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The Szeged and Wiener Indices for Coprime Graph of Dihedral Groups

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Abstract. The coprime graph is defined as a graph where two distinct vertices are adjacent if and only if the order of both vertices are coprime. The Szeged index is the summation of the products of the number of vertices which are lying closer to x than y and vice versa. Meanwhile, the Wiener index is the half-sum of the distances for all vertices of the graph. In this paper, the Szeged index and the Wiener index of the coprime graph for certain order of dihedral groups are computed. Then, the general form of the Szeged and Wiener indices of the coprime graph for the dihedral groups are determined.

INTRODUCTION

Topological indices have been widely used in chemistry. A topological index is a numerical value that can be used to characterize the graph of a molecule [1]. It was first introduced by Wiener in 1947 [2] to predict the physico-chemical properties specifically for alkanes. There are many types of topological indices such as the Wiener index, the Zagreb index, the Harary index, the Hosoya index, and the Szeged index. The concept of topological index is based on the connectivity of the graph and the distance where the degree of the atom and the shortest distance between two atoms are computed to determine the index [1]. The value of index gives different characterization and prediction. For example, if the Wiener index is smaller, then it shows that the molecule is more compact and it leads to the lower intermolecular force. Hence, the boiling point is lower.

Furthermore, a topological index is known as the molecular descriptor that is calculated based on the molecular graph of chemical compound. In mathematical chemistry, the graph consists of the set of vertices and edges which represent the atoms and bonds between two atoms, respectively. The application of topological index is not limited to the prediction of physicochemical properties only, but can also be used in some models such as quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR). In this paper, two types of topological indices, the Szeged index and Wiener index of a specific graph and group will be determined and called the coprime graph and dihedral groups, respectively.

This paper consists of four sections which are the introduction, preliminaries, results and discussion, and conclusion. In the preliminaries section, the concepts, definitions and previous results are stated. Then, the results and discussion section includes the general form of the Szeged and Wiener indices of the coprime graph for a group will be presented. In the conclusion section, the results are concluded.

PRELIMINARIES

In order to compute the Szeged and Wiener indices of a graph and determine their general formula, some basic concepts and definitions in group theory and graph theory are needed. This paper focuses on these two topological

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indices of one type of graph, namely the coprime graph associated to dihedral group.

A dihedral group is a group that consists a set of elements which involves rotations and reflections, denoted as D_{2n}. According to [3], the presentation of the dihedral group is given as follows :

$$D_{2n} =< a, b|a^n = b^2, bab = a^{-1} > .$$

Many researchers have been done on dihedral groups, but none of them focuses on finding the topological indices based on the groups. Most of them determined the topological indices directly from the molecular structure.

The first type of the topological indices is the Wiener index which is originally introduced for molecular graph of alkanes. In 2009, Eliasi and Taeri [4] introduced four new types of graphs and their Wiener indices are found. Then, Vijayabarathi and Anjaneyulu [5] analyzed the structure of some organic molecules in chemistry by using the Wiener index. Meanwhile, Yu *et al.* [6] extended the research on the Wiener index in finding its sufficient condition for bipartite graph. The Wiener index is defined as half-sum of the distances between every pair of vertices of the graph [2], which can be written as in the following :

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

An example of the Wiener index for a connected graph is given as follows.

Example 1 *Let Γ be the multipartite graph with two independent sets, as shown in the following figure.*

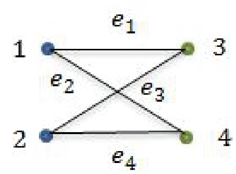

FIGURE 1. A complete bipartite graph, $K_{2,2}$

By definition, the Wiener index of the graph,

$$\begin{aligned}
W(\Gamma_G) &= \frac{1}{2}\sum_{i=1}^{4}\sum_{j=1}^{4} d(i, j) \\
&= \frac{1}{2}[(d(1,1) + d(1,2) + d(1,3) + d(1,4)) + \\
&\quad (d(2,1) + d(2,2) + d(2,3) + d(2,4)) + \\
&\quad (d(3,1) + d(3,2) + d(3,3) + d(3,4)) + \\
&\quad (d(4,1) + d(4,2) + d(4,3) + d(4,4))] \\
&= \frac{1}{2}[(0 + 2 + 1 + 1) + (2 + 0 + 1 + 1) + (1 + 1 + 0 + 2) + (1 + 1 + 2 + 0)] \\
&= \frac{1}{2}(18) \\
&= 9.
\end{aligned}$$

Meanwhile, the Szeged index has been proposed by Gutman [4] in 1998. It is the generalization of Wiener's formula for cyclic molecules. The value of the Wiener index and Szeged index are the same if the graph is a tree [4]. The Szeged index is defined as follows :

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

where

$$n_1(e|\Gamma) = |\{v|v \in V(\Gamma), d(v, x|\Gamma) < d(v, y|\Gamma)\}|$$
$$n_2(e|\Gamma) = |\{v|v \in V(\Gamma), d(v, x|\Gamma) > d(v, y|\Gamma)\}|.$$

In other words, $n_1(e|\Gamma)$ counts the vertices that have a shorter distance to vertex x than the distance to vertex y. Meanwhile, $n_2(e|\Gamma)$ counts the vertices that have a shorter distance to vertex y than vertex x [4].

An example of the Szeged index is shown in the following.

Example 2 *Let Γ be a multipartite graph which has four vertices and four edges as shown in Figure 1. Note that, $N_1(e_i|\Gamma)$ is the vertices of Γ lying closer to one endpoint x of the edge e_i than to its other endpoint y while $N_2(e_i|\Gamma)$ is vice versa. First, $N_1(e_i|\Gamma)$ and $N_2(e_i|\Gamma)$ are calculated for all i,*
$i = 1, e_1 = \{1, 3\}$:

$$\begin{aligned} N_1(e_1|\Gamma) &= \{x \in V(\Gamma) : d(x, 1) < d(x, 3)\}, \\ &= \{1, 4\}. \ Thus, \ n_1(e_1|\Gamma) = 2, \\ N_2(e_1|\Gamma) &= \{y \in V(\Gamma) : d(y, 1) > d(y, 3)\}, \\ &= \{2, 3\}. \ Thus, \ n_2(e_1|\Gamma) = 2. \end{aligned}$$

$i = 2, e_2 = \{1, 4\}$:

$$\begin{aligned} N_1(e_2|\Gamma) &= \{x \in V(\Gamma) : d(x, 1) < d(x, 4)\}, \\ &= \{1, 3\}. \ Thus, \ n_1(e_2|\Gamma) = 2, \\ N_2(e_2|\Gamma) &= \{y \in V(\Gamma) : d(y, 1) > d(y, 4)\}, \\ &= \{2, 4\}. \ Thus, \ n_2(e_2|\Gamma) = 2. \end{aligned}$$

$i = 3, e_3 = \{2, 3\}$:

$$\begin{aligned} N_1(e_3|\Gamma) &= \{x \in V(\Gamma) : d(x, 2) < d(x, 3)\}, \\ &= \{2, 4\}. \ Thus, \ n_1(e_3|\Gamma) = 2, \\ N_2(e_3|\Gamma) &= \{y \in V(\Gamma) : d(y, 2) > d(y, 3)\}, \\ &= \{1, 3\}. \ Thus, \ n_2(e_3|\Gamma) = 2. \end{aligned}$$

$i = 4, e_4 = \{2, 4\}$:

$$\begin{aligned} N_1(e_4|\Gamma) &= \{x \in V(\Gamma) : d(x, 2) < d(x, 4)\}, \\ &= \{2, 3\}. \ Thus, \ n_1(e_4|\Gamma) = 2, \\ N_2(e_4|\Gamma) &= \{y \in V(\Gamma) : d(y, 2) > d(y, 4)\}, \\ &= \{1, 4\}. \ Thus, \ n_2(e_4|\Gamma) = 2. \end{aligned}$$

Hence,

$$\begin{aligned} Sz(\Gamma) &= \sum_{i=1}^{4} n_1(e_i|\Gamma)n_2(e_i|\Gamma) \\ &= n_1(e_1|\Gamma)n_2(e_1|\Gamma) + n_1(e_2|\Gamma)n_2(e_2|\Gamma) + n_1(e_3|\Gamma)n_2(e_3|\Gamma) + \\ &\quad n_1(e_4|\Gamma)n_2(e_4|\Gamma) \\ &= (2 \times 2) + (2 \times 2) + (2 \times 2) + (2 \times 2) \\ &= 16. \end{aligned}$$

The research on the Szeged index has been extended to polycyclic and monocyclic graph by Dobrynin and Gutman [7] and Gutman *et al.* [8], respectively. In 2008, Gutman and Ashrafi [9] have introduced the edge version of Szeged index and found that the edge-Szeged index of a tree is the difference of its Szeged index and its Wiener index. Nadjafi-Arani *et al.* [10] also found the relation between the Wiener and Szeged indices of a graph and proved that $Sz(\Gamma) = W(\Gamma)$, where Γ is a graph. Then, Wang *et al.* [11] identified the minimum edge-Szeged index for $n-$vertex unicyclic graphs with a given diameter in 2018.

The topological indices are computed based on the connected graph. In this paper, the Szeged index and Wiener index are determined based on the coprime graph.

The coprime graph of a group G is defined as a graph that consists a set of vertices, where the vertices are the elements in G, and two vertices are adjacent if the order of vertices x and y are coprime, written as $(|x|, |y|) = 1$ [12]. In 2014, Ma *et al.* in [12] found that one of the types of coprime graphs for the dihedral groups is the multipartite graph.

A multipartite graph, denoted as k-partite graph is defined as a graph that can be partitioned into k different independent sets. Two examples for multipartite graphs with three independent sets are as follows :

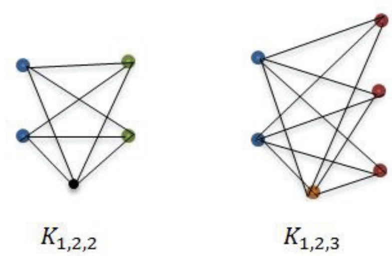

FIGURE 2. Examples of multipartite graph

Next, the star graph is also one of the multipartite graphs with two different independent sets, which consists of a vertex and k vertices. Two examples of the star graph are shown in the following figures.

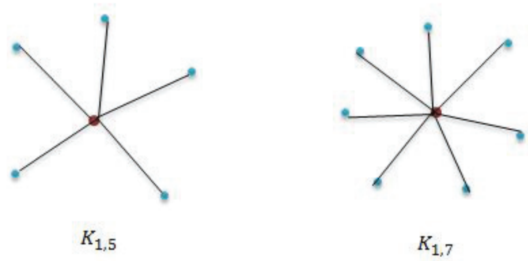

FIGURE 3. Examples of star graph

Some results of the coprime graph associated to the dihedral groups which are used in the proving of the theorems are stated in the following propositions.

Proposition 1 *[12] Let Γ_G be the coprime graph associated to the dihedral groups of order $2n$. If n is an odd prime, then, the coprime graph of G is a multipartite graph, $K_{1,n-1,n}$.*

Proposition 2 *[12] Let Γ_G be the coprime graph associated to the dihedral groups of order $2n$. If $n = 2^k$, where $k \in \mathbb{Z}^+$, then, the coprime graph of G is a multipartite graph, $K_{1,2^{k+1}-1}$.*

In 2016, Dorbidi has found some properties of the coprime graph which are the clique number and the chromatic number. He proved that the clique number of the coprime graph and the chromatic number of the coprime graph are the same [13]. Also in [13], Dorbidi had studied on the automorphism of the coprime graph that gives the result; the group is isomorphic to the automorphism of the coprime graph if and only if the group is isomorphic to the cyclic group of order two. Both researches focus on the coprime graph of finite groups, but this paper focuses on the coprime graph of a specific group, which is the dihedral group.

RESULTS AND DISCUSSION

In this section, the main results are determined, namely the Szeged index and the Wiener index of the coprime graph for dihedral group, D_{2n}. Based on Propositions 1 and 2, there are two cases to be considered, namely when n is an odd prime and when $n = 2^k, k \in \mathbb{Z}^+$. The generalization of Szeged index of the coprime graph for dihedral group, D_{2n} is stated in the following two theorems.

Theorem 1 *Let G be a dihedral group of order* $2n$, *where* $n \geq 3$ *and* Γ_G *is coprime graph of G. Then, if n is an odd prime, the Szeged index of coprime graph for* D_{2n} *is as follows :*

$$Sz(\Gamma_G) = n^4 - 2n^3 + 3n^2 - 2n + 1.$$

Proof *Let* Γ_G *be coprime graph of the dihedral groups. If n is odd prime and* $n \geq 3$, *coprime graph of G is represented as multipartite graph,* $K_{1,n-1,n}$. *There are* $(n-1)$ *edges that have* $n_1(e|\Gamma) = n-1$ *and* $n_2(e|\Gamma) = 1$, *n edges have* $n_1(e|\Gamma) = n$ *and* $n_2(e|\Gamma) = 1$, *and the other edges have* $n_1(e|\Gamma) = n-1$ *and* $n_2(e|\Gamma) = n$. *Then, the Szeged index of the coprime graph for* D_{2n} *when n is odd prime can be simplified as follows :*

$$\begin{aligned} Sz(\Gamma_G) &= \sum_{e \in E(\Gamma)} n_1(e|\Gamma) n_2(e|\Gamma) \\ &= [(n-1) \times (n-1) \times 1] + [n \times (n \times 1)] + [(|E(\Gamma_G)| - (2n-1)) \times n(n-1)] \\ &= (n^2 - 2n + 1) + n^2 + (n^2 + n - 1 - 2n + 1)(n^2 - n) \\ &= (2n^2 - 2n + 1) + (n^2 - n)^2 \\ &= n^4 - 2n^3 + 3n^2 - 2n + 1. \qquad \blacksquare \end{aligned}$$

Theorem 2 *Let G be a dihedral group of order* $2n$, *where* $n \geq 3$ *and* Γ_G *is coprime graph of G. Then, if* $n = 2^k$, *where* $k \in \mathbb{Z}^+$, *the Szeged index of coprime graph for* D_{2n} *is as follows :*

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

Proof *Let* Γ_G *be coprime graph of the dihedral groups. If* $n = 2^k, k \in \mathbb{Z}^+$ *and* $n \geq 3$, *coprime graph is the star graph,* $K_{1,2^{k+1}-1}$. *There are* $2^{k+1} - 1$ *edges that have* $n_1(e|\Gamma) = 2^{k+1} - 1$ *and* $n_2(e|\Gamma) = 1$. *Hence, the Szeged index of the coprime graph for* D_{2n} *when* $n = 2^k, k \in \mathbb{Z}^+$ *can be simplified as follows :*

$$\begin{aligned} Sz(\Gamma_G) &= \sum_{e \in E(\Gamma)} n_1(e|\Gamma) n_2(e|\Gamma) \\ &= (2^{k+1} - 1) \times [(2^{k+1} - 1) \times 1] \\ &= 2^{2k+2} - 2(2^{k+1}) + 1 \\ &= 4(2^{2k}) - 4(2^k) + 1 \\ &= 4n^2 - 4n + 1. \qquad \blacksquare \end{aligned}$$

Next, the Wiener index of the coprime graph for the dihedral group is determined in the following two theorems.

Theorem 3 *Let G be the dihedral group of order* $2n$, *where* $n \geq 3$ *and* Γ_G *is coprime graph of G. Then, if n is an odd prime, the Wiener index of coprime graph for* D_{2n} *is as follows :*

$$W(\Gamma_G) = 3n^2 - 3n + 1.$$

Proof *If n is an odd prime, coprime graph of D_{2n} is the multipartite graph, $K_{1,n-1,n}$. By the definition of the Wiener index,*

$$\begin{aligned}W(\Gamma_G) &= \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m} d(i,j)\\ &= (n-1)(n+1) + n + 2\left[\frac{(n-1)(n-2)}{2}\right] + 2\left[\frac{n(n-1)}{2}\right]\\ &= (n-1)(n+1) + n + (n-1)(n-2) + n(n-1)\\ &= 3n^2 - 3n + 1. \qquad \blacksquare\end{aligned}$$

Theorem 4 *Let G be dihedral group of order 2n, where $n \geq 3$ and Γ_G is coprime graph of G. Then, if $n = 2^k$, where $k \in \mathbb{Z}^+$, the Wiener index of coprime graph for D_{2n} is as follows :*

$$W(\Gamma_G) = (2n-1)^2.$$

Proof *If $n = 2^k$, where $k \in \mathbb{Z}^+$, the coprime graph of D_{2n} is a multipartite graph which is also known as star graph, $K_{1,2^{k+1}-1}$. Thus,*

$$\begin{aligned}W(\Gamma_G) &= \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m} d(i,j)\\ &= \frac{1}{2}\left[(2^{k+1}-1) + (2^{k+1}-1) + 2(2^{k+1}-2)(2^{k+1}-1)\right]\\ &= \frac{1}{2}\left[(2n-1) + (2n-1) + 2(2n-2)(2n-1)\right]\\ &= \frac{1}{2}\left[(2n-1)(2 + 2(2n-2))\right]\\ &= (2n-1)(1 + 2n - 2)\\ &= (2n-1)^2. \qquad \blacksquare\end{aligned}$$

Despite the long computation of finding the topological indices, this paper provides the general form of the Szeged and Wiener indices of coprime graph for dihedral group in terms of n. From the order of the group, the indices can be determined.

CONCLUSION

In this paper, the general forms of Szeged and Wiener indices of the coprime graph for the dihedral groups are found. This generalization will help chemists to determine the physicochemical properties of the molecular structure. Despite the long laboratory work in finding the chemical and physical properties of the molecular structure, this paper provides the general form of the Szeged and Wiener indices of coprime graph for dihedral group in terms of n where both indices can be used to predict their properties in a faster way. From the order of group, the indices can be determined. In future, other topological indices could be computed which include the Zagreb index and Harary index.

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REFERENCES

[1] N. Trinajstić, *Chemical Graph Theory* (Florida:CRC Press,1982).
[2] H. Wiener, Journal of the American Chemical Society, **69**, 17-20 (1947).
[3] J.F. Humphreys, *A Course in Group Theory* (New York:Oxford University Press,1996).
[4] M. Eliasi and B. Taeri, Discrete Applied Mathematics, **157**(4), 794-803 (2009).
[5] A. Vijayabarathi, and G. Anjaneyulu, International Journal of ChemTech Research, **5**(4) 1847-1853 (2013).
[6] G. Yu, L. Ren, and X. Li, Applied Mathematics-A Journal of Chinese Universities, **34**(2), 162-172 (2009).
[7] I. Gutman and A.A. Dobrynin, Graph Theory Notes NY, **34**, 37-44 (1998).
[8] I. Gutman, L. Popović, P.V. Khadikar, S. Karmarkar, S. Joshi, and M. Mandloi, Communications in Mathematical and in Computer Chemistry (MATCH), **35**, 91-103 (1997).
[9] I. Gutman and A.R. Ashrafi, Croatica Chemica Acta, **81**(2), 263-266 (2008).
[10] M.J. Nadjafi-Arani, H. Khodashenas, and A. Ashrafi, Discrete Mathematics, **311**(20), 2233-2237 (2011).
[11] G. Wang, S. Li, D. Qi, and H. Zhang, Applied Mathematics and Computation, **336**, 94-106 (2018).
[12] X.Ma, H.Wei, and L.Yang, International Journal of Group Theory, **3**(3), 13-23 (2014).
[13] H.R. Dorbidi, International Journal of Group Theory, **5**(4), 17-22 (2016).