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Topological Indices of the Prime Power Cayley Graph for a Dihedral Group

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Abstract
A Wiener index is a topological index of a molecule described as the sum of the length of the shortest paths among all pairs of vertices in the chemical graph. Based on the chemical application of graph theory, this index is used to calculate the number of bonds between pairs of atoms in molecules by computing the total distance between all pairs of atoms in molecules by computing the total distance between all pairs by creating a distance matrix. Meanwhile, a Cayley graph is a graph that encodes the abstract structure of a group. An example of the applications of Cayley graph is in solving the Rubik's Cube. Various transformations and configurations of the cube constitute a subgroup within a permutation group, derived from the distinct horizontal and vertical rotations of the puzzle. In other words, each position of the cube corresponds to a vertex of the Cayley graph. One of the important groups that is always associated to graph theory is the dihedral group since this group represents the symmetries of a regular polygon including rotations and reflections. This is due to the applications of this group in various fields including computer graphics, crystallography, and chemistry. In chemistry, the dihedral groups are used to characterize the symmetry of molecules. Therefore, in this paper, a variant of Cayley graph namely the prime power Cayley graph is constructed for the dihedral group of order 12, and the Wiener index and mean distance of this graph is computed.
Keywords: Cayley graph; Dihedral group; Wiener index; Group theory

1. Introduction

Graph theory is an essential field within mathematics and plays a vital role in constructing structural models. In mathematics, a graph Γ consists of a pair of set of vertices $V(\Gamma)$ and set of edges $E(\Gamma)$ where $V(\Gamma)$ is a finite non-empty set containing elements called vertices, and $E(\Gamma)$ is a set of unordered pairs of distinct vertices called edges [1].

A group G is defined as a set together with an associative binary operation which possesses identity an identity and such that each element of G has an inverse [2]. In group theory, a graph of groups is related with the Cayley graph. A Cayley graph was introduced by Cayley in 1878 to illustrate the concept of abstract groups defined by a set of generators [3].

Meanwhile, a new variation of Cayley graph has been introduced in 2022, namely the prime power Cayley graph [4]. In [4], the prime power Cayley graph is constructed for a cyclic group of order $p,$ where p is a prime. The prime power Cayley graph is denoted as $\widetilde{Cay}(G,S)$ where a set of vertices which comprises the elements of G. If $xy^{-1} \in S$, then any two vertices, x and y in G are adjacent.

The topological indices represent numerical values associated with chemical constitutions for the purpose of correlating chemical structure with various properties. A most commonly topological indices which are the Wiener index and the mean distance. The Wiener index was introduced by Harold Wiener in 1947, originated from working on the boiling point of paraffin [5].

In this paper, the prime power Cayley graph of the dihedral group of order 12 is constructed. Then, the Wiener index and the mean distance of these graph are computed.

2. Preliminaries

In this section, some basic concepts of group theory and graph theory which are used in this research are included.

Definition 1 [6] (Dihedral Group)
For any $n \geq 3,$ the dihedral group D_{2n} of order $2n$ is defined by :

$$D_{2n} = \langle a, b : a^n = b^2 = e, b^{-1}ab = a^{-1} \rangle.$$

Definition 2 [4] (Graph of a Group)
A graph of a group G denoted as Γ_G consists of a finite nonempty set of objects called vertices and set of unordered pairs of distinct vertices of Γ_G called edges. The vertex set of Γ_G denoted by $\mathrm{V}(\Gamma_G)$ represents the elements of a group, while the edge set denoted by $\mathrm{E}(\Gamma_G)$ represents the adjacency of the vertices.

Definition 3 [7] (Complete Graph)
A complete graph is a graph in which each pair of vertices is joined by an edge, a complete graph of n vertices is denoted by K_n and it has $\binom{n}{2}$ edges.

Definition 4 [3] (Cayley Graph)
Given a group G and a subset *S* of G. The Cayley graph, $Cay(G,S)$ is associated to group G with $V\big(Cay(G,S)\big) = G$, and two vertices *g* and *h* are adjacent if and only if $gh^{-1} \in S$.

Definition 5 [4] (Prime Power Cayley Graph)
Let G be a group and $|G| = p_1^{\alpha_1} \cdot p_2^{\alpha_2} \cdot \ldots \cdot p_k^{\alpha_k}$ where p_i are primes. Let S be non-empty subset of G in which $S = \{x \in G : |x| = p_i^{r_i}, 1 \leq r_i \leq \alpha_i, i = 1,2,\ldots,k\}$ and $S = S^{-1} := \{s^{-1} | s \in S\}$. The prime power Cayley graph of G with respect to S, denoted as $\widetilde{Cay}(G,S)$, is a graph where the set of vertices of the graph are the elements of G, and two distinct vertices, g and h, are adjacent if $gh^{-1} \in S$ for all $g, h \in G$.

Definition 6 [1] (Distance of Vertices)
In a connected graph, the distance between two vertices u and v is the minimum length of a path from u and v, and is denoted by $d(u,v)$.

Definition 7 [8] (Wiener Index)
A Wiener index of a simple graph Γ is the sum of distances between all ordered pairs of vertices of Γ.

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

Definition 8 [5] (Mean Distance)
Let Γ be a connected graph of order *n*. Then, the mean distance of Γ, denoted as $\sigma(\Gamma)$ is as follows :

$$\sigma(\Gamma) = \frac{W(\Gamma)}{\binom{n}{2}} = \frac{2W(\Gamma)}{n(n-1)}$$

where $W(\Gamma)$ is the Wiener index of Γ.

3. Research Methodology

In this paper, the prime power Cayley graph of the dihedral group of order 12 is constructed by using definition of the graph as in Definition 5 and the group presentation of D_{12} as follows :

$$D_{12} = \langle a, b : a^6 = b^2 = e, b^{-1}ab = a^{-1} \rangle$$

$$= \{e, a, a^2, a^3, a^4, a^5, b, ab, a^2b, a^3b, a^4b, a^5b\}.$$

Next, based on the group presentation, the Cayley table of D_{12} is computed.

Table 3.1 The Cayley Table of D_{12}.

$*$	$\boldsymbol{e}$	$\boldsymbol{a}$	$\boldsymbol{a^2}$	$\boldsymbol{a^3}$	$\boldsymbol{a^4}$	$\boldsymbol{a^5}$	$\boldsymbol{b}$	$\boldsymbol{ab}$	$\boldsymbol{a^2b}$	$\boldsymbol{a^3b}$	$\boldsymbol{a^4b}$	$\boldsymbol{a^5b}$
$\boldsymbol{e}$	e	a	a^2	a^3	a^4	a^5	b	ab	a^2b	a^3b	a^4b	a^5b
$\boldsymbol{a}$	a	a^2	a^3	a^4	a^5	e	ab	a^2b	a^3b	a^4b	a^5b	b
$\boldsymbol{a^2}$	a^2	a^3	a^4	a^5	e	a	a^2b	a^3b	a^4b	a^5b	b	ab
$\boldsymbol{a^3}$	a^3	a^4	a^5	e	a	a^2	a^3b	a^4b	a^5b	b	ab	a^2b
$\boldsymbol{a^4}$	a^4	a^5	e	a	a^2	a^3	a^4b	a^5b	b	ab	a^2b	a^3b
$\boldsymbol{a^5}$	a^5	e	a	a^2	a^3	a^4	a^5b	b	ab	a^2b	a^3b	a^4b
$\boldsymbol{b}$	b	a^5b	a^4b	a^3b	a^2b	ab	e	a^5	a^4	a^3	a^2	a
$\boldsymbol{ab}$	ab	b	a^5b	a^4b	a^3b	a^2b	a	e	a^5	a^4	a^3	a^2
$\boldsymbol{a^2b}$	a^2b	ab	b	a^5b	a^4b	a^3b	a^2	a	e	a^5	a^4	a^3
$\boldsymbol{a^3b}$	a^3b	a^2b	ab	b	a^5b	a^4b	a^3	a^2	a	e	a^5	a^4
$\boldsymbol{a^4b}$	a^4b	a^3b	a^2b	ab	b	a^5b	a^4	a^3	a^2	a	e	a^5
$\boldsymbol{a^5b}$	a^5b	a^4b	a^3b	a^2b	ab	b	a^5	a^4	a^3	a^2	a	e

The prime power Cayley graph of D_{12} is constructed and order of D_{12} the elements of is determined from the Cayley table. Lastly, the Wiener index and the mean distance of order D_{12} are computed by referring to the distance between the vertices of the graph.

4. Results and discussion

4.1. Construction of the Prime Power Cayley Graph of the Dihedral Group of order 12

By referring to the group presentation and Cayley table for D_{12} as in Table 3.1, the order of each element in D_{12} is obtained.

Table 3.2 The order of element D_{12}.

$\boldsymbol{g \in D_{12}}$	e	a	a^2	a^3	a^4	a^5	b	ab	a^2b	a^3b	a^4b	a^5b
$\lvert g \rvert$	1	6	3	2	3	6	2	2	2	2	2	2

Then, using the Definition 5, the prime power Cayley graph of D_{12}, $\widetilde{Cay}(D_{12}, S)$ is associated to subset $S = \{x \in D_{12} \mid |x| = 2, 3\} = \{a^2, a^3, a^4, b, ab, a^2b, a^3b, a^4b, a^5b\}$.

By Deifintion 5, $V[\widetilde{Cay}(D_{12},S)] = \{e, a, a^2, a^3, a^4, a^5, b, ab, a^2b, a^3b, a^4b, a^5b\}$, two distinct vertices g and h in $\widetilde{Cay}(D_{12},S)$ are adjacent if $gh^{-1} \in S$. Let $s \in S$, then $g \sim h$ if $gh^{-1} \in S$ equivalently, $g \sim h$ if $g = sh$.

The vertex a is adjacent to a^4 since $a(a^4)^{-1} = a(a^2) = a^3$ in S.

And the vertex a is non adjacent to a^2 since $a(a^2)^{-1} = a(a^4) = a^5$ not in S.

By using similar steps, the set of edges of $\widetilde{Cay}(D_{12},S)$ is given as follows :

$$E(\widetilde{Cay}(D_{12},S)) = \{(a,e),(a,a^2),(a,a^3),(a,a^4),(a,a^5),(a,b),(a,ab),(a,a^2b),(a,a^3b),(a.a^4b),(a,a^5b),$$
$$(a^2,e),(a^2,a^3),(a^2,a^4),(a^2,a^5),(a^2,b),(a^2,ab),(a^2,a^2b),(a^2,a^3b),(a^2.a^4b),(a^2,a^5b),$$
$$(a^3,e),(a^3,a^4),(a^3,a^5),(a^3,b),(a^3,ab),(a^3,a^2b),(a^3,a^3b),(a^3.a^4b),(a^3,a^5b),(a^4,e),$$
$$(a^4,a^5),(a^4,b),(a^4,ab),(a^4,a^2b),(a^4,a^3b),(a^4.a^4b),(a^4,a^5b),(a^5,e),(a^5,b),(a^5,ab),$$
$$(a^5,a^2b),(a^5,a^3b),(a^5.a^4b),(a^5,a^5b),(b,e),(b,ab),(b,a^2b),(b,a^3b),(b.a^4b),(b,a^5b),$$
$$(ab,e),(ab,a^2b),(ab,a^3b),(ab.a^4b),(ab,a^5b),(a^2b,e),(a^2b,a^3b),(a^2b.a^4b),(a^2b,a^5b),$$
$$(a^3b,e),(a^3b,a^4b),(a^3b,a^5b),(a^4b,e),(a^4b,a^5b),(a^5b,e)\}.$$

The prime power Cayley graph, D_{12}, $\widetilde{Cay}(D_{12},S)$ is constructed as follows.

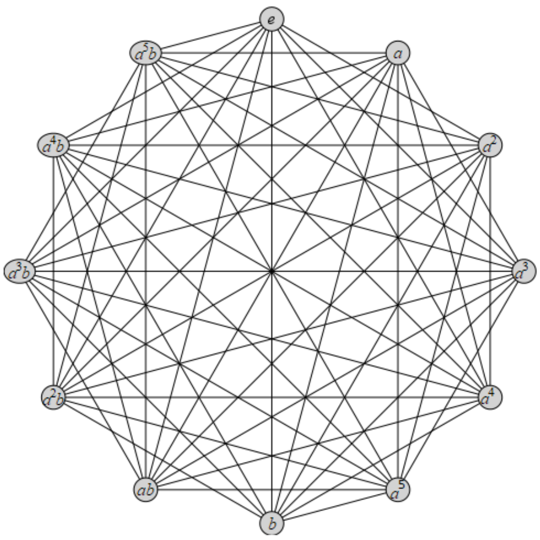

Figure 4.1 The Prime Power Cayley Graph of D_{12}

From Figure 4.1, it can be observed that the prime power Cayley graph of dihedral group of order 12 is a connected and regular graph.

4.2. The Wiener Index

By Definition 7, the Wiener index of $\widetilde{Cay}(D_{12},S)$ is

$$W(\widetilde{Cay}(D_{12}, S)) = \sum_{u,v \in V(\widetilde{Cay}(D_{12},S))} d(u,v)$$

$d(e,a) = 2, d(e,a^2) = 1, d(e,a^3) = 1, d(e,a^4) = 1, d(e,a^5) = 2, d(e,b) = 1, d(e,ab) = 1,$

$d(e,a^2b) = 1, d(e,a^3b) = 1, d(e,a^4b) = 1, d(e,a^5b) = 1, d(a,a^2) = 2, d(a,a^3) = 1,$

$d(a,a^4) = 1, d(a,a^5) = 1, d(a,b) = 1, d(a,ab) = 1, d(a,a^2b) = 1, d(a,a^3b) = 1,$

$d(a,a^4b) = 1, d(a,a^5b) = 1, d(a^2,a^3) = 2, d(a^2,a^4) = 1, d(a^2,a^5) = 1, d(a^2,b) = 1,$

$d(a^2,ab) = 1, d(a^2,a^2b) = 1, d(a^2,a^3b) = 1, d(a^2,a^4b) = 1, d(a^2,a^5b) = 1, d(a^3,a^2) = 2,$

$d(a^3,a^4) = 2, d(a^3,a^5) = 1, d(a^3,b) = 1, d(a^3,ab) = 1, d(a^3,a^2b) = 1, d(a^3,a^3b) = 1,$

$d(a^3,a^4b) = 1, d(a^3,a^5b) = 1, d(a^4,a^5) = 2, d(a^4,b) = 1, d(a^4,ab) = 1, d(a^4,a^2b) = 1,$

$d(a^4,a^3b) = 1, d(a^4,a^4b) = 1, d(a^4,a^5b) = 1, d(a^5,b) = 1, d(a^5,ab) = 1, d(a^5,a^2b) = 1,$

$d(a^5,a^3b) = 1, d(a^5,a^4b) = 1, d(a^5,a^5b) = 1, d(b,ab) = 2, d(b,a^2b) = 1, d(b,a^3b) = 1,$

$d(b,a^4b) = 1, d(b,a^5b) = 2, d(ab,a^2b) = 2, d(ab,a^3b) = 1, d(ab,a^4b) = 1,$

$d(ab,a^5b) = 1, d(a^2b,a^3b) = 2, d(a^2b,a^4b) = 1, d(a^2b,a^5b) = 1, d(a^3b,a^4b) = 2,$

$d(a^3b,a^5b) = 1, d(a^4b,a^5b) = 2.$

Therefore, $W(\widetilde{Cay}(D_{12}, S)) = 80$.

4.3. The Mean Distance

By Definition 8, the mean distance of $\widetilde{Cay}(D_{12}, S)$

$$\sigma(\widetilde{Cay}(D_{12}, S)) = \frac{W(\widetilde{Cay}(D_{12}, S))}{\binom{n}{2}} = \frac{2W(\widetilde{Cay}(D_{12}, S))}{n(n-1)}$$

$$= \frac{2(80)}{12(12-1)} = \frac{40}{33}$$

Conclusion

In this paper, the construction of the prime power Cayley graph of the dihedral group of order 12 is presented.it is found that this graph not complete. Then, the Wiener index and the mean distance of this graph are computed. Therefore, the Wiener index of $\widetilde{Cay}(D_{12}, S)$ is 80 while the mean distance of $\widetilde{Cay}(D_{12}, S)$ is $\frac{40}{33}$.

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