 2, 3, 4, 5$.

- Case III: At $n = 5$, Figure 3, the Laplacian eigenvalues for W_6 are $\{5+1, 3 - 2\cos\frac{2\pi j}{5}$, where $j \in \{1,2,3,4\}, 0\} = \{6, 4.618, 4.618, 2.382, 2.382, 0\}$. From Table 2, we have

$$S_k(W_6) \leq e(W_6) + \binom{k+1}{2} = 10 + \frac{k(k+1)}{2},$$

for all $k = 1, 2, 3, 4, 5, 6$.

Table 2. $S_k(W_6)$ and $e(W_6) + \frac{k(k+1)}{2}$.

k	$S_k(W_6)$	$e(W_6) + \binom{k+1}{2}$
1	6	11
2	10.618	13
3	15.236	16
4	17.618	20
5	20	25
6	20	31

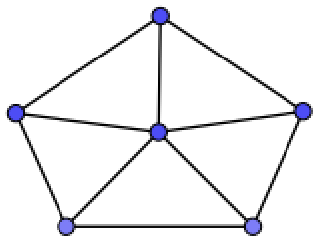

Figure 3. W_6.

Therefore, Brouwer's conjecture holds for W_6 for all $k = 1, 2, 3, 4, 5, 6$.

Now, we are ready to present the main theorem.

Theorem 3. *Brouwer's conjecture holds for the wheel graph W_{n+1}, where $n \geq 3$, i.e.,*

$$S_k(W_{n+1}) \leq 2n + \frac{k(k+1)}{2},$$

where $n \geq 3$ for $k = 1, 2, \ldots, n+1$.

Proof of Theorem 3. We have to show that

$$S_k(W_{n+1}) \leq 2n + \frac{k(k+1)}{2},$$

for all $k = 1, 2, \ldots, n+1$.

Now, for $1 \leq k \leq n+1$, we have

$$\begin{aligned} S_k(W_{n+1}) &= (n+1) + \mu_2 + \mu_3 + \cdots + \mu_k \\ &\leq (n+1) + 5(k-1) \\ &= n + 5k - 4. \end{aligned}$$

Then, $n + 5k - 4 \leq 2n + \frac{k(k+1)}{2}$ if $k^2 - 9k + 2n + 8 \geq 0$. To achieve this inequality, consider the polynomial $f(k) = k^2 - 9k + 2n + 8$. The discriminant for f is $D = (9)^2 - 4(2n+8) = 81 - 8n - 32 = 49 - 8n$, which implies that $f(k) \geq 0$ for all $k = 1, 2, \ldots, n+1$ when $D \leq 0$. Now, $49 - 8n \leq 0$, which implies that $n \geq \frac{49}{8}$, which is $n \geq 7$. Therefore, when $n \geq 7$, $n + 5k - 4 \leq 2n + \frac{k(k+1)}{2}$, which implies that $S_k(W_n) \leq 2n + \frac{k(k+1)}{2}$, Brouwer's conjecture is satisfied. $\square$

We compare the upper bound obtained for $S_k(W_{n+1})$ using the Grone–Merris–Bai theorem and that obtained using Brouwer's conjecture. Here, we review the Grone–Merris–Bai theorem. We present the conjugate of a degree d_i^* as

$$d_i^* = |\{j : d_j \geq i\}|.$$

Theorem 4. *The Grone–Merris–Bai theorem states that for a graph G and $1 \leq k \leq n$,*

$$S_k(G) \leq \sum_{i=1}^{k} d_i^*(G).$$

Clearly, for W_{n+1}, $d_1^* = d_2^* = d_3^* = n+1$, $d_4^* = d_5^* = \ldots = d_n^* = 1$, and $d_{n+1}^* = 0$. Therefore,

$$\sum_{i=1}^{k} d_i^* = \begin{cases} n+1 & \text{if } k = 1 \\ 2n+2 & \text{if } k = 2 \\ 3n+k & \text{if } 3 \leq k \leq \ n \\ 4n & \text{if } k = n+1. \end{cases}$$

Now, we present some examples for a comparison between the upper bound obtained for $S_k(W_{n+1})$ using the Grone–Merris–Bai theorem and that obtained using Brouwer's conjecture.

Consider the wheel graph W_9. The Laplacian eigenvalues for W_9 are

$$\begin{aligned} \sigma(W_9) &= \{9, 3 - 2\cos\frac{2\pi j}{8} \text{ where } j \in \{1,2,3,4,5,6,7\}, 0\} \\ &= \{9, 5, 4.4142, 4.4142, 3, 3, 1.5858, 1.5858, 0\}. \end{aligned}$$

As shown in Table 3, the Grone–Merris–Bai theorem resulted in a better approximation for the upper bound compared to that obtained using Brouwer's conjecture when $k = 1$, $k = 2$, and $k \geq 5$. However, this does not apply when $k = 3$ and $k = 4$, as Brouwer's conjecture provides a better upper bound.

Table 3. The Brouwer and Grone–Merris–Bai upper bounds for $S_k(W_9)$.

k	$S_k(W_9)$	$\sum_{i=1}^{k} d_i^*$	$e(W_9) + \binom{k+1}{2}$
1	9	9	17
2	14	18	19
3	18.4142	27	22
4	22.8284	28	26
5	25.8284	29	31
6	28.8284	30	37
7	30.4142	31	44
8	32	32	52
9	32	32	61

Consider the wheel graph W_{10}. The Laplacian eigenvalues for W_{10} are

$$\begin{aligned}\sigma(W_{10}) &= \{10, 3 - 2\cos\frac{2\pi j}{9} \text{ where } j \in \{1,2,3,4,5,6,7,8\}, 0\} \\ &= \{10, 4.8794, 4.8794, 4, 4, 2.6527, 2.6527, 1.4679, 1.4679, 0\}.\end{aligned}$$

From Table 4, it can be observed that at $k = 1$, $k = 2$, and $k \geq 5$, the Grone–Merris–Bai theorem provides a more accurate upper bound than Brouwer's conjecture. But at $k = 3$ and $k = 4$, the upper bound obtained using Brouwer's conjecture is better than that obtained using the Grone–Merris–Bai theorem.

Table 4. The Brouwer and Grone–Merris–Bai upper bounds for $S_k(W_{10})$.

k	$S_k(W_{10})$	$\sum_{i=1}^{k} d_i^*$	$e(W_{10}) + \binom{k+1}{2}$
1	10	10	19
2	14.8794	20	21
3	19.7588	30	24
4	23.7588	31	28
5	27.7588	32	33
6	30.4115	33	39
7	33.0642	34	46
8	34.5321	35	54
9	36	36	63
10	36	36	73

Now, we will look at some cases where the upper bound for $S_k(W_{n+1})$ using the Grone–Merris–Bai theorem is more accurate than that using Brouwer's conjecture.

Theorem 5. *Let W_{n+1} be a wheel graph. Then, the upper bound for $S_k(W_{n+1})$ using the Grone–Merris–Bai theorem is better than that using Brouwer's conjecture at $k = 1$, $k = 2$, and $k \geq \frac{1+\sqrt{1+8n}}{2}$.*

Proof of Theorem 4. At $k = 1$,

$$\begin{aligned}d_1^* &= n + 1 \\ &\leq 2n + \frac{1(2)}{2} \\ &= 2n + 1.\end{aligned}$$

At $k = 2$,

$$\begin{aligned} d_1^* + d_2^* &= 2n + 2 \\ &\leq 2n + \frac{2(3)}{2} \\ &= 2n + 3. \end{aligned}$$

At $3 \leq k \leq n$, $\sum_{i=1}^{k} d_i^* = 3n + k$,

$$3n + k \leq 2n + \frac{k(k+1)}{2},$$

if

$$6n + 2k \leq 4n + k^2 + k,$$

that is,

$$k^2 - k - 2n \geq 0.$$

Consider $f(k) = k^2 - k - 2n$, where the roots of f are

$$\frac{1 \pm \sqrt{1+8n}}{2},$$

where $f(k) \geq 0$ for all $k \geq \frac{1 \pm \sqrt{1+8n}}{2}$. Therefore, the upper bound obtained for $S_k(W_{n+1})$ using the Grone–Merris-Bai theorem is better than that obtained using Brouwer's conjecture if $k \geq \frac{1 \pm \sqrt{1+8n}}{2}$. $\square$

From Theorems 4 and 5, we find the following:

Corollary 1. *Let W_{n+1} be a wheel graph. Then, $UB(S_k(W_{n+1})) = Min(\sum_{i=1}^{k} d_i^*,\ e(W_{n+1}) + \binom{k+1}{2})$, $k = 1, \ldots n+1$, $n \geq 3$, provides an upper bound for $S_k(W_{n+1})$ that is closer to its actual value compared to the values obtained using the Grone–Merris–Bai theorem and Brouwer's conjecture.*

Example 2. *For W_{21}:*

$$\sigma(W_{21}) = \{21, 3 - 2\cos\frac{2\pi j}{20}, \textit{where } j \in \{1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18, 19\}, 0\}$$

Therefore,

$$\sigma(W_{21}) = \{21, 5, 4.9, 4.9, 4.618, 4.618, 4.1756, 4.1756, 3.618, 3.618, 3, 3, 2.382, 2.382, 1.8244, 1.8244, 1.382, 1.382, 1.0979, 1.0979, 0\}$$

For W_{26}:

$$\sigma(W_{26}) = \{26, 3 - 2\cos\frac{2\pi j}{25}, \textit{where } j \in \{1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16, 17,18,19,20,21,22,23,24\}, 0\}$$

Therefore,

$$\sigma(W_{26}) = \{26, 4.9842.4.9842, 4.8596, 4.8596, 4.618, 4.618, 4.2748, 4.2748, 3.8516, 3.8516, 3.3748, 3.3748, 2.8744, 2.8744, 2.382, 2.382, 1.9283, 1.92831.5421, 1.5421, 1.2474, 1.2474, 1.0628, 1.0628, 0\}$$

From Tables 5 and 6, we can observe that the difference between $S_k(W_n)$ and $e(W_{n+1}) + \binom{k+1}{2}$ is increasing. This means that when n is large, the upper bound obtained using the Grone–Merris–Bai theorem is more accurate than that obtained using Brouwer's conjecture when n is very large. Also, the equality in the Grone–Merris–Bai theorem holds at $k = 1, n, n+1$. To verify this equality, we can see that

- $S_1(W_{n+1}) = d_1^* = n+1.$
- $S_n(W_{n+1}) = S_{n+1}(W_{n+1}) = \sum_{i=1}^{n} d_i^*$. *As*

$$\begin{aligned}\sum_{i=1}^{n} d_i^* &= d_1^* + \ldots + d_n^* \\ &= (n+1) + (n+1) + (n+1) + 1 + 1 + \ldots + 1 \\ &= 3n + 3 + n - 3 \\ &= 4n\end{aligned}$$

$$\begin{aligned}S_n(W_{n+1}) &= \sum_{i=1}^{n} \mu_i \\ &= \sum_{i=1}^{n+1} \mu_i \\ &= tr(L(W_n)) \\ &= \sum_{i=1}^{n+1} d_i \\ &= n + 3 + \ldots + 3 \\ &= n + 3n \\ &= 4n.\end{aligned}$$

The above result directly follows from the previous results [11,12], which show that the sum of the Laplacian spectra equals the sum of the degrees of all the vertices of the graph, which can be readily seen to be $4n$ for W_{n+1}.

Table 5. The Brouwer and Grone–Merris–Bai upper bounds for $S_k(W_{21})$.

k	$S_k(W_{21})$	$\sum_{i=1}^{k} d_i^*$	$e(W_{21}) + \binom{k+1}{2}$
1	21	21	41
2	26	42	43
3	30.9	63	46
4	35.8	64	50
5	40.418	65	55
6	45.036	66	61
7	49.2116	67	68
8	53.3872	68	76
9	57.0052	69	85
10	60.6232	70	95
11	63.6232	71	106
12	66.6232	72	118

Table 5. *Cont.*

k	$S_k(W_{21})$	$\sum_{i=1}^{k} d_i^*$	$e(W_{21}) + \binom{k+1}{2}$
13	69.0052	73	131
14	71.3872	74	145
15	73.2116	75	160
16	75.036	76	176
17	76.418	77	193
18	77.8	78	211
19	78.8979	79	230
20	79.9958	80	250
21	79.9958	80	271

Table 6. The Brouwer and Grone–Merris–Bai upper bounds for $S_k(W_{26})$.

k	$S_k(W_{26})$	$\sum_{i=1}^{k} d_i^*$	$e(W_{26}) + \binom{k+1}{2}$
1	26	26	51
2	30.9842	52	53
3	35.9684	78	56
4	40.828	79	60
5	45.6876	80	65
6	50.3056	81	71
7	54.9236	82	78
8	59.1984	83	86
9	63.4732	84	95
10	67.3248	85	105
11	71.1764	86	116
12	74.5512	87	128
13	77.926	88	141
14	80.8004	89	155
15	83.6748	90	170
16	86.0568	91	186
17	88.4388	92	203
18	90.3671	93	221
19	92.2954	94	240
20	93.8375	95	260
21	95.3796	96	281
22	96.627	97	303
23	97.8744	98	326
24	98.9372	99	350
25	100	100	375
26	100	100	401

4. Application

In this section, we provide an application of our study.

Example 3. *Consider the airports RUH (Riyadh), ALG (Algeria), CAI (Cairo), LHR (London), AMM (Amman), IST (Istanbul), ADD (Addis Ababa), BOM (Mumbai), GYD (Baku), DXB (Dubai), BAH (Manama) as vertices and the flight paths as edges. Then, we have the graph* W_{11}*, Figure 4, with Table 7.*

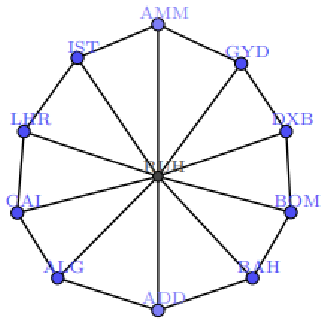

Figure 4. W_{11}.

The Laplacian eigenvalues for W_{11} *are*

$$\begin{aligned}\sigma(W_{11}) &= \{11, 3 - 2\cos\frac{2\pi j}{10} \text{ where } j \in \{1,2,3,4,5,6,7,8,9\}, 0\} \\ &= \{11, 5, 4.6180, 4.6180, 3.6180, 3.6180, 2.3820, 2.3820, 1.3820, 1.3820, 0\}.\end{aligned}$$

Table 7. Upper bounds for $S_k(W_{11})$.

k	$S_k(W_{11})$	$\sum_{i=1}^{k} d_i^*$	$e(W_{11}) + \binom{k+1}{2}$
1	11	11	21
2	16	22	23
3	20.618	33	26
4	25.236	34	30
5	28.854	35	35
6	32.472	36	41
7	34.854	37	48
8	37.236	38	56
9	38.618	39	65
10	40	40	75
11	40	40	86

5. Discussion

In this section, a discussion related to our work is presented, including an essential interpretation of a problem and conjecture in algebraic graph theory. Some invariants of wheel graphs are calculated. New results and findings for Brouwer's conjecture are calculated and presented in majorization tables and figures.

The literature review in Section 1.1 can be compared to our findings and results. This work can be extended to further research and future studies.

There are many open questions and problems in algebraic graph theory that are related to wheel graphs and their invariants. There are unanswered questions and computations that could lead to potential future research in this regard.

6. Conclusions

In this paper, we study a problem in algebraic graph theory. We provide a sufficient background and a review of the relevant literature. The design of this paper is standard. Brouwer's conjecture holds for the wheel graph W_{n+1}, where $n \geq 3$. The Grone–Merris–Bai theorem results in a better approximation of the upper bound than Brouwer's conjecture for W_{n+1} when $k = 1, 2$ and $k \geq \frac{1+\sqrt{1+8n}}{2}$. On the other hand, if $2 < k < \frac{1+\sqrt{1+8n}}{2}$, then the upper bound obtained using Brouwer's conjecture is better than that obtained using the Grone–Merris–Bai theorem. Also, if n is increasing, the difference between $S_k(W_{n+1})$ and $e(W_{n+1}) + \binom{k+1}{2}$ is increasing, as shown in Figures 5–7. However, the upper bound obtained using the Grone–Merris–Bai theorem is more accurate than that obtained using Brouwer's conjecture when n is large enough. The equality in the Grone–Merris–Bai theorem holds for

W_{n+1} at $k = 1, n, n+1$. Therefore, $UB(S_k(W_{n+1}))$ results in a more accurate upper bound compared to the Grone–Merris–Bai and Brouwer upper bounds. We provide an application of this work using the subject of international airports, resulting in the wheel graph W_{11}. Then, we apply Brouwer's conjecture. We visualize our results using some curves that depict the relationship between the Grone–Merris–Bai inequality, Brouwer's conjecture, and $UB(S_k(W_{n+1}))$ as in Figure 8–11.

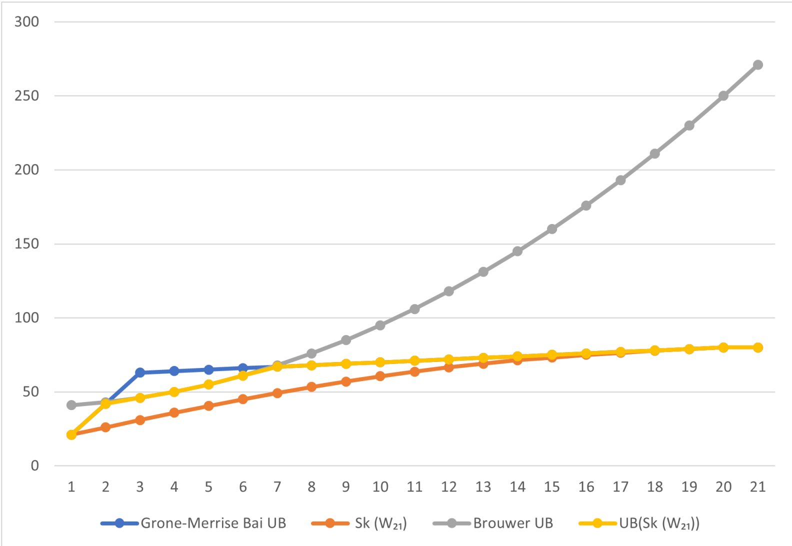

Figure 5. Comparison of the upper bounds obtained using the Grone–Merris–Bai theorem, Brouwer's conjecture, and $UB(S_k(W_{21}))$ for W_{21}.

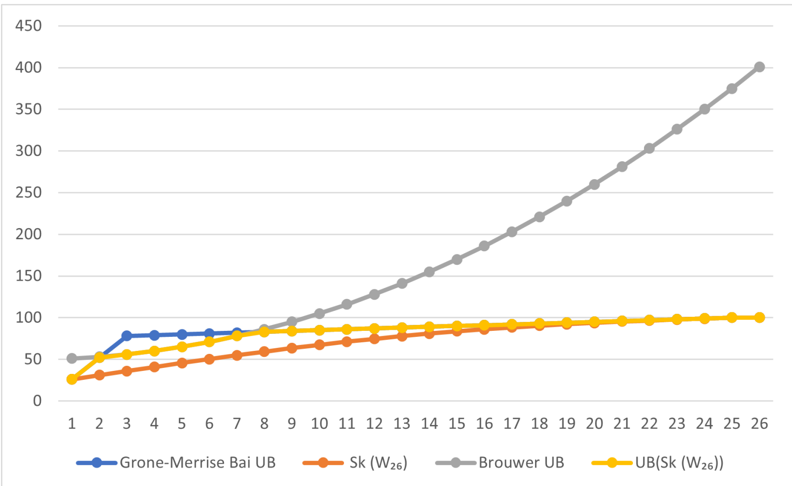

Figure 6. Comparison of the upper bounds obtained using the Grone–Merris–Bai theorem, Brouwer's conjecture, and $UB(S_k(W_{26}))$ for W_{26}.

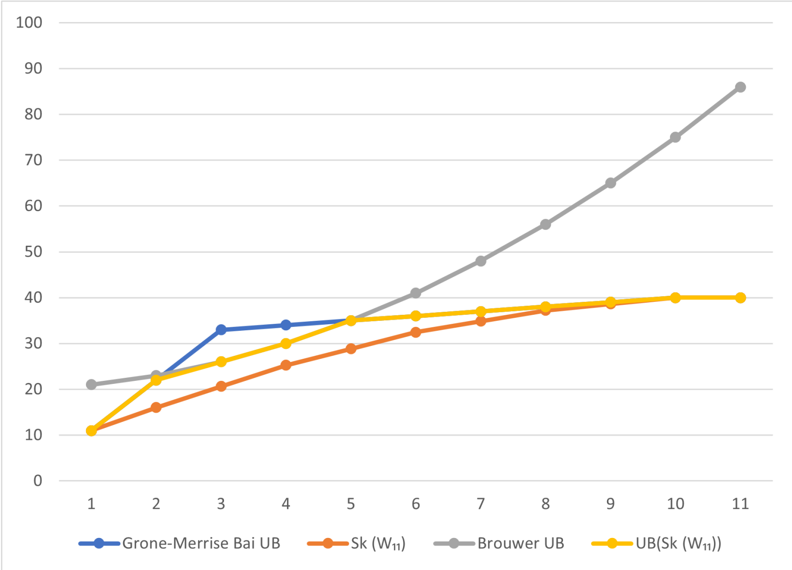

Figure 7. Comparison of the Grone–Merris–Bai inequality, Brouwer's conjecture, and $UB(S_k(W_{11}))$ for W_{11}.

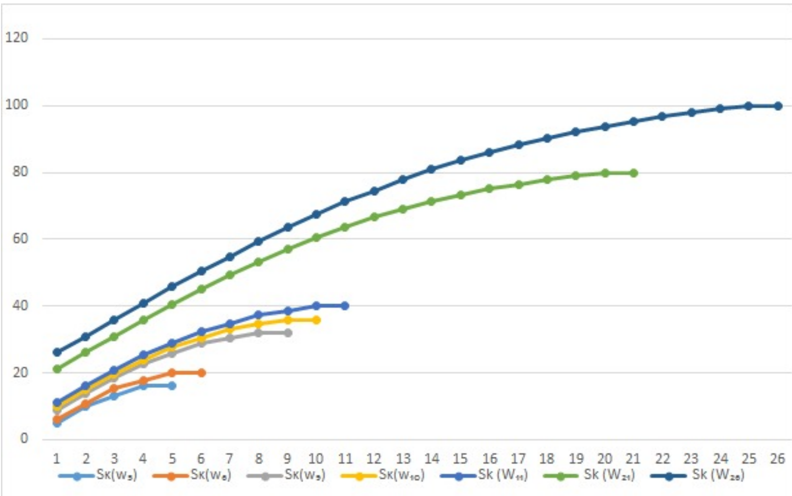

Figure 8. $S_k(W_{n+1})$ for specific wheel graphs.

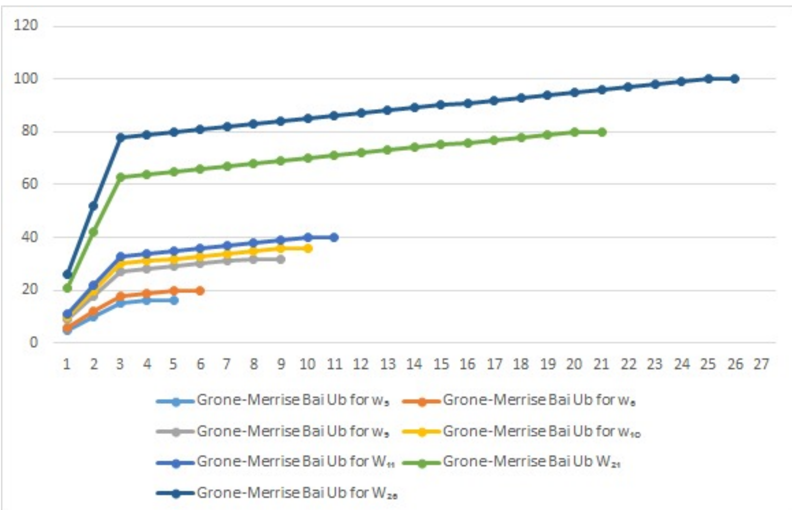

Figure 9. Grone –Merris–Bai upper bound for specific wheel graphs.

As we indicated in the Discussion section, there is work that can be extended to further research and future studies in the field of algebraic graph theory.

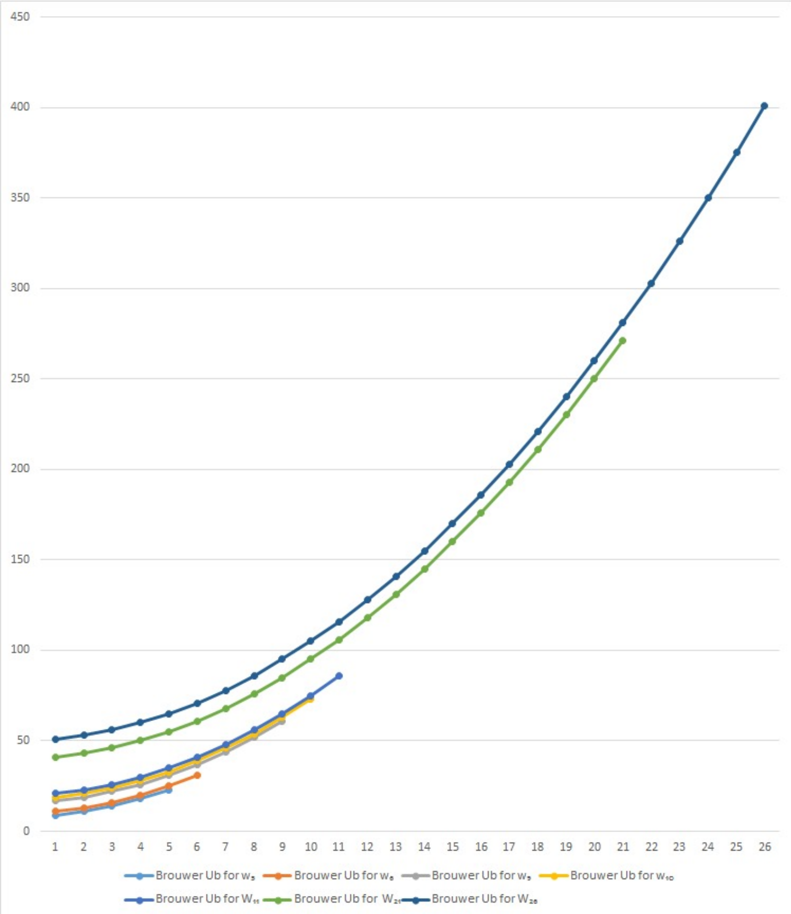

Figure 10. Brouwer's conjecture upper bound for specific wheel graphs.

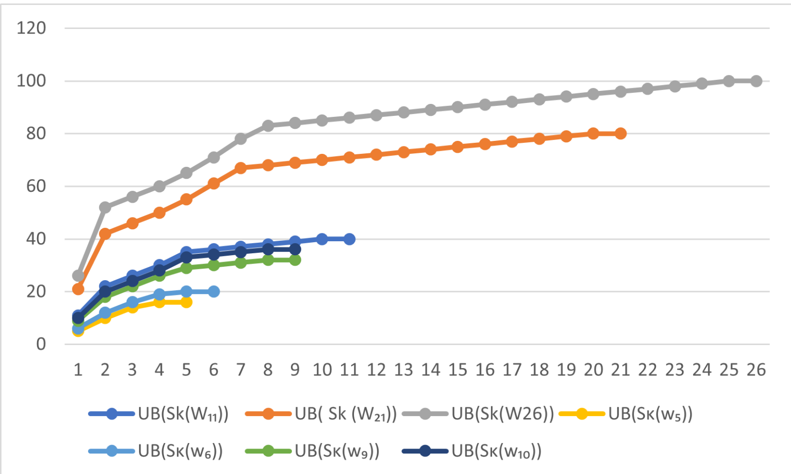

Figure 11. $UB(S_k(W_{n+1}))$ for specific wheel graphs.

Author Contributions: Formal analysis and writing—original draft, M.A.; Project administration and supervision, H.A.; Validation and visualization, A.A.; Resources and writing—review and editing, H.A. and A.A. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: All data are included in the paper.

Acknowledgments: This project was supported by the Researchers Supporting Project Number (RSP2023R317) King Saud University, Riyadh, Saudi Arabia. The authors would like to thank the two reviewers for their valuable comments and suggestions, which led to a great improvement in the original manuscript.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Dharwadker, A.; Pirzada, S. *Graph Theory*, 3rd ed.; Institute of Mathematics: Hyderabad, India, 2011; pp. 1–190.
2. Ganie, H.A.; Alghamdi, A.m.; Pirzada, S. On the sum of the Laplacian eigenvalues of a graph and Brouwer's conjecture. *Linear Algebra Appl.* **2016**, *501*, 376–389. [CrossRef]
3. Bai, H. The grone-merris conjecture. *Trans. Am. Math. Soc.* **2011**, *363*, 4463–4474. [CrossRef]
4. Brouwer, A.; Haemers, W. Spectra of Graph. *Personal. Individ. Differ.* **2012**, xiv+250. [CrossRef]
5. Trevisan, V.; Helmberg, C. Spectral threshold dominance, Brouwer's conjecture and maximality of Laplacian energy. *Linear Algebra Appl.* **2017**, *512*, 0024–3795.
6. Mayank. On Variants of the Grone-Merris Conjecture. Master's Thesis, Endhoven University of Tichnology, Einhoven, The Netherlands, 2010.
7. Haemers, W.H.; Mohammadian, A.; Tayfeh-Rezaie, B. On the sum of Laplacian eigenvalues of graphs. *Linear Algebra Appl.* **2010**, *432*, 2214–2221. [CrossRef]
8. Molitierno, J.J. *Applications of Combinatorial Matrix Theory to Laplacian Matrices of Graphs*, 3rd ed.; CRC Press: Boca Raton, FL, USA, 2016; pp. 1–171.
9. Cvetkovic, D.M.; Doob, M.; Sachs, H. *Spectra of Graphs. Theory and Application*; Academic Press: London, UK; New York, NY, USA; San Francisco, CA, USA, 1980.
10. Coulson, C.A.; Mallion, R.B. *Huckel Theory for Organic Chemists*; Academic Press: London, UK; New York, NY, USA; San Francisco, CA, USA, 1978.
11. Balasubramanian, K. Laplacians of Fullerenes (C42–C90). *J. Phys. Chem.* **1995**, *99*, 6509–6518. [CrossRef]
12. Balasubramanian, K. Computation of spanning tree generators of fullerenes. *Mol. Phys.* **1995**, *85*, 335–348. [CrossRef]
13. Babic', D.; Klien, D.J.; Lukovits, I.; Nikolic', S.; Trinajstic, N. Resistance-Distance Matrix: A Computational Algorithm and Its Application. *Int. J. Quantum Chem.* **2001**, *90*, 166–176. [CrossRef]
14. Wang, W.; Yang, D.; Luo, Y. The Laplacian polynomial and Kirchhoff index of graphs derived from regular graphs. *Discret. Appl. Math.* **2013**, *161*, 3063–3071. [CrossRef]
15. Balasubramanian, K. Characteristic polynomials, spectral-based Riemann-Zeta functions and entropy indices of n-dimensional hypercubes. *J. Math. Chem.* **2023**, *61*, 1570–1591. [CrossRef]
16. Balasubramanian, K. Topological indices, graph spectra, entropies, laplacians, and matching polynomials of n-dimensional hypercubes. *Symmetry* **2023**, 15, 557. [CrossRef]
17. Zhang, Y.; Liub, X.; Yong, X. Which wheel graphs are determined by their Laplacian spectra? *Comput. Math. Appl.* **2009**, *85*, 1887–1890. [CrossRef]
18. Wen, F.; Huang, Q.; Huang, X.; Liu, F. The spectral characterization of wind-wheel graphs. *Indian J. Pure Appl. Math.* **2015**, *46*, 613–631. [CrossRef]
19. Chu, Z.Q.; Munir, M.; Yousaf, A.; Qureshi, M.I.; Liu, J.B. Laplacian and signless laplacian spectra and energies of multi-step wheels. *Math. Biosci. Eng.* **2020**, *17*, 3649–3659. [CrossRef] [PubMed]
20. Sun, D.; Zhao, Z.; Li, X.; Cao, J.; Yang, Y. On subtree number index of generalized book graphs, fan Graphs, and wheel graphs. *J. Math.* **2021**, *2021*, 5511214. [CrossRef]
21. Kuswardi, Y.; Almira, L.; Nurussakbana, N.; Pinilih, A.C. Chromatic Number of Amalgamation of Wheel Graph-Star Graph and Amalgamation of Wheel Graph-Sikel Graphs. *J. Math. Math. Educ.* **2022**, *12*, 1–100. [CrossRef]
22. Wei, Y.; Gao, Z.; Lu, X. The Complexity of Wheel Graphs with Multiple Edges and Vertice. *Asian Res. J. Math.* **2023**, *19*, 1–12. [CrossRef]
23. Greeni, A.B.; Joshwa, P.L. Embedding complete bipartite graphs into wheel related graphs. *J. Adv. Comput. Intell. Intell. Inform.* **2023**, *27*, 645–648. [CrossRef]
24. Selig, T. Combinatorial aspects of sandpile models on wheel and fan graphs. *Eur. J. Comb.* **2023**, *110*, 103663. [CrossRef]
25. Buseck, P.R.; Tsipursky, S.J.; Hettich, R. Fullerenes from the geological environment. *Science* **1992**, *257*, 215–217. [CrossRef]
26. Cox, D.M.; Behal, S.; Disko, M.; Gorun, S.M.; Greaney, M.; Hsu, C.S.; Kollin, E.B.; Millar, J.; Robbins, J. Characterization of C60 and C70 clusters. *J. Am. Chem. Soc.* **1991**, *113*, 2940–2944. [CrossRef]
27. Dance, I.G.; Fisher, K.J.; Willett, G.D.; Wilson, M.A. C60 and liquid-crystal mesophase. *J. Phys. Chem.* **1991**, *95*, 8425–8428. [CrossRef]

28. Tully, C. Symmetric random walks on wheel-and-spokes graphs. *SIAM Undergrad. Res. Online* **2021**, *14*, 604–620. [CrossRef]
29. Balasubramanian, K. Symmetry Groups of Chemical Graphs. *Int. J. Quantum Chem.* **1982**, *21*, 411–418. [CrossRef]
30. Potanka, K.S. Groups, Graphs, and Symmetry-Breaking. Ph.D. Dissertation, Virginia Tech, Blacksburg, VA, USA, 1998; pp. 1–100.
31. Kavi, L.C. Symmetry breaking in graphs and matroids. *AIMS* **2015**. [CrossRef]
32. Boutin, D.L. Identifying graph automorphisms using determining sets. *Electron. J. Comb.* **2006**, *13*, R78. [CrossRef]
33. Deligeorgaki, D. Smallest graphs with given automorphism groups. *J. Algebr. Comb.* **2022**, *56*, 609–633. [CrossRef]
34. Mirafzal, S.M. On the automorphism groups of connected bipartite irreducible graphs. *Proc.-Math. Sci.* **2020**, *130*, 1–15. [CrossRef]
35. Ibarra, S.; Rivera, L.M. The automorphism groups of some token graphs. *arXiv* **2019**, arXiv:1907.06008.