The topological indices of non-commuting graph for quasidihedral group

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Abstract: A topological index is a single value that can be calculated from a graph which represents the molecule in Chemistry and it is computed by applying a specific algorithm using information obtained from the graph. Meanwhile, non-commuting graph is the graph of vertex set whose vertices are non-central elements and two distinct vertices are joined by an edge if and only if they do not commute. In this paper, the topological indices including Wiener index, first Zagreb index and second Zagreb index of the non-commuting graph for quasidihedral group are determined.

Keywords: Non-commuting graph, Wiener index, Zagreb index, Quasidihedral group.

1 Introduction

Graph theory has very wide applications in various field such as engineering, computer sciences, physical and biological sciences, and numerous other areas to solve real world problems. A graph can be used to represent almost any physical situations where it consists a set of vertices or points and edges or lines. For example, the points might be the destinations with the lines of travel path form one destination to the others [1].

In addition, the topological indices have become increasingly important in the prediction of physical properties in chemistry and biology as it is free of cost without involving any laboratory work. The topological indices are numerical values that can be obtained from the graph where it is used in chemistry to analyzed the chemical properties of the molecular structure such as in predicting the boiling point of the inorganic molecules. The molecular structure can be represented as a graph where the atoms represent the set of vertices while the bond between them are the edges.

Various topological indices have been studied by many researchers but this paper only focuses on the Wiener index, first Zagreb index and second Zagreb index of the non-commuting graph of quasidihedral groups.

The presentation of the quasidihedral groups, QD_{2^n} is given in the following:

$$QD_{2^n} =< a, b|a^{2^{n-1}} = b^2 = 1,\ bab^{-1} = a^{2^{n-2}} - 1 >, \qquad n \geq 4.$$

This paper consists of three sections. The first section is the introduction section, followed by the second section, namely the preliminaries where some basic concepts, definitions and previous results on group theory and graph theory are stated. In the third section, the main results which are the new theoretical results on the generalisation of Wiener index and Zagreb index of the non-commuting graph of quasidihedral groups are presented.

2 Preliminaries

In this section, some basic concepts, definitions and previous results in group theory and graph theory that will be used in the main theorems are stated.

Definition 2.1 (2). **(Centralizer)** The centralizer of x in G, is a subset of the elements in G that commute with x, written as $C_G(x) = g \in G \mid gx = xg$.

Definition 2.2 (3). **(Non-commuting Graph)** Let G be a finite group. The non-commuting graph of G, denoted by Γ_G, is the graph of vertex set $G - Z(G)$ and two distinct vertices x and y are joined by an edge whenever $xy \neq yx$.

The main objective of this study is to determine some topological indices of the non-commuting graph of the quasidihedral groups. The topological indices are defined in the following.

Definition 2.3 (4). **(Wiener Index)** Let v_i and v_j be two distinct vertices where $i \neq j$ and Γ be the connected graph with n vertices. The Wiener index of a graph is defined as the sum of the half of the distances between every pair of vertices of Γ, written as,

$$W(\Gamma) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} d(v_i, v_j),$$

where $d(v_i, v_j)$ is the shortest distance of v_i and v_j.

Definition 2.4 (5). **(The First Zagreb Index)** Let Γ be a connected graph. Then, the first Zagreb index is the sum of squares of the degrees of the vertices of Γ, written as,

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

where $\deg(u)$ is the number of edges connected to vertex u.

Definition 2.5 (5). **(The Second Zagreb Index)** Let Γ be a connected graph. Then, the second Zagreb index is the sum of the product of the degrees of pairs of adjacent vertices of Γ, written as,

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

where u, v are the vertices on the edge connected them.

Now, some works related to group theory, graph theory and the topological indices of the non-commuting graph of finite groups are stated. The following propositions are some concepts that will be used in the later sections.

Proposition 2.1 (2). *Let G be a quasidihedral group, QD_{2^n} of order 2^n and $Z(G)$ be the center of G. Then, $Z(G) = \{1,\ a^{2^{n-2}}\}$.*

Proposition 2.2 (6). *Let G be a finite group and Γ_G be the non-commuting graph of G. Then,*

$$2|E(\Gamma_G)| = |G|^2 - k(G),$$

where $k(G)$ is the number of conjugacy classes of G.

Next, the following propositions are the previous results of some types of topological indices of the non-commuting graph of a finite group.

Proposition 2.3 (7). *Let G be a quasidihedral group, QD_{2^n} of order 2^n where $n \geq 4$, $n \in \mathbb{Z}^+$. Then, the conjugacy class graph of G is $\Gamma_G^{cl} = K_{2^{n-2}+1}$ where it is a complete graph with $2^{n-2}+1$ vertices.*

Proposition 2.4 (8). *Let G be a finite group and Γ_G be the non-commuting graph. Then, the Wiener index of Γ_G is,*

$$W(\Gamma_G) = \frac{1}{2}\left[(|G| - |Z(G)|)(|G| - 2|Z(G)| - 2) + |G|(k(G) - |Z(G)|)\right],$$

where $k(G)$ denotes the number of conjugacy classes of G and $|Z(G)|$ is the number of centers of G.

Proposition 2.5 (9). *Let G be a finite group and Γ_G be the non-commuting graph. Then, the first Zagreb index of Γ_G is,*

$$M_1(\Gamma_G) = |G|^2(|G| + |Z(G)| - 2k(G)) - \sum_{x \in G - Z(G)} |C_G(x)|^2,$$

where $k(G)$ is the number of conjugacy classes and $C_G(x)$ is the centralizer of x.

Proposition 2.6 (10). *Let G be a finite group and Γ_G be the non-commuting graph. Then, the second Zagreb index of Γ_G is,*

$$M_2(\Gamma_G) = -|G|^2|E(\Gamma_G)| + |G| M_1(\Gamma_G) + \sum_{x,y \in E(\Gamma_G)} |C_G(x)||C_G(y)|.$$

3 Results and discussion

In this section, the Wiener index, the first Zagreb index, and the second Zagreb index of the non-commuting graph of quasidihedral groups are determined. Lemma 1 shows the number of conjugacy classes of quasidihedral groups while Lemma 2 and Lemma 3 show the summation of centralizers of elements in $G - Z(G)$ that will be used in the main theorems.

Lemma 3.1. *Let G be a quasidihedral group, QD_{2^n} and $k(G)$ be the number of conjugacy classes of G. Then,*

$$k(G) = 2^{n-2} + 3,$$

where $n \geq 4$.

Proof By Proposition 3, we know that the number of non-central conjugacy classes of the quasidihedral group is $2^{n-2}+1$. So that, the total number of conjugacy classes, $k(G)$ is $2^{n-2}+1+|Z(G)|$. Hence, by Proposition 1, we now have $k(G) = 2^{n-2}+3$. ∎

Lemma 3.2. *Let G be a quasidihedral group, $QD_{2^n} = \langle a, b | a^{2^{n-1}} = b^2 = 1,\ bab^{-1} = a^{2^{n-2}} - 1 \rangle$ of order 2^n where $n \geq 4$ and $C_G(x)$ is the centralizer of an element $x \in G$. Then,*

$$\sum_{x \in G - Z(G)} |C_G(x)|^2 = 2^{3n-3} - 2^{2n-1} + 2^{n+3}.$$

Proof By Definition 1, $C_G(x)$ is the set of all elements in G that commute with element x in G. We know that $a^i a^j = a^j a^i$ where $i \neq j$ and $i, j = 0, 1, \ldots, 2^{n-1} - 1$. There will be 2^{n-1} elements which have $|C_G(x)| = 4$ since a^i and b^j does not commute where $i, j = 0, 1, \ldots, 2^{n-1} - 1$. Then, there will be $2^{n-1} - |Z(G)| = 2^{n-1} - 2$ elements which have $|C_G(x)| = 2^{n-1}$ since all a^i commute each other where $i = 0, 1, \ldots, 2^{n-1} - 1$ and $|Z(G)| = 2$ which can see in Proposition 1. Then,

$$\sum_{x \in G - Z(G)} |C_G(x)|^2 = 4^2 \left(2^{n-1}\right) + \left(2^{n-1}\right)^2 \left(2^{n-1} - 2\right)$$

$$= 2^{3n-3} - 2^{2n-1} + 2^{n+3}.$$

■

Lemma 3.3. *Let G be a quasidihedral group, $QD_{2^n} =< a, b | a^{2^{n-1}} = b^2 = 1,\ bab^{-1} = a^{2^{n-2}} - 1 >$ of order 2^n where $n \geq 4$ and $C_G(x)$ is the centralizer of an element $x \in G$. Then,*

$$\sum_{x \in G - Z(G)} |C_G(x)| |C_G(y)| = 2^n \left(2^{2n-1} - 8\right).$$

Proof By Definition 2, the non-commuting graph is the graph of vertex set $G - Z(G)$ and two distinct vertices x and y are joined by an edge if they do not commute. So that, the non-commuting graph of quasidihedral group consists an edge if and only if $a^i b^j \neq b^j a^i$ where $i = \{0, 1, 2, \ \ldots, \ 2^{n-1}\}$ and $j = 0, 1$. By Definition 1, $C_G(x)$ is the set of all elements in G that commute with element x in G.

There will be $\left(2^{n-1}\right)\left(2^{n-1} - 2\right)$ edges that connect two vertices x and y which have $|C_G(x)| = 2^{n-1}$ and $|C_G(x)| = 4$ while the another $|E(\Gamma_G)| - \left(2^{n-1}\right)\left(2^{n-1} - 2\right)$ edges connect two distinct vertices x and y which have $|C_G(x)| = 4$ and $|C_G(y)| = 4$. then, after simplified,

$$\sum_{x \in G - Z(G)} |C_G(x)| |C_G(y)| = 2^n \left(2^{2n-1} - 8\right).$$

■

The following theorems are the new theoretical results of some topological indices of the non-commuting graph of the quasidihedral groups.

Theorem 3.1. *Let G be a quasidihedral group, QD_{2^n} of order 2^n where $n \geq 4$, Γ_G is the non-commuting graph of G and $W(\Gamma_G)$ is the Wiener index of the non-commuting graph of G. Then,*

$$W(\Gamma_G) = 2^{2n-1} + 2^{2n-3} - 7\left(2^{n-1}\right) + 6.$$

Proof From Proposition 4,

$$W(\Gamma_G) = \frac{1}{2}\left[\left(|G| - |Z(G)|\right)\left(|G| - 2|Z(G)| - 2\right) + |G|\left(k(G) - |Z(G)|\right)\right].$$

By Lemma 1, $k(G) = 2^{n-2} + 3$, by Proposition 1, we can see that $|Z(G)| = 2$ and by Proposition 2, the number of edges of the non-commuting graph, $|E(\Gamma_G)| \frac{|G|^2-k(G)|G|}{2}$. Then,

$$\begin{aligned}
W(\Gamma_G) &= \frac{1}{2}\left[(|G|-|Z(G)|)(|G|-2|Z(G)|-2)+|G|(k(G)-|Z(G)|)\right] \\
&= \frac{1}{2}\left[(2^n-2)(2^n-2(2)-2)+2^n\left(2^{n-2}+3-2\right)\right] \\
&= \frac{1}{2}\left[2^{2n}-7(2^n)+12+2^{2n-2}\right] \\
&= 2^{2n-1}+2^{2n-3}-7\left(2^{n-1}\right)+6,
\end{aligned}$$

where $n \geq 4$. ■

Theorem 3.2. *Let G be a quasidihedral group, QD_{2^n} of order 2^n where $n \geq 4$, Γ_G is the non-commuting graph of G and $M_1(\Gamma_G)$ is the first Zagreb index of the non-commuting graph of G. Then,*

$$M_1(\Gamma_G) = 2^n\left[5\left(2^{2n-3}\right)-9\left(2^{n-1}\right)+8\right].$$

Proof From Proposition 5,

$$M_1(\Gamma_G) = |G|^2(|G|+|Z(G)|-2k(G)) - \sum_{x\in G-Z(G)} |C_G(x)|^2.$$

By Lemma 1, $k(G) = 2^{n-2}+3$, by Proposition 1, we can see that $|Z(G)| = 2$ and by Proposition 2, the number of edges of the non-commuting graph, $|E(\Gamma_G)| \frac{|G|^2-k(G)|G|}{2}$. From Lemma 2,

$$\sum_{x\in G-Z(G)} |C_G(x)|^2 = 2^{3n-3}-2^{2n-1}+2^{n+3}.$$

Then,

$$\begin{aligned}
M_1(\Gamma_G) &= |G|^2(|G|+|Z(G)|-2k(G)) - \sum_{x\in G-Z(G)} |C_G(x)|^2 \\
&= 2^{2n}\left(2^n+2-2\left(2^{n-2}+3\right)\right)+\left(2^{2(n-1)}\left(2^{n-1}-2\right)+4^2\left(2^{n-1}\right)\right) \\
&= 2^{3n}-2^{3n-1}-4\left(2^{2n}\right)+2^{3n-3}-2^{2n-1}+4^2\left(2^{n-1}\right) \\
&= 2^n\left[5\left(2^{2n-3}\right)-9\left(2^{n-1}\right)+8\right],
\end{aligned}$$

where $n \geq 4$. ■

Theorem 3.3. *Let G be a quasidihedral group, QD_{2^n} of order 2^n where $n \geq 4$, Γ_G is the non-commuting graph of G and $M_2(\Gamma_G)$ is the second Zagreb index of the non-commuting graph of G. Then,*

$$M_2(\Gamma_G) = 2^n\left[2^{3n-2}-5\left(2^{2n-1}\right)+8\left(2^n\right)-8\right].$$

Proof From Proposition 6,

$$M_2(\Gamma_G) = -|G|^2 |E(\Gamma_G)| + |G| M_1(\Gamma_G) + \sum_{x,y \in E(\Gamma_G)} |C_G(x)| |C_G(y)|.$$

By Lemma 1, $k(G) = 2^{n-2} + 3$, by Proposition 1, we can see that $|Z(G)| = 2$ and by Proposition 2, the number of edges of the non-commuting graph, $|E(\Gamma_G)| \frac{|G|^2 - k(G)|G|}{2}$. From Lemma 3,

$$\sum_{x \in G - Z(G)} |C_G(x)| |C_G(y)| = 2^n \left(2^{2n-1} - 8\right).$$

Then,

$$\begin{aligned} M_2(\Gamma_G) &= -|G|^2 |E(\Gamma_G)| + |G| M_1(\Gamma_G) + \sum_{x,y \in E(\Gamma_G)} |C_G(x)| |C_G(y)| \\ &= -2^{2n} \left[\frac{2^{2n} - \left(2^{n-2} + 3\right)\left(2^n\right)}{2}\right] + 2^{2n}\left[\frac{5}{8}2^{2n} - \frac{9}{2}2^n + 8\right] + 2^n\left(2^{2n-1} - 8\right) \\ &= \frac{1}{4}2^{4n} - \frac{5}{2}2^{3n} + 8\left(2^{2n}\right) - 8\left(2^n\right) \\ &= 2^n\left[2^{3n-2} - 5\left(2^{2n-1}\right) + 8\left(2^n\right) - 8\right], \end{aligned}$$

where $n \geq 4$. ∎

4 Conclusion

In this paper, the generalisation of the Wiener index, the first Zagreb index and the second Zagreb index of the non-commuting graph for quasidihedral groups are determined. The results obtained can help the related industry especially chemists to analyze the chemical properties of the molecular structure.

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Competing interests

The authors declare that they have no competing interests.

Authors' contributions

All authors have contributed to all parts of the article. All authors read and approved the final manuscript.

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