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Sombor Index and Sombor Polynomial of the Noncommuting Graph Associated to Some Finite Groups

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ABSTRACT

Sombor index is a newly developed degree-based topological index which involves the degree of the vertex in a simple connected graph. The Sombor index is known as the square root of the sum of the squared degrees of two adjacent vertices in a graph. Meanwhile, the noncommuting graph associated to a group is a graph where its vertices are the non-central elements of the group and two vertices are adjacent if and only if they do not commute. In this study, a new notion called the Sombor polynomial is introduced. Then, the general formula of the Sombor index and the Sombor polynomial of the noncommuting graph associated to some finite groups are determined by using their definitions and some preliminaries. The groups involved in this research are the dihedral groups, the quasidihedral groups, and the generalized quaternion groups. The results found can help the chemists and biologists to predict the chemical and physical properties of the molecules without involving any laboratory work.

1. Introduction

A topological index is a numerical quantity associated with a chemical compound that captures some aspect of its molecular topology, or the way its constituent atoms are connected in three-dimensional space [1]. The purpose of a topological index is typically to provide insight into some chemical or physical property of the compound, such as its solubility, reactivity, or biological activity [2]. In addition, the topological indices can be broadly divided into two categories: distance and degree-based topological indices. Distance-based indices are computed based on the distances between pairs of atoms in the molecule, while degree-based indices are computed based on the number of bonds or other topological features that each atom in the molecule possesses.

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Topological index has been introduced since 1947 by Wiener [3] where the first type of topological index, namely the Wiener index is developed. The study in [3] focuses on computing the Wiener number of some types of paraffins and their boiling points are predicted. Then, the results were compared to their observed boiling points. Since then, many new concepts and formulas of the topological indices have been introduced in mathematical chemistry field for both degree and distance-based topological indices. Other than the Wiener index [3-5], other examples of commonly used topological indices include the Randić index [6-8], the Zagreb index [9-12], and the Harary index [13,14]. Each of these indices captures a different aspect of molecular topology and has its own specific mathematical formula for calculation. In 2021, a new topological index called the Sombor index has been introduced by Gutman [15], where Sombor is the name of a city in Serbia, also Gutman's hometown. Its formula is given in Definition 1. Many findings on the Sombor index have been determined since then, where they can be found in the previous studies [16-19].

The topological indices have found applications in a wide range of fields, including drug design, environmental chemistry, and materials science. They provide a valuable tool for predicting and understanding the properties of chemical compounds and continue to be an active area of research in the field of computational chemistry. Besides that, they are closely related to graph theory, which is the mathematical study of graphs or networks. A set of objects (vertices or nodes) can be mathematically represented as a graph and the connections between them (edges) [20]. In the context of chemistry, graphs are often used to represent molecular structures, where the atoms of the molecule correspond to the vertices and the bonds between them correspond to the edges.

Graph theory provides a rich set of mathematical tools for analysing the properties of graphs, including the degree distribution, clustering coefficient, diameter, and many others. By applying these tools to the graph of a molecule, researchers can gain insights into its topological properties and predict its behaviour in various chemical or physical contexts. In graph theory, there are topological indices that are associated with graph polynomials and have certain practical applications such as found in the previous studies [21,22]. The study of polynomials discusses the structures of graphs, but they do not always solve the characterization of graph since non-isomorphic graphs appear to have the same polynomial. Nevertheless, graph polynomials such as the Zagreb polynomial [23] and the Harmonic polynomial [24] are important in studying several types of topological indices and describing the properties of graphs and networks. They have several important applications in topology and graph theory.

The study on Sombor index is getting much attention from the researchers where more than 50 related articles have been published in a year. The concept of Sombor polynomial is not introduced yet. Hence, in this paper, the definition of Sombor polynomial is introduced based on the Sombor index. The Sombor polynomial and Sombor index are determined for the noncommuting graph associated to some finite groups.

2. Preliminaries

Some definitions and fundamental ideas in group theory and graph theory are given in this section. The definition of the Sombor index is included. Besides that, some previous results and studies that have been done by other researchers in the scope of Sombor index, the noncommuting graph and some finite groups are also stated, and they are used to prove the main theorems in the next section.

2.1 Definition 1 [20] Sombor Index

Let Γ be a graph. The Sombor index of Γ is defined as $SO(\Gamma)=\sum_{uv\in E(\Gamma)}\sqrt{d_u^{\,2}+d_v^{\,2}}$, where d_u and d_v represent the degree of the edges u and v in Γ, respectively.

An essential component of understanding molecular structure is graph theory. Hence, the study on the topological index in graph theory is increasingly developing. The following definitions are some important concepts in graph theory, particularly in this study.

2.2 Definition 2 [25] Complete Multipartite Graph

A complete multipartite graph, also known as a k −partite graph, is a graph where the vertices can be divided into k distinct independent sets. In other words, it is a graph that can have k colors applied so that no two edge endpoints have the same color.

2.3 Definition 3 [26] The Noncommuting Graph

Let G be a finite group. The noncommuting graph of G is the graph with the non-central vertex set and two distinct vertices x and y are connected by an edge whenever they do not commute to each other.

In 2018, Mahmoud *et al.,* [27] found the noncommuting graph of dihedral groups, the quasidihedral groups and the generalized quaternion groups. Their general formulas are stated in the following propositions and are used to prove the main theorems.

Proposition 1 [27] Let G be the dihedral groups of order $2n,\ n\ge 3$ and Γ_G be the noncommuting graph of G. Then,

$$\Gamma_G=\begin{cases} K_{\underbrace{1,1,\ldots,1}_{n\text{ times}},n-1}, & n\text{ is odd,}\\ K_{\underbrace{2,2,\ldots,2}_{\frac{n}{2}\text{ times}},n-2}, & n\text{ is even.}\end{cases}$$

Proposition 2 [27] Let G be the generalized quaternion groups of order $4n,\ n\ge 2$ and Γ_G be the noncommuting graph of G. Then,

$$\Gamma_G=K_{\underbrace{2,2,\ldots,2}_{n\text{ times}},2n-2}.$$

Proposition 3 [27] Let G be the quasidihedral groups of order $2^n,\ n\ge 4$ and Γ_G be the noncommuting graph of G. Then,

$$\Gamma_G=K_{\underbrace{2,2,\ldots,2}_{2^{n-2}\text{ times}},\,2^{n-1}-2}.$$

In addition, the number of edges of the non-commuting graph for the finite groups has been determined by Abdollahi *et al.,* [26].

Proposition 4 [26] Let G be a finite group and Γ_G be the noncommuting graph of . Then, the number of edges of Γ_G, $|E(\Gamma_G)| = \frac{|G|^2 - k(G)|G|}{2}$, where $k(G)$ is the number of conjugacy classes of G.

This study involves three types of non-abelian finite groups which are the dihedral groups, D_{2n}, the quasidihedral groups, Q_{4n} and the generalised quaternion groups, QD_{2^n}. Their group presentations are as follows.

$$D_{2n} = \left\langle a,b \middle| a^n = b^2 = 1, bab = a^{-1} \right\rangle, n \geq 3.$$

$$QD_{2^n} = \left\langle a,b \middle| a^{2^{n-1}} = b^2 = 1, bab = a^{2^{n-2}-1} \right\rangle, n \geq 4.$$

$$Q_{4n} = \left\langle a,b \middle| a^n = b^2, a^{2n} = b^4 = 1, bab = a^{-1} \right\rangle, n \geq 2.$$

The centre of the dihedral group can be presented as follows:

Proposition 5 [28] Let G be a dihedral group of order $2n$, where $n \geq 3, n \in \mathrm{N}$. Then, the centre of G,

$$Z(G) = \begin{cases} \{1\}, & n \text{ is odd,} \\ \left\{1, a^{\frac{n}{2}}\right\}, & n \text{ is even.} \end{cases}$$

The conjugacy class of $a \in G$ is the set $cl(a) = \left\{xax^{-1} \middle| x \in G\right\}$ [29]. The number of the conjugacy classes of the dihedral group is given in the next proposition.

Proposition 6 [30] The number of the conjugacy class of the dihedral group of order $2n$, $n \geq 3, n \in \mathrm{N}$ is

$$k(G) = \begin{cases} \frac{n+3}{2}, & n \text{ is odd,} \\ \frac{n+6}{2}, & n \text{ is even.} \end{cases}$$

3. Results

In this section, the Sombor index of the noncommuting graph associated to the dihedral groups, the quasidihedral groups and the generalised quaternion groups are determined. Then, their Sombor polyomials are also computed. At the end of the paper, the Sombor index and Sombor polynomial of k −regular graph is presented.

The Sombor polynomial of the graph Γ is given in Definition 4, which it satisfies the condition $SO'(\Gamma;1) = SO(\Gamma)$.

Definition 4 Sombor Polynomial

Let Γ be a graph. The Sombor polynomial of Γ is defined as $SO(\Gamma;x)=\sum_{uv\in E(\Gamma)}\frac{1}{\sqrt{d_u{}^2+d_v{}^2}}x^{d_u{}^2+d_v{}^2}$, where d_u and d_v represent the degree of u and v in Γ, respectively.

3.1 The Sombor Index of the Noncommuting Graph Associated to Some Finite Groups

Theorem 1 Let Γ_G be the noncommuting graph of G where G is the dihedral groups of order $2n$, $n\geq 3.$ Then, the Sombor index of Γ_G,

$$SO(\Gamma_G)=\begin{cases} n(n-1)\left[\sqrt{2}(n-1)+\sqrt{4(n-1)^2+n^2}\right], & n \text{ is odd,}\\ n(n-2)\left[\sqrt{2}(n-2)+\sqrt{4(n-2)^2+n^2}\right], & n \text{ is even.}\end{cases}$$

Proof Based on Proposition 1, the noncommuting graph of D_{2n}, Γ_G, are split into two categories; n is odd and n is even, where $n\geq 3.$

For n is odd:

$\Gamma_G=K_{\underbrace{1,1,\ldots,1}_{n\text{ times}},n-1}$ and by Propositions 4 and 6, $|E(\Gamma_G)|=\frac{3}{2}n(n-1).$ Then, there are $n(n-1)$ edges which connect two vertices of Γ_G that has degree $2n-2$ and $n.$ Meanwhile, there are $\frac{1}{2}n(n-1)$ edges which connect two vertices of Γ_G that both have degrees $2n-2$. By Definition 1,

$$\begin{aligned}SO(\Gamma_G)&=\sum_{uv\in E(\Gamma_G)}\sqrt{d_u{}^2+d_v{}^2}=\frac{1}{2}n(n-1)\sqrt{(2n-2)^2+(2n-2)^2}+n(n-1)\sqrt{(2n-2)^2+n^2}\\ &=n(n-1)\left[\sqrt{2}(n-1)+\sqrt{4(n-1)^2+n^2}\right].\end{aligned}$$

For n is even:

$\Gamma_G=K_{\underbrace{2,2,\ldots,2}_{\frac{n}{2}\text{ times}},n-2}$ and by Propositions 4 and 6, $|E(\Gamma_G)|=\frac{3}{2}n(n-2).$ There are $n(n-2)$ edges which connect two vertices of Γ_G that has degree $2n-4$ and n. Meanwhile, there are $\frac{1}{2}n(n-2)$ edges which connect two vertices in Γ_G of degrees $2n-4.$ By Definition 1,

$$\begin{aligned}SO(\Gamma_G)&=\sum_{uv\in E(\Gamma_G)}\sqrt{d_u{}^2+d_v{}^2}=\frac{1}{2}n(n-2)\sqrt{(2n-4)^2+(2n-4)^2}+n(n-2)\sqrt{(2n-4)^2+n^2}\\ &=n(n-2)\left[\sqrt{2}(n-2)+\sqrt{4(n-2)^2+n^2}\right].\end{aligned} \tag{1}$$

Theorem 2 Let Γ_G be the noncommuting graph of G where G is the quasidihedral groups of order 2^n, $n\geq 4.$ Then, the Sombor index of Γ_G,

$$SO(\Gamma_G)=\sqrt{2}\left(2^n-4\right)\left(2^{2n-3}-2^{n-1}\right)+\left(2^{2n-2}-2\right)\sqrt{\left(2^n-4\right)^2+2^{2n-2}}.$$

Proof Based on Proposition 3, the noncommuting graph of D_{2n}, $\Gamma_G=K_{\underbrace{2,2,\ldots,2}_{2^{n-2}\text{ times}},2^{n-1}-2}$, where $n\geq 4$. By Proposition 4, $|E(\Gamma_G)|=3\left(2^{2n-3}-2^{n-1}\right)$. Then, there are $2^{n-1}\left(2^{n-1}-2\right)$ edges which connect two vertices of Γ_G that has degree 2^n-4 and 2^{n-1}. Meanwhile, there are $\frac{2^{2n}}{2^3}-2\left(2^{n-1}\right)$ edges which connect two vertices in Γ_G of degrees 2^n-4. Hence, by Definition 1,

$$\begin{aligned}SO(\Gamma_G)&=\sum_{uv\in E(\Gamma_G)}\sqrt{d_u^{\,2}+d_v^{\,2}}=\left[\frac{2^{2n}}{2^3}-\frac{2^n}{2}\right]\sqrt{\left(2^n-4\right)^2+\left(2^n-4\right)^2}+2^{n-1}\left(2^{n-1}-2\right)\sqrt{\left(2^n-4\right)^2+\left(2^{n-1}\right)^2}\\&=\sqrt{2}\left(2^{2n-3}-2^{n-1}\right)\left(2^n-4\right)+\left(2^{2n-2}-2^n\right)\sqrt{\left(2^n-4\right)^2+2^{2n-2}}.\end{aligned}\tag{2}$$

Theorem 3 Let Γ_G be the noncommuting graph of G where G is the generalized quaternion groups of order $4n$, $n\geq 2$. Then, the Sombor index of Γ_G,

$$SO(\Gamma_G)=8n(n-1)\left[\sqrt{2}(n-1)+\sqrt{4(n-1)^2+n^2}\right].$$

Proof Based on Proposition 2, the noncommuting graph of D_{2n}, $\Gamma_G=K_{\underbrace{2,2,\ldots,2}_{n\text{ times}},2n-2}$, where $n\geq 2$. By Proposition 4, $|E(\Gamma_G)|=6n(n-1)$. Then, there are $2n(2n-2)$ edges which connect two vertices of Γ_G that has degree $4n-4$ and $2n$. Meanwhile, there are $2n(n-1)$ edges which connect two vertices in Γ_G of degrees $4n-4$. Hence, by Definition 1,

$$\begin{aligned}SO(\Gamma_G)&=\sum_{uv\in E(\Gamma_G)}\sqrt{d_u^{\,2}+d_v^{\,2}}=2n(n-1)\sqrt{(4n-4)^2+(4n-4)^2}+2n(2n-2)\sqrt{(2n-4)^2+n^2}\\&=8n(n-1)\left[\sqrt{2}(n-1)+\sqrt{4(n-1)^2+n^2}\right].\end{aligned}\tag{3}$$

3.2 The Sombor Polynomial of the Noncommuting Graph Associated to Some Finite Groups

Theorem 4 Let Γ_G be the noncommuting graph of G where G is the dihedral groups of order $2n$, $n\geq 3$. Then, the Sombor polynomial of Γ_G,

$$SO(\Gamma_G;x)=\begin{cases}n(n-1)\left[\dfrac{x^{8(n-1)^2}}{4\sqrt{2}(n-1)}+\dfrac{x^{4(n-1)^2+n^2}}{\sqrt{4(n-1)^2+n^2}}\right], & n\text{ is odd,}\\[2ex] n(n-2)\left[\dfrac{x^{8(n-2)^2}}{4\sqrt{2}(n-2)}+\dfrac{x^{4(n-2)^2+n^2}}{\sqrt{4(n-2)^2+n^2}}\right], & n\text{ is even.}\end{cases}$$

Proof Based on Proposition 1, the noncommuting graph of D_{2n}, Γ_G, are split into two categories; n is odd and n is even, where $n\geq 3$.

For n is odd:
By Propositions 4, 6 and Definition 4,

$$SO(\Gamma_G;x)=\sum_{uv\in E(\Gamma_G)}\frac{1}{\sqrt{d_u^{\,2}+d_v^{\,2}}}x^{d_u^{\,2}+d_v^{\,2}}=\frac{\frac{n(n-1)}{2}}{\sqrt{(2n-2)^2+(2n-2)^2}}x^{(2n-2)^2+(2n-2)^2}+\frac{n(n-1)}{\sqrt{(2n-2)^2+n^2}}x^{(2n-2)^2+n^2}$$
$$=n(n-1)\left[\frac{x^{8(n-1)^2}}{4\sqrt{2}(n-1)}+\frac{x^{4(n-1)^2+n^2}}{\sqrt{4(n-1)^2+n^2}}\right].$$

For n is even:
By Propositions 4, 6 and Definition 4,

$$SO(\Gamma_G;x)=\sum_{uv\in E(\Gamma_G)}\frac{1}{\sqrt{d_u^{\,2}+d_v^{\,2}}}x^{d_u^{\,2}+d_v^{\,2}}=\frac{\frac{n(n-2)}{2}}{\sqrt{(2n-4)^2+(2n-4)^2}}x^{(2n-4)^2+(2n-4)^2}+\frac{n(n-2)}{\sqrt{(2n-4)^2+n^2}}x^{(2n-4)^2+n^2}$$
$$=n(n-2)\left[\frac{x^{8(n-2)^2}}{4\sqrt{2}(n-2)}+\frac{x^{4(n-2)^2+n^2}}{\sqrt{4(n-2)^2+n^2}}\right]. \tag{4}$$

Theorem 5 Let Γ_G be the noncommuting graph of G where G is the quasidihedral groups of order 2^n, $n\geq 4$. Then, the Sombor polynomial of Γ_G,

$$SO(\Gamma_G;x)=\frac{2^{2n-3}-2^{n-1}}{\sqrt{2}(2^n-4)}x^{2(2^n-4)^2}+\frac{2^{2n-2}-2^n}{\sqrt{(2^n-4)^2+2^{2n-2}}}x^{(2^n-4)^2+2^{2n-2}}.$$

Proof Based on Proposition 3, the noncommuting graph of QD_{2^n}, $\Gamma_G=K_{\underbrace{2,2,\ldots,2}_{2^{n-2}\text{ times}},2^{n-1}-2}$, where $n\geq 4$.

Then, the Sombor polynomial of Γ_G,

$$SO(\Gamma_G;x)=\sum_{uv\in E(\Gamma_G)}\frac{1}{\sqrt{d_u^{\,2}+d_v^{\,2}}}x^{d_u^{\,2}+d_v^{\,2}}=\frac{2^{2n-3}-2^{n-1}}{\sqrt{(2^n-4)^2+(2^n-4)^2}}x^{(2^n-4)^2+(2^n-4)^2}+\frac{2^{2n-2}-2^n}{\sqrt{(2^n-4)^2+(2\cdot 2^{n-2})^2}}x^{(2^n-4)^2+(2^{n-1})^2}$$
$$=\frac{2^{2n-3}-2^{n-1}}{\sqrt{2}(2^n-4)}x^{2(2^n-4)^2}+\frac{2^{2n-2}-2^n}{\sqrt{(2^n-4)^2+2^{2n-2}}}x^{(2^n-4)^2+2^{2n-2}}. \tag{5}$$

Theorem 6 Let Γ_G be the noncommuting graph of G where G is the generalized quaternion groups of order $4n$, $n\geq 2$. Then, the Sombor polynomial of Γ_G,

$$SO(\Gamma_G;x)=\frac{\sqrt{2}n}{4(n-1)}x^{32(n-1)^2}+\frac{2n(n-1)}{\sqrt{4(n-1)^2+n^2}}x^{16(n-1)^2+4n^2}.$$

Proof Based on Proposition 2, the noncommuting graph of Q_{4n}, $\Gamma_G=K_{\underbrace{2,2,\ldots,2}_{n\text{ times}},2n-2}$, where $n\geq 2$.

By Proposition 4 and the Definition 4,

$$SO(\Gamma_G;x)=\sum_{uv\in E(\Gamma_G)}\frac{1}{\sqrt{d_u^{\,2}+d_v^{\,2}}}x^{d_u^2+d_v^2}=\frac{2n(n-1)}{\sqrt{(4n-4)^2+(4n-4)^2}}x^{(4n-4)^2+(4n-4)^2}+\frac{2n(2n-2)}{\sqrt{(4n-4)^2+(2n)^2}}x^{(4n-4)^2+(2n)^2}$$

$$=\frac{\sqrt{2}n}{4(n-1)}x^{32(n-1)^2}+\frac{2n(n-1)}{\sqrt{4(n-1)^2+n^2}}x^{16(n-1)^2+4n^2}. \tag{6}$$

Next, the Sombor index and Sombor polynomial of k −regular graph is presented.

Theorem 7 Let Γ be k −regular graph where k is the degree of each vertex and m is the total number of edges in Γ. Then, the Sombor index of Γ, $SO(\Gamma)=\sqrt{2}km.$

Proof Based on Definition 1,

$$SO(\Gamma)=\sum_{uv\in E(\Gamma)}\sqrt{d_u^{\,2}+d_v^{\,2}}=\sum_{uv\in E(\Gamma)}\sqrt{2d_u^{\,2}}=\sqrt{2}\left|E(\Gamma)\right|d_u=\sqrt{2}km. \tag{7}$$

Theorem 8 Let Γ be k −regular graph where k is the degree of each vertex and m is the total number of edges in Γ. Then, the Sombor polynomial of Γ, $SO(\Gamma;x)=\frac{m}{\sqrt{2}k}x^{2k^2}$.

Proof Based on the definition of Sombor polynomial of the graph,

$$SO(\Gamma;x)=\sum_{uv\in E(\Gamma)}\frac{1}{\sqrt{d_u^{\,2}+d_v^{\,2}}}x^{d_u^2+d_v^2}=\sum_{uv\in E(\Gamma)}\frac{1}{\sqrt{2d_u^{\,2}}}x^{2d_u^2}=\frac{\left|E(\Gamma)\right|}{\sqrt{2}k}x^{2k^2}=\frac{m}{\sqrt{2}k}x^{2k^2}. \tag{8}$$

4. Conclusions

In this paper, the Sombor polynomial is introduced. Then, the general formulas of the Sombor index and Sombor polynomial of the non-commuting graph associated to the dihedral groups, the quasidihedral groups and the generalised quaternion groups are determined. The Sombor index and Sombor polynomial for k −regular graph is also found. These formulas can be used to help chemists, biologist and scientists to predict the physical and chemical properties of some molecules without involving any laboratory work. In future, this study can be extended to determine the Sombor index and Sombor polynomial of other types of graphs and groups. Some properties of the Sombor index and Sombor polynomial can also be found, such as obtaining the Sombor polynomial of certain classical graph operations and deriving the bounds of the Sombor index of some graph operations.

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