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Some Results on Topological Indices of Graphs Associated to Groups and Rings

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Abstract

A topological index is a numerical value associated with a chemical compound that provides information about its molecular structure and properties. Researches on topological indices are initially related to graphs obtained from chemical structures to predict the biological activities and reactivity. Recently, the research on this topic has evolved on graphs in general and even on graphs obtained from algebraic structures, such as groups, rings or modules. This paper will present various researches and results on topological indices of graphs associated to groups, including the non-commuting graph and the co-prime graph, and a graph associate to rings, namely the non-zero divisor graph.

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1 Introduction

Topological indices provide numerical descriptors that capture important structural features of molecules, and serve as powerful tools for the analysis and prediction of various physicochemical properties and biological activities. The significance of topological indices lies in their ability to transform complex molecular structures into numerical representations, enabling the development of computational models and the efficient exploration of chemical space for various applications in drug discovery, materials science, and reaction chemistry [1].

One of the primary applications of topological indices is in the prediction of properties related to the biological activity of compounds, such as drug-likeness, toxicity, and bioactivity [2]. By analyzing the connectivity and arrangement of atoms within a molecule, topological indices can provide insights into how a compound interacts with biological targets, aiding in the design and optimization of new drugs. In addition to drug discovery, topological indices find applications in various other areas of mathematical chemistry and materials science. For example, they can be used to predict physical properties of molecules, such as boiling points, solubilities, and partition coefficients, aiding in the selection of appropriate solvents or understanding the behavior of compounds in different environments [3].

The first type of topological index has been discovered by Wiener [4] in 1947, in which the concept of Wiener number considering the path in a graph is introduced. In [4], the Wiener number of some paraffins are determined and their boiling points are also predicted. Then, Hosoya [5] reformulated the formula of Wiener number, known as Wiener index of a graph, $W(\Gamma)$, and its formula is given in the following.

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

where $d(i,j)$ is the distance between vertices i and j, and m is the total number of vertices in a graph Γ.

Since then, various types of topological indices have been developed based on either chemistry or mathematical perspectives. In 1972, Gutman and Trinajstić [6] introduced the degree-based topological index, Zagreb index, which is divided into two types; first Zagreb index, M_1, and second Zagreb index, M_2, defined as follows.

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

and

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

In addition, the Szeged and Harary indices are given in the following definitions.

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Definition 1.1. ***[7] The Szeged Index***
Let Γ be a simple connected graph with vertex set $V(\Gamma) = \{1,2,\ldots,n\}$. 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 1.2. ***[8] The Harary Index***
Let Γ be a connected graph with vertex set $V = \{1,2,\ldots,n\}$. Half the elements' sum in the reciprocal distance matrix, $D^r = D^r(\Gamma)$, is what is known as the Harary index, written as

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

where
$D^r(i,j) = \begin{cases} \frac{1}{d(i,j)} & if \quad i \neq j, \\ 0 & if \quad i = j, \end{cases}$ *and $d(i,j)$ is the shortest distance between vertex i and j.*

The Randić index is a graph-theoretical descriptor that quantifies the complexity or branching structure of a molecular graph. It was introduced by Milan Randić [9] in 1975 and has found applications in various fields of chemistry. The Randić index of a molecular graph is calculated based on the topological distances between pairs of vertices (atoms) in the graph. It is defined as the sum of the reciprocal square roots of the product of the degrees of connected pairs of vertices, written as

$$R(\Gamma) = \sum_{u,v\in E(\Gamma)} \frac{1}{\sqrt{deg(u)deg(v)}}.$$

Then, the Randić index is modified and introduced a concept of general zeroth order Randić index, which is defined as

$${}^0R_\alpha = \sum_{u\in V(\Gamma)} (deg(u))^\alpha,$$

where α can be any non-zero real number [10]. In 2018, the general inequalities of ${}^0R_\alpha$ is determined, as stated in the following.

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Theorem 1.1. *[11] Let α be a positive integer and Γ be any graph, then*

$$^{0}R_{\alpha} \leq \frac{1}{c}(^{0}R_{\frac{1}{\alpha}}(\Gamma))^{\alpha}$$

holds for $c = 1$ whereas the inequailty is not always true for $c > 1$. The equality sign in the above inequality holds if and only if $\alpha > 1$ or Γ has size zero.

Recently, in 2020, a new topological index, Sombor index has been established by Gutman [12]. The Sombor index of a graph, $SO(\Gamma)$, is defined as follows.

$$SO(\Gamma) = \sum_{u,v \in E(\Gamma)} \sqrt{\deg(u)^2 + \deg(v)^2}.$$

In this paper, some results on the topological indices of some graphs associated to groups and rings are presented.

2 Topological Indices of Graphs Associated to Groups

The study on topological indices have received attention from many researchers, from multidisciplinary field. In this paper, some results on both degree and distance based topological indices of some graphs of groups are stated.

Following theorem presents the Wiener index of some graphs associated to some finite groups. The graphs that include in this paper are the non-commuting graph and coprime graph.

Theorem 2.1. *[15] Let G be the generalised quaternion group, Q_{4n} of order $4n$ where $n \geq 2$, Γ_G is the non-commuting graph of G and $W(\Gamma_G^{NC})$ is the Wiener index of Γ_G. Then,*

$$W(\Gamma_G^{NC}) = 2n(5n-7)+6.$$

In addition, the coprime graph of a group G is denoted as Γ_G^{CO} and its Wiener index has been determined by Alimon et al [17] in 2020.

Theorem 2.2. *[17] Let G be the dihedral group of order $2n$, where $n \geq 3$. Then, if n is an odd prime, $W(\Gamma_G^{CO}) = 3n^2 - 3n + 1$. Meanwhile, if $n = 2^k, k \in Z^+$, then $W(\Gamma_G^{CO}) = (2n-1)^2$.*

Next, the first and second Zagreb index of the non-commuting graph for some finite groups, denoted as $M_1(\Gamma_G^{NC})$ and $M_2(\Gamma_G^{NC})$, respectively, are stated in the following theorems.

Theorem 2.3. *[16] Let G be a dihedral group, D_{2n} of order $2n$ where $n \geq 3$. Then,*

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$$M_1(\Gamma_G^{NC}) = \begin{cases} n(5n-4)(n-1) & \textit{if} \quad n \textit{ is odd}, \\ n(5n-8)(n-2) & \textit{if} \quad n \textit{ is even}, \end{cases}$$

and

$$M_2(\Gamma_G^{NC}) = \begin{cases} 2n(n-1)^2(2n-1) & \textit{if} \quad n \textit{ is odd}, \\ 4n(n-2)^2(n-1) & \textit{if} \quad n \textit{ is even}. \end{cases}$$

Theorem 2.4. *[15] Let G be the generalised quaternion group, Q_{4n} of order $4n$ where $n \geq 2$. Then,*

$$M_1(\Gamma_G^{NC}) = 8n(5n^2-9n+4),$$

and

$$M_2(\Gamma_G^{NC}) = 32n(2n^3-5n^2+4n-1).$$

Theorem 2.5. *[17] Let G be a dihedral group, D_{2n} and Γ_G^{CO} is coprime graph of G. Then, if $n = 2^k$, where $k \in Z^+$, the Szeged index of coprime graph for D_{2n} is as follows :*

$$Sz(\Gamma_G^{CO}) = 4n^2-4n+1.$$

Furthermore, the Harary index of the non-commuting graph associated to the dihedral groups are stated in the next theorem.

Theorem 2.6. *[18] Let G be a dihedral group, D_{2n} and Γ_G^{NC} is a non-commuting graph of G. Then,*

$$H(\Gamma_G^{NC}) = \begin{cases} \frac{1}{4}\left[(n-2)(7n-3)+n\right] & \textit{if} \quad n \textit{ is even}, \\ \frac{1}{4}\left[(n-1)(7n-2)\right] & \textit{if} \quad n \textit{ is odd}. \end{cases}$$

In 2023, Roslly et al. [19] determined the general formula of Randić index of the non-commuting graph associated to three finite groups, namely the dihedral groups, the generalised quaternion groups and the quasidihedral groups, as presented in Theorems 2.8, 2.9 and 2.10, respectively.

Theorem 2.7. *[19] Let G be a dihedral group, D_{2n} and Γ_G^{NC} is a non-commuting graph of G. Then,*

$$R(\Gamma_G^{NC}) = \begin{cases} \frac{n\sqrt{2n(n-1)}+4n(n-1)}{4\sqrt{2n(n-1)}} & \textit{if} \quad n \textit{ is odd}, \\ \frac{n\sqrt{2n(n-2)}+4n(n-2)}{4\sqrt{2n(n-2)}} & \textit{if} \quad n \textit{ is even}. \end{cases}$$

Theorem 2.8. *[19] Let G be the generalised quaternion group, Q_{4n} and Γ_G^{NC} is a non-commuting graph of G. Then,*

$$R(\Gamma_G^{NC}) = \frac{4n(n-1)}{\sqrt{8n(n-1)}} + \frac{n}{2}.$$

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Theorem 2.9. *[19] Let G be the quasidihedral group, QD_{2^n} and Γ_G^{NC} is a non-commuting graph of G. Then,*

$$R(\Gamma_G^{NC}) = \frac{2^{n-1}(2^{n-1}-2)}{\sqrt{(2^{n-1})(2^n-4)}} + \frac{2^{n-1}(2^{n-2}-1)}{2^n-4}.$$

Some results on Sombor index of the non-commuting graph related to groups are found by Khasraw et al. [13].

Theorem 2.10. *[13] Let G_1 be the dihedral groups, G_2 be the generalised quaternion groups and G_3 be the quasidihedral groups. Then,*

$$SO(\Gamma_{G_1}^{NC}) = \begin{cases} n(n-1)\left[\sqrt{2}(n-1)+\sqrt{4(n-1)^2+n^2}\right] & \text{if } n \text{ is odd}, \\ n(n-2)\left[\sqrt{2}(n-2)+\sqrt{4(n-2)^2+n^2}\right] & \text{if } n \text{ is even}, \end{cases}$$

$$SO(\Gamma_{G_2}) = 8n(n-1)\left[\sqrt{2}(n-1)+\sqrt{4(n-1)^2+n^2}\right],$$

$$SO(\Gamma_{G_3}) = \sqrt{2}(2^n-4)(2^{2n-3}-2^{n+1}) + (2^{2n-2}-2)\sqrt{(2^n-4)^2+2^{2n-2}}.$$

3 Topological Indices of Graphs Associated to Rings

In this section, some results on the topological indices of zero divisor graph for some commutative rings, found by [21] and [22] are presented.

Theorem 3.1. *[21] The first Zagreb index of zero divisor graph for Z_{p^k} is $2(p^{k-1}-p^k)\left(k-1+\lceil\frac{k-1}{2}\rceil\right)+(p^k+1)(p^{k-1}-1)+3\left(p^{\lceil\frac{k-1}{2}\rceil}-1\right)$ where $k \geq 3$ for $p=2$ and $k \geq 2$ for odd prime p.*

Theorem 3.2. *[22] The general zeroth-order Randić index of the zero divisor graph for the ring $Z_{p^k q}$ when $\alpha = 1$,*

$$R_1^0 = k(p^k - p^{k-1})(2q-1) - p^k - p + 2 - \left(\frac{p^k - p^{\lceil\frac{k+3}{2}\rceil}}{p^{\lceil\frac{k+1}{2}\rceil}}\right).$$

4 Conclusion

In this paper, some results on a few types of topological indices of some graphs associated to some finite groups and commutative rings are stated. These theoretical results can benefit other disciplines in predicting the chemical and physical properties of the molecules.

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