Proceedings of Science and Mathematics
Faculty of science, universiti teknologi malaysia
https://science.utm.my/procscimath/
Volume 26 (2024) 53-58

Topological Indices of Coprime Graph of Generalized Quaternion Group

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Abstract
Topological indices are crucial tools in molecular chemistry, used to predict molecular properties by analyzing the relationships between vertices in a graph. This article focuses on deriving general formulas for various topological indices of the coprime graph associated with the quaternion group of prime power order. Specifically, we investigate the Wiener index, Gutman index, Harmonic index, Zagreb index, and Harary index. By establishing these formulas, we aim to enhance the understanding of the structural properties of such graphs and their implications in chemical informatics and related fields.
Keywords: topological index;quaternion group;coprime graph;chemical graph theory;algebraic graph theory

Introduction

Graphs are everywhere, like in strait, telecommunication networks, and chemical structures. In chemistry, graphs are used in chemical graph theory. In chemical graph theory there are named topological index of chemical compounds that are represented by a graph. Topological indices are crucial tools in molecular chemistry to predict molecular properties by analyzing the relationship between vertices in the graph. In this age, algebraic graph theory is very famous among mathematicians. Algebraic graph theory makes a group or a ring or maybe a module represented by a graph. Chemical graph theory and algebraic graph theory have the same idea. So, we can make and compute the topological index of the graph representing abstract algebra objects (García-Domenech et. al., 2008).

These indices provide various measures of the coprime graph's structure, capturing different aspects of its complexity and connectivity. Each index reflects a unique perspective: the Gutman Index offers insights into the graph's energy and connectivity; the Harmonic Index measures the balance in the reciprocal of vertex degrees; the First Zagreb Index is related to the sum of the squares of the vertex degrees, indicating vertex degree distribution; the Second Zagreb Index focuses on the degree of vertex pairs, showing interaction strength; the Wiener Index measures the total distance between all pairs of vertices; and the Harary Index provides a measure related to the reciprocal of distances in the graph. Understanding these indices helps in analyzing the coprime graph's properties and behaviours within the mathematical framework of the generalized quaternion group (Ningrum et. all, 2024).

Some mathematicians computed topological indices of some graph-represented algebraic objects. In 2022, Husni et. al. wrote an article discussing the harmonic and Gutman index of the coprime graph of integer group with modulo addition operation. In 2023, Putra et. al. discussed the power graph of integer group modulo n with modulo addition operation and its indices. In the same year, Gayatri et. al. also found some of the topological indices of the coprime graph of the dihedral group.

This article focuses on deriving general formulas for various topological indices associated with the quaternion group. It is based on the article that was written by Nurhabibah in 2021. Some topological indices that will be investigated in this article are the formula of the Gutman index, harmonic index, first Zagreb index, second Zagreb index, Wiener index, and Harary index. By establishing these formulas, we aim to enhance the understanding of the structural properties of such graphs and their implication in chemical informatics and related fields.

A quaternion group is a group formed by eight elements that is $Q_8 = \{\pm 1, \pm i, \pm j, \pm k | i^2 = j^2 = k^2 = ijk = -1\}$ (Girard, 1983). If $a = i, b = j$, then the form of $Q_8 = \{1, a, a^2, a^3, b, ab, a^2b, a^3b\} =< a, b | a^4 = 1, a^2 = b^2, b^{-1}ab = a^{-1} >$. If we generalized it, we get generalized quaternion group Q_{4n} where $n \geq 2$.

Definition 1

Generalized quaternion group denoted by Q_{4n} with $n \geq 2$ is a group with an order $4n$ and defined by

$$Q_{4n} =< a, b | a^{2n} = e, a^n = b^2, b^{-1}ab = a^{-1} >.$$

In 2014, Ma et. al. defined a graph that can represent a finite group by checking if two distinct elements of the group G have orders that are coprime or $a, b \in G$, $\gcd(|a|, |b|) = 1$, then they are adjacent. This graph is called the coprime graph of G.

Definition 2

Let G be finite group, the coprime graph of G denoted by Γ_G is a graph with vertices are elements of G and two distinct vertices u and v are adjacent if and only if $\gcd(|u|, |y|) = 1$.

Some indices use the degree of vertex and distance of two vertices of the graph Γ. So, below are definitions of degree and distance in the graph.

Definition 3(Rosen, 2019)

Let $V(\Gamma)$ denoted set of vertices of the graph Γ. Degree of vertex $v \in V(\Gamma)$ is the number of edges incident with v. Distance between $u, v \in V(\Gamma)$ is the length of the shortest path between u and v is denoted by $d(u, v)$.

Results and discussion

These are some properties that can help us investigate topological indices of the coprime graph of the generalized quaternion group.

Theorem 1 (Nurhabibah, et. al., 2021)

Consider $\Gamma_{Q_{4n}}$ as the coprime graph associated with the generalized quaternion group where $n = 2^k, k \in \mathbb{N}$ then the coprime graph of Q_{4n} is a complete bipartite.

Proof. Let $Q_{4n} = \{e, a, a^2, \dots, a^{2n-1}, b, ab, a^2b, \dots, a^{2n-1}b\}$. Clear that $|e| = 1$, so $\gcd(|e|, |u|), \forall u \in Q_{4n} \backslash \{e\}$, hence e is adjacent to all other vertices. For all $x \in Q_{4n} \backslash \{e\}$, order of x is 2^i with $i = 1, 2, \dots, k + 1$. So $\forall u, v \in Q_{4n} \backslash \{e\}, 2 | \gcd(|u|, |v|)$, hence u and v are not adjacent. Then, $\Gamma_{Q_{4n}}$ is a complete bipartite graph with $P_1 = \{e\}$ and $P_2 = Q_{4n} \backslash \{e\}$.

This theorem indirectly states that the coprime graph of Q_{4n} is star graph when n is the power of 2. So clear that $\deg(e) = 4n - 1$ and $\deg(v) = 1, v \in Q_{4n} \backslash \{e\}$.

Definition 4 (Andova, et. al., 2012)

Let $V(\Gamma)$ be the set of vertices of a connected graph Γ. The Gutman index is defined as

$$Gut(\Gamma) = \sum_{u,v \in V(\Gamma)} \deg(u) \deg(v)\, d(u, v).$$

By the definition above, we compute the Gutman index of the coprime graph of the generalized quaternion group.

Theorem 2
Consider $\Gamma_{Q_{4n}}$ as the coprime graph associated with the generalized quaternion group where $n = 2^k, k \in \mathbb{N}$ then $Gut(\Gamma_{Q_{4n}}) = (4n-1)(8n-3)$.

Proof. By using Theorem 1 that $\Gamma_{Q_{4n}}$ is a complete bipartite graph with $P_1 = \{e\}, P_2 = \{u \in Q_{4n} | u \neq e\}$ then $\deg(e) = 4n-1$ and $\deg(u) = 1$ and $d(e,v) = 1, d(u,v) = 2,\ u,v \in P_2$. So by definition of the Gutman index, we get

$$\begin{aligned}
Gut(\Gamma_{Q_{4n}}) &= \sum_{u,v \in V(\Gamma_{Q_{4n}})} \deg(u)\deg(v)\, d(u,v) \\
&= \sum_{v \in P_2} \deg(e)\deg(v)\, d(e,v) + \sum_{u,v \in P_2} \deg(u)\deg(v)\, d(u,v) \\
&= (4n-1)(4n-1)(1)(1) + \binom{4n-1}{2}(1)(1)(2) \\
&= (4n-1)^2 + (4n-1)(4n-2) \\
&= (4n-1)(4n-3)
\end{aligned}$$

Below is the definition of the harmonic index of a connected graph. The harmonic index simply is the summation of 2 divided by the addition of two degrees of vertices.

Definition 5 (Zhong, 2012)
Let $E(\Gamma)$ be the set of edges of a connected graph Γ. The harmonic index is defined as

$$H(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{2}{\deg(u) + \deg(v)}.$$

By definition above, below is the harmonic index of the coprime graph of the generalized quaternion group.

Theorem 3
Consider $\Gamma_{Q_{4n}}$ as the coprime graph associated with the generalized quaternion group where $n = 2^k, k \in \mathbb{N}$ then $H(\Gamma_{Q_{4n}}) = \frac{4n-1}{2n}$.

Proof. By using Theorem 1 that $\Gamma_{Q_{4n}}$ is a complete bipartite graph with $P_1 = \{e\}, P_2 = \{u \in Q_{4n} | u \neq e\}$ then $\deg(e) = 4n-1$ and $\deg(u) = 1, u \in P_2$. So by definition of harmonic index, we get

$$\begin{aligned}
H(\Gamma_{Q_{4n}}) &= \sum_{uv \in E(\Gamma_{Q_{4n}})} \frac{2}{\deg(u) + \deg(v)} \\
&= (4n-1)\frac{2}{4n-1+1} \\
&= \frac{4n-1}{2n}.
\end{aligned}$$

Below is the definition of the Zagreb indices that is the first Zagreb index and the second Zagreb index.

Definition 6 (Gutman, et. al., 2015)

Let $V(\Gamma)$ and $E(\Gamma)$ be the set of vertices and edges of a connected graph Γ. The first Zagreb index M_1 and second Zagreb index M_2 is defined as follows

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

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

By definition above, we compute both of the Zagreb indices in Theorem 4 and Theorem 5 below.

Theorem 4
Consider $\Gamma_{Q_{4n}}$ as the coprime graph associated with the generalized quaternion group where $n = 2^k, k \in \mathbb{N}$ then $M_1(\Gamma_{Q_{4n}}) = 16n^2 - 4n$.

Proof. By using Theorem 1 that $\Gamma_{Q_{4n}}$ is a complete bipartite graph with $P_1 = \{e\}, P_2 = \{u \in Q_{4n} | u \neq e\}$ then $\deg(e) = 4n - 1$ and $\deg(u) = 1, u \in P_2$. So by definition of the first Zagreb index, we get

$$\begin{aligned} M_1(\Gamma_{Q_{4n}}) &= \sum_{u \in V(\Gamma_{Q_{4n}})} \deg(u)^2 \\ &= (4n-1)^2 + (4n-1)(1)^2 \\ &= 16n^2 - 4n. \end{aligned}$$

Theorem 5
Consider $\Gamma_{Q_{4n}}$ as the coprime graph associated with the generalized quaternion group where $n = 2^k, k \in \mathbb{N}$ then $M_2(\Gamma_{Q_{4n}}) = (4n-1)^2$.

Proof. By using Theorem 1 that $\Gamma_{Q_{4n}}$ is a complete bipartite graph with $P_1 = \{e\}, P_2 = \{u \in Q_{4n} | u \neq e\}$ then $\deg(e) = 4n - 1$ and $\deg(u) = 1, u \in P_2$. So by definition of the second Zagreb index, we get

$$\begin{aligned} M_2(\Gamma_{Q_{4n}}) &= \sum_{uv \in E(\Gamma_{Q_{4n}})} \deg(u)\deg(v) \\ &= (4n-1)(4n-1)(1) \\ &= (4n-1)^2. \end{aligned}$$

Below is the definition of the Wiener index. Wiener index is the summation of half of the distance between two vertices.

Definition 7 (Graovac and Pisanski, 1991)
Let $V(\Gamma)$ be the set of vertices of a connected graph Γ. The Wiener index is defined as

$$W(\Gamma) = \frac{1}{2} \sum_{u,v \in V(\Gamma)} d(u,v).$$

By definition above, we compute the Wiener index of the coprime graph of the generalized quaternion group.

Theorem 6
Consider $\Gamma_{Q_{4n}}$ as the coprime graph associated with the generalized quaternion group where $n = 2^k, k \in \mathbb{N}$ then $W(\Gamma_{Q_{4n}}) = \frac{(4n-1)^2}{2}$.

Proof. By using Theorem 1 that $\Gamma_{Q_{4n}}$ is a complete bipartite graph with $P_1 = \{e\}, P_2 = \{u \in Q_{4n} | u \neq e\}$ then $d(e,u) = 1, d(u,v) = 2, u,v \in P_2$. So by definition of the Wiener index, we get

$$\begin{aligned} W(\Gamma_{Q_{4n}}) &= \frac{1}{2} \sum_{u,v \in V(\Gamma_{Q_{4n}})} d(u,v) \\ &= \frac{1}{2}\left((4n-1)(1) + \binom{4n-1}{2}(2)\right) \\ &= \frac{1}{2}\big((4n-1) + (4n-1)(4n-2)\big) \\ &= \frac{1}{2}\big((4n-1)(4n-1)\big) \\ &= \frac{(4n-1)^2}{2} \end{aligned}$$

Below is the definition of the Harary index of a connected graph.

Definition 8 (Zhou, et. al., 2008)
Let $V(\Gamma)$ be the set of vertices of a connected graph Γ. The Harary index is defined as

$$\mathcal{H}(\Gamma) = \frac{1}{2} \sum_{u,v \in V(\Gamma)} \frac{1}{d(u,v)}.$$

By definition above, below is the Harary index of the coprime graph of the generalized quaternion group.

Theorem 7
Consider $\Gamma_{Q_{4n}}$ as the coprime graph associated with the generalized quaternion group where $n = 2^k, k \in \mathbb{N}$ then $\mathcal{H}(\Gamma_{Q_{4n}}) = \frac{(4n-1)(4n+1)}{4}$.

Proof. By using Theorem 1 that $\Gamma_{Q_{4n}}$ is a complete bipartite graph with $P_1 = \{e\}, P_2 = \{u \in Q_{4n} | u \neq e\}$ then $d(e,u) = 1, d(u,v) = 2,\ u,v \in P_2$. So by definition of the Harary index, we get

$$\begin{aligned} W(\Gamma_{Q_{4n}}) &= \frac{1}{2} \sum_{u,v \in V(\Gamma_{Q_{4n}})} d(u,v) \\ &= \frac{1}{2}\left((4n-1)\left(\frac{1}{1}\right) + \binom{4n-1}{2}\left(\frac{1}{2}\right)\right) \\ &= \frac{1}{2}\left((4n-1) + \frac{(4n-1)(4n-2)}{2}\right) \\ &= \frac{1}{2}\left(\frac{2(4n-1) + (4n-1)(4n-1)}{2}\right) \\ &= \frac{(4n-1)(4n+1)}{4} \end{aligned}$$

Corollary 1
Consider $\Gamma_{Q_{4n}}$ as the coprime graph associated with the generalized quaternion group where $n = 2^k, k \in \mathbb{N}$ then $M_2(\Gamma_{Q_{4n}}) = 2W(\Gamma_{Q_{4n}})$.

Conclusion

Gutman index, harmonic index, first Zagreb index, second Zagreb index, Wiener index, and Harary index of the coprime graph of the generalized quaternion group Q_{4n} with $n = 2^k, k \in \mathbb{N}$ is $(4n-1)(4n-3)$, $\frac{4n-1}{2n}, 16n^2 - 4n, (4n-1)^2, \frac{(4n-1)^2}{2}$, and $\frac{(4n-1)(4n+1)}{4}$ respectively. These indices provide various measures of the coprime graph's structure, capturing different aspects of its complexity and connectivity.

Acknowledgement

We would like to express our gratitude for the guidance and financial support from the algebraic and combinatorics group, department of Mathematics, Universitas Mataram.

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