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On Topological Indices of a Graph Associated to the Direct Product of Two Groups

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ABSTRACT— The topological structure or connectedness of a molecular network can be understood through the use of topological indices, which are numerical values. The topological indices are widely used in various disciplines including chemistry, mathematics, physics and many applications including the drug design and chemical property studies. In this paper, the topological indices of the non-commuting for the direct product of an abelian group and the dihedral groups are determined. The non-commuting graph is a graph where two of its vertices are adjacent if and only if they represent elements in a group that do not commute with one another. Moreover, the vertices of this graph correspond to the noncentral elements of the group. The general formula of the non-commuting graph for the direct product of an abelian group and the dihedral groups is established. Then, it is used to find its topological indices by using some preliminaries. The topological indices involve in this study are the Wiener index, Zagreb index, Szeged index and Harary index. It is found that their general formulas have relation between the order of an abelian group and the topological indices of the non-commuting graph for the dihedral groups.

KEYWORDS: Topological index, Non-commuting graph, Direct product, Graph theory.

1. INTRODUCTION

The term "topological index" refers to an algorithm that calculates a molecular descriptor from a molecular graph. In this graph, the vertices represent atoms of the molecule, while the edges represent the bonds between these atoms [1]. The information in the molecular graph must be transformed into numerical characteristics to connect the molecular topology to any molecular property [2]. The number of elements forming the graph and the information about their connection are retrieved from the hydrogen-suppressed graph and used in a specific algorithm to compute the topological indices [3].

Recent years have seen a significant increase in the use of topological indices and have been employed in QSPR (quantitative structure-property relationship) and QSAR (quantitative structure activity relationship) studies. The literature on mathematical chemistry has seen the development of numerous new topological indices and got many attentions among researchers [4]. Wiener index, which was introduced by Wiener, is one of the earliest types of topological indices in 1947 [5]. Then, its formula has been modified by Hosoya [6] since Wiener does not take into account the ring molecule. The idea of introducing the Wiener index's formula is by first implementing the polynomial expression and the latest formula is stated in Definition 1.1. Many studies have been done and new concepts of the Wiener index have been established [7- 9]. In addition, the Wiener, the Szeged and the Harary indices are classified as the distance-based topological index. Meanwhile, the Zagreb index is classified as the degree-based topological index.

Definition 1.1 [5] The Wiener Index
Let Γ be a simple connected graph with a vertex set $V(\Gamma)=\{1,2,\cdots,n\}$. The Wiener index of Γ, denoted by $W(\Gamma)$, is half of the sum of the distances between all pair of vertices in Γ, written as

$$W(\Gamma)=\sum_{i=1}^{n}\sum_{j=1}^{n}d(i,j),$$

where $d(i,j)$ is the distance between vertices i and j.

In 1972, [10] developed the Zagreb index, which is divided into first and second Zagreb indices, defined in the following definition. Some recent studies on the Zagreb index can be found in [11- 13].

Definition 1.2 [10] The First and Second Zagreb Indices
Let Γ be a simple connected graph with a vertex set $V(\Gamma)=\{1,2,\cdots,n\}$. The first Zagreb index, $M_1(\Gamma)$, is defined as the total summation of square of the degree of each vertex in Γ while the second Zagreb index, $M_2(\Gamma)$ is defined as the summation of the product of the degree of two vertices for each edge, respectively, written as

$$M_1(\Gamma)=\sum_{v\in V(\Gamma)}(\deg(v))^2$$

and

$$M_2(\Gamma)=\sum_{\{u,v\}\in E(\Gamma)}\deg(u)\deg(v).$$

The concepts of Szeged and Harary indices are then introduced from the Wiener index [14], as stated in the following definitions.

Definition 1.3 [15] The Szeged Index
Let Γ be a simple connected graph with vertex set $V(\Gamma)=\{1,2,\cdots,n\}$. The Szeged index, $Sz(\Gamma)$ is given as in the following:

$$Sz(\Gamma)=\sum_{e\in E(\Gamma)}n_1(e|\Gamma)n_2(e|\Gamma),$$

where the summation embraces all edges of Γ,

$$n_1(e|\Gamma)=|\{v|v\in V(\Gamma),d(v,x|\Gamma)<d(v,y|\Gamma)\}|$$

and

$$n_2(e|\Gamma)=|\{v|v\in V(\Gamma),d(v,y|\Gamma)<d(v,x|\Gamma)\}|$$

which means that $n_1(e|\Gamma)$ counts the Γ's vertices are closer to one edge's terminal x than the other while $n_2(e|\Gamma)$ is vice versa.

Definition 1.4 [16] The Harary Index
Let Γ be a connected graph with vertex set $V(\Gamma)=\{1,2,\cdots,n\}$. Half the elements' sum in the reciprocal distance matrix, $D^r=D^r(\Gamma)$, is what is known as the Harary index, written as

$$H(\Gamma)=\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}D^r(i,j),$$

where

$$D^r(i,j)=\begin{cases}\dfrac{1}{d(i,j)}, & \text{if} \quad i\neq j,\\ 0, & \text{if} \quad i=j,\end{cases}$$

and $d(i,j)$ is the shortest distance between vertex i and j.

The Harary index of certain types of graphs and its properties have been done by many researchers and many interesting findings have been found such as in [17- 19].

In this paper, the general formula of some topological indices of the non-commuting graph associated to the direct product of an abelian group and the dihedral groups are established. The main results and their proofs are presented in Section 4. Next, the non-commuting graph is defined as follows.

Definition 1.5 [20] Non-commuting Graph
Let G be a finite group. The non-commuting graph of G, denoted as Γ_G, is the graph with vertex set $G-Z(G)$ and two distinct vertices x and y are joined by an edge whenever $xy\neq yx$.

2. Prelimiaries

Some preliminaries that are used to prove the main theorems are stated in this section. The number of conjugacy classes of D_{2n} are found as given in the following proposition.

Proposition 2.1 Let G be the dihedral group, D_{2n} and $k(G)$ denotes the number of the conjugacy classes of G. Then,

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

The center of the dihedral group is presented in the following proposition.

Proposition 2.2 [21] Let G be a dihedral group, D_{2n} where $n\geq 3, n\in\mathbb{Z}$ and $Z(G)$ is the center of G. Then,

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

Next, the general formula of the non-commuting graph of dihedral groups has been determined by [22].

Proposition 2.3 [22] Let G be the dihedral groups of order $2n$ where $n\geq 3, n\in\mathbb{Z}$ and the non-commuting graph of G is denoted by Γ_G. Then,

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

Proposition 2.4 [23] Let G be the dihedral groups of order $2n$ where $n \geq 3, n \in \mathbb{Z}$. Then, the Harary index of the non-commuting graph of G,

$$H(\Gamma_G) = \begin{cases} \frac{1}{4}[7n^2 - 9n + 2], & \text{if} \quad n \text{ is odd,} \\ \frac{1}{4}[7n^2 - 16n + 6], & \text{if} \quad n \text{ is even.} \end{cases}$$

3. The Non-commuting Graph of $G \times D_{2n}$

In this section, the degree of the vertices in the non-commuting graph of an abelian group and the dihedral groups, $G \times D_{2n}$ is stated in the following lemma. In addition, the general formula of the non-commuting graph for $G \times D_{2n}$ is also found, which is presented in Proposition 3.1. These results will be used to prove the main theorems.

Lemma 3.1 Let $G \times D_{2n}$ be the direct product of an abelian group and the dihedral group of order $2n$ and $\Gamma_{G\times D_{2n}}$ be the non-commuting graph of $G \times D_{2n}$. Then, the degree of the vertices of $\Gamma_{G\times D_{2n}}$,

$$deg_{\Gamma_{G\times D_{2n}}}(g, x) = |G| deg_{\Gamma_{D_{2n}}}(x),$$

where $deg_{\Gamma_{D_{2n}}}(x)$ is the degree of vertex x in $\Gamma_{D_{2n}}$.

Proof. The center of an abelian group G is G. Hence, the center of $G \times D_{2n}$ is $G \times Z(D_{2n})$. Then,

$$\begin{aligned} V\left(\Gamma_{G\times D_{2n}}\right) &= (G \times D_{2n}) \backslash G \times Z(D_{2n}) \\ &= \{(g, x) | g \in G, x \in D_{2n} \backslash Z(D_{2n})\}. \end{aligned}$$

If $(g, x) \in V\left(\Gamma_{G\times D_{2n}}\right)$, then

$$\begin{aligned} deg_{\Gamma_{G\times D_{2n}}}(x) &= \left|\{a \in V(\Gamma_{D_{2n}}) | a \text{ is adjacent to } x\}\right| \\ &= \left|\{a \in V(\Gamma_{D_{2n}}) | ax \neq xa\}\right| \\ &= \left|\{a \in V(\Gamma_{D_{2n}}) | a \in C_{D_{2n}}(x)\}\right| \\ &= \left|D_{2n} \backslash C_{D_{2n}}(x)\right|. \end{aligned}$$

Then,

$$\begin{aligned} deg_{\Gamma_{G\times D_{2n}}}(g, x) &= \left|(G \times D_{2n}) \backslash C_{G\times D_{2n}}(g, x)\right| \\ &= |G \times D_{2n}| - \left|C_{G\times D_{2n}}(g, x)\right| \\ &= |G||D_{2n}| - |G|\left|C_{D_{2n}}(x)\right| \\ &= |G|\left(|D_{2n}| - \left|C_{D_{2n}}(x)\right|\right) \\ &= |G| deg_{\Gamma_{D_{2n}}}(x). \end{aligned}$$

□

Next, the general form of the non-commuting graph for $G \times D_{2n}$ is stated, as follows.

Proposition 3.1 Let $\Gamma_{G\times D_{2n}}$ be the non-commuting graph of the direct products of an abelian group, G, and the dihedral groups, D_{2n}, which is denoted as $G \times D_{2n}$. Then,

$$\Gamma_{G\times D_{2n}} = \begin{cases} K_{\underbrace{|G|,|G|,\cdots,|G|}_{n\ times},(n-1)|G|}, & \text{if} \quad n \text{ is odd,} \\ K_{\underbrace{2|G|,2|G|,\cdots,2|G|}_{\frac{n}{2}\ times},(n-2)|G|}, & \text{if} \quad n \text{ is even.} \end{cases}$$

Proof. The vertices of the non-commuting graph for $G \times D_{2n}$,

$$V(\Gamma_{G\times D_{2n}}) = (G \times D_{2n}) \backslash Z(G \times D_{2n})$$
$$= (G \times D_{2n}) \backslash (G \times Z(D_{2n})).$$

By Proposition 2.3, there are two cases of the non-commuting graph of dihedral groups, which are n is odd and n is even. By Proposition 2.2, there is a center of D_{2n} when n is odd and two centers of D_{2n} when n is even.

For n is odd, there are $|G| \times (n-1)$ elements that do not commute to each other and there are n sets of $|G|$ elements which do not commute to each other. Then,

$$K_{\underbrace{|G|,|G|,\cdots,|G|}_{n\ times},(n-1)|G|}.$$

For n is even, there are $|G| \times (n-2)$ elements that do not commute to each other and there are $\frac{n}{2}$ sets of $2|G|$ elements that do not commute to each other. Then,

$$K_{\underbrace{2|G|,2|G|,\cdots,2|G|}_{\frac{n}{2}\ times},(n-2)|G|}.$$

Therefore,

$$\Gamma_{G\times D_{2n}} = \begin{cases} K_{\underbrace{|G|,|G|,\cdots,|G|}_{n\ times},(n-1)|G|}, & \text{if} \quad n \text{ is odd,} \\ K_{\underbrace{2|G|,2|G|,\cdots,2|G|}_{\frac{n}{2}\ times},(n-2)|G|}, & \text{if} \quad n \text{ is even.} \end{cases}$$

□

4. The Topological Indices of $\Gamma_{G\times D_{2n}}$

This section states the topological indices for $\Gamma_{G\times D_{2n}}$ which includes the Wiener index, the first Zagreb index, the second Zagreb index, the Szeged index and the Harary index.

4.1 The Wiener Index of $\Gamma_{G\times D_{2n}}$

In this subsection, the Wiener index of the non-commuting graph for $G \times D_{2n}$, denoted as $W(G \times D_{2n})$, is computed and its general formula is found by using Proposition 3.1, as stated in the following theorem.

Theorem 4.1 Let the group be the direct product of an abelian group with dihedral groups, $G \times D_{2n}$. Then,

$$W(\Gamma_{G\times D_{2n}}) = \begin{cases} |G|^2 W(\Gamma_{D_{2n}}) + |G|(|G|-1)(2n-1), & \text{if} \quad n \text{ is odd,} \\ |G|^2 W(\Gamma_{D_{2n}}) + 2|G|(|G|-1)(n-1), & \text{if} \quad n \text{ is even.} \end{cases}$$

Proof. Based on Proposition 3.1, the number of vertices of the non-commuting graph for $G \times D_{2n}$ is $|G \times D_{2n}| - 1$. There are $|G|^2$ sets of elements that have the Wiener index of the non-commuting graph of $G \times D_{2n}$ which is the same as the Wiener index of the non-commuting graph for D_{2n}. Since G is abelian, then all the elements do not commute and the distance between each other is two. Then, there are $(|G|^2 - |G|)(2n - |Z(D_{2n})|)$ elements in $\Gamma_{G\times D_{2n}}$ where they have distance two. Thus, the Wiener index of the non-commuting graph for $G \times D_{2n}$,

$$W(\Gamma_{G\times D_{2n}}) = |G|^2 W(\Gamma_{D_{2n}}) + (|G|^2 - |G|)(2n - |Z(D_{2n})|).$$

Since $Z(D_{2n}) = 1$ if n is odd and $Z(D_{2n}) = 2$ if n is even, then,

$$W\left(\Gamma_{G\times D_{2n}}\right)=\begin{cases}|G|^2W\left(\Gamma_{D_{2n}}\right)+|G|(|G|-1)(2n-1), & \text{if } n \text{ is odd},\\ |G|^2W\left(\Gamma_{D_{2n}}\right)+2|G|(|G|-1)(n-1), & \text{if } n \text{ is even}.\end{cases}$$

4.2 The Zagreb Index of $\Gamma_{G\times D_{2n}}$

In this subsection, the general formula of the first and second Zagreb indices of the non-commuting graph for $G\times D_{2n}$, denoted as $M_1\left(\Gamma_{G\times D_{2n}}\right)$ and $M_2\left(\Gamma_{G\times D_{2n}}\right)$, respectively, are found by using their definitions, as stated in the following theorems.

Theorem 4.2 Let the group be the direct product of an abelian group with dihedral groups, $G\times D_{2n}$. Then,

$$M_1\left(\Gamma_{G\times D_{2n}}\right)=|G|^3M_1\left(\Gamma_{D_{2n}}\right).$$

Proof. Let X be the elements in G and Y be the elements in D_{2n}. Then, $X=\{x_1,x_2,\cdots,x_m\}$ where m is the total number of elements in X and $Y=\{y_1,y_2,\cdots,y_n\}$, where n is the total number of vertices in Y.
For $G\times D_{2n}$, where G is abelian, based on Definition 1.2,

$$\begin{aligned}M_1\left(\Gamma_{G\times D_{2n}}\right)&=\sum_{x,y\in V\left(\Gamma_{G\times D_{2n}}\right)}(\deg(x,y))^2\\
&=\left[|G|deg_{\Gamma_{D_{2n}}}(y_1)\right]^2+\left[|G|deg_{\Gamma_{D_{2n}}}(y_2)\right]^2+\cdots+\left[|G|deg_{\Gamma_{D_{2n}}}(y_n)\right]^2+\cdots+\\
&\quad\left[|G|deg_{\Gamma_{D_{2n}}}(y_1)\right]^2+\left[|G|deg_{\Gamma_{D_{2n}}}(y_2)\right]^2+\cdots+\left[|G|deg_{\Gamma_{D_{2n}}}(y_n)\right]^2\\
&=|G|^2\sum_{i=1}^{n}deg^2_{\Gamma_{D_{2n}}}(y_i)+|G|^2\sum_{i=1}^{n}deg^2_{\Gamma_{D_{2n}}}(y_i)+\cdots+|G|^2\sum_{i=1}^{n}deg^2_{\Gamma_{D_{2n}}}(y_i)\\
&=[|G|^2+|G|^2+\cdots+|G|^2]\sum_{i=1}^{n}deg^2_{\Gamma_{D_{2n}}}(y_i)\\
&=m|G|^2\sum_{i=1}^{n}deg^2_{\Gamma_{D_{2n}}}(y_i)\\
&=|G|^3M_1\left(\Gamma_{D_{2n}}\right).\end{aligned}$$

□

Theorem 4.3 Let the group be the direct product of an abelian group with dihedral groups, $G\times D_{2n}$. Then,

$$M_2\left(\Gamma_{G\times D_{2n}}\right)=|G|^4M_2\left(\Gamma_{D_{2n}}\right).$$

Proof. Let X be the elements in G and Y be the elements in D_{2n}. $X=\{x_1,x_2,\cdots,x_m\}$, where m is the total number of elements in X and $Y=\{y_1,y_2,\cdots,y_n\}$, where n is the total number of vertices in Y.
For $G\times D_{2n}$, where G is abelian, based on Definition 1.2,

$$\begin{aligned}M_2\left(\Gamma_{G\times D_{2n}}\right)&=\sum_{\left((x_i,y_j),(x_k,y_l)\right)\in E\left(\Gamma_{G\times D_{2n}}\right)}deg\left(x_i,y_j\right)deg(x_k,y_l)\\
&=\sum_{(y_j,y_l)\in E\left(\Gamma_{D_{2n}}\right)}deg\left(y_j\right)deg(y_l)[|G|^2+|G|^2+\cdots+|G|^2]\times m\\
&=m\times m\times|G|^2\sum_{(y_j,y_l)\in E\left(\Gamma_{D_{2n}}\right)}deg\left(y_j\right)deg(y_l)\\
&=|G|^4M_2\left(\Gamma_{D_{2n}}\right).\end{aligned}$$

□

4.3 The Szeged Index of $\Gamma_{G\times D_{2n}}$

In this subsection, the general form of the Szeged index of the non-commuting graph associated to the direct product of an abelian group, G, and the dihedral groups, D_{2n} and its proof are presented in the following theorem.

Theorem 4.4 Let the group be the direct product of an abelian group with the dihedral groups, $G \times D_{2n}$. Then, the Szeged index of the non-commuting graph for $G \times D_{2n}$,

$$Sz(\Gamma_{G\times D_{2n}}) = |G|^4 Sz(\Gamma_{D_{2n}}).$$

Proof. By Proposition 3.1, the non-commuting graph of $G \times D_{2n}$ has a multiple of $|G|$ elements in each independent set of the multipartite graph for both cases, when n is even and n is odd, compared to the elements in each independent set of the non-commuting graph of D_{2n}. So that, there are multiple of $|G|$ elements that an element is closer to the other element of an edge in a graph, and vice versa. In addition, there are multiple of $|G|^2$ edges in the non-commuting graph of $G \times D_{2n}$, compared to in the non-commuting graph of D_{2n} Therefore, the Szeged index of the non-commuting graph of $G \times D_{2n}$ is multiple of $|G|^4$ of the Szeged index of the non-commuting graph for D_{2n}, as written in the following.

$$Sz(\Gamma_{G\times D_{2n}}) = |G|^4 Sz(\Gamma_{D_{2n}}).$$

□

4.4 The Harary Index of $\Gamma_{G\times D_{2n}}$

In this subsection, the Harary index of the non-commuting graph associated to the direct product of an abelian group, G and the dihedral groups, D_{2n}, denoted as $H(\Gamma_{G\times D_{2n}})$, is found.

Theorem 4.5 Let the group be the direct product of an abelian group and a non-abelian dihedral groups, $G \times D_{2n}$. Then,

$$H(\Gamma_{G\times D_{2n}}) = \begin{cases} |G|^2 H(\Gamma_{D_{2n}}) + \dfrac{|G|}{4}(|G|-1)(2n-1), & \text{if } \ n \text{ is odd,} \\ |G|^2 W(\Gamma_{D_{2n}}) + \dfrac{|G|}{2}(|G|-1)(n-1), & \text{if } \ n \text{ is even.} \end{cases}$$

Proof. By Definition 1.4 and Proposition 2.4, the Harary index of $\Gamma_{G\times D_{2n}}$ is proved as follows. There are$|G|^2$ sets of elements which have the same value of Harary index of the non-commuting graph ofD_{2n}. All the entries are the same as the entries for calculating the $H(\Gamma_{D_{2n}})$ but there are $(|G|^2-|G|)(2n-|Z(D_{2n})|)$ elements that have reciprocal distance $\frac{1}{2}$. Then,

$$H(\Gamma_{G\times D_{2n}}) = |G|^2 H(\Gamma_{D_{2n}}) + \frac{1}{4}(|G|^2-|G|)(2n-|Z(D_{2n})|).$$

Therefore, by Proposition 2.2,

$$H(\Gamma_{G\times D_{2n}}) = \begin{cases} |G|^2 H(\Gamma_{D_{2n}}) + \dfrac{|G|}{4}(|G|-1)(2n-1), & \text{if } \ n \text{ is odd,} \\ |G|^2 W(\Gamma_{D_{2n}}) + \dfrac{|G|}{2}(|G|-1)(n-1), & \text{if } \ n \text{ is even.} \end{cases}$$

5. Conclusion

In this paper, some topological indices of the non-commuting graph associated to the direct product of an abelian group and the dihedral groups are presented. Their general formulas in terms of the order of the groups are stated in the main theorem and have been proved by using some preliminaries and definitions. These results can be used to predict the chemical and physical properties of molecules by developing a new mathematical model which consists the topological index as the variable. In addition, future studies on the relation between these general formulas and some molecular structures can be done.

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