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The Energy of the Cayley Graph Associated to the Dihedral Group of Order Six with Subsets of Order Three

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ABSTRACT

The Hückel Molecular Orbital (HMO) theory, which was used to calculate the energy associated with π-electron orbitals in molecules, is where the idea of graph energy first originated. In this research, subsets of order three are used to compute the energy of Cayley graphs associated with dihedral groups of orders six. The method involves constructing the Cayley graph for each subset of the dihedral group and then determining the corresponding adjacency matrices to obtain the eigenvalues. These eigenvalues are then used to compute the energy of the graphs. The findings indicate that two types of Cayley graphs are identified within the dihedral group of order six, using subsets of order three. The energies calculated for these two graphs are 8 and 6, respectively.

Keywords: Cayley graph, energy of graph, dihedral group, graph theory, group theory

INTRODUCTION

Arthur Cayley first proposed the idea of Cayley graphs in 1878. A graph known as a Cayley graph is one whose vertices represent the members of a group G. If and only if there is an element s in a subset S of G such that the product of s and v_1 equals v_2, then there is an edge connecting two vertices in G, v_1 and v_2. The subset S has the inverse-closed property, which indicates that for each element in S, its inverse under the group operation is also included in S. It also excludes the identity member of G. $Cay(G, S)$ is the standard notation for the Cayley graph of G related to the subset S (Beineke & Wilson, 2004).

Cayley graphs have a wide range of real-world applications across various fields, including computer science, biology, and chemistry. In chemistry, for instance, they are utilized to track atoms through reaction pathways, offering valuable insights into the structural evolution of molecules. Through the years, many researchers show significant interest in this field. For example, Adiga and Ariamanesh (2012) specifically focused on Cayley graphs associated with symmetric groups. Additionally, Ramaswamy and Veena (2009) obtained the energy of the unitary Cayley graphs, which was extended from Balakrishnan (2004).

The concept of graph energy was first explored by Gutman (1978). He defined the energy of a graph as the sum of the absolute values of the eigenvalues of its adjacency matrix, drawing inspiration from the Hückel Molecular Orbital (HMO) theory proposed in the 1930s by Hückel.

Chemists have used the Hückel Molecular Orbital Theory to estimate the energy levels associated with π-electron orbitals in conjugated hydrocarbons. The study of graph energy also has significant scientific applications. For instance, it has been employed to model protein properties (Wu et al., 2015) and used to look into the genetic reason of Alzheimer's Disease (Daianu et al., 2015).

Using subsets of order three, the energy of Cayley graphs connected to the order six dihedral groups is calculated in this study. The methodology involves generating the Cayley graphs using the subset S, determining the adjacency matrices, and then obtaining the eigenvalues of these matrices to compute the energy of the Cayley graphs obtained.

This paper has the following structure. The first part summarizes previous work on Cayley graphs and their associated energy. Then, the next section presents the preliminary results used in this study. Subsequently, we provide the main results in the form of theorems. In the end, we conclude with a summary of the main findings.

MATERIALS AND METHODS

In this section, some definitions that are used in this research are included, utilizing concepts from graph theory, group theory, and linear algebra.

Definition 1 (Gallian, 1994) Dihedral Groups
The dihedral group of order $2n$, denoted by D_{2n}, is the group of symmetries of an n-gon. These symmetries include rotations, denoted by a, and reflections, denoted b. The group presentation is $D_{2n} = \langle a, b \mid a^n = b^2 = 1 \; and \; bab = a^{-1} \rangle$.

Definition 2 (Beineke and Wilson, 2004) Cayley Graph of a Group
Let G be a finite group with identity 1. Let S be a subset of G such that $1 \notin S$ and that $S = S^{-1}$; in other words, $s \in S$ if and only if $s^{-1} \in S$. The following is the definition of the Cayley graph $Cay(G, S)$ on G with subset S:

- the elements of G are the vertices.
- there is an edge joining v_1 and v_2 if and only if $v_2 = sv_1$ for some $s \in S$.

The set of edges is denoted as $E\big(Cay(G, S)\big) = \Big\{\{v_{i,} v_{i,}\} | v_i \text{ is adjacent to } v_j\Big\}$.
Remark: The relation between the two vertices can also be rewritten as $v_2 v_1^{-1} = s$ for some $s \in S$.

Definition 3 (Bondy & Murty, 1982) Bipartite Graph and Complete Bipartite Graph
Bipartite graphs are those whose vertex set is split into two separate subsets, X and Y, so that every edge has a single end in X as well as one end in Y. This type of partition (X, Y) is known as a bipartition of the graph. A full bipartite graph is a simple bipartite graph with bipartition (X, Y) where every vertex of X is connected to every vertex of Y; such a graph is represented by $K_{m,n}$ if $|X| = m$ and $|Y| = n$.

Definition 4 (Bapat, 2010) Adjacency Matrix
Let R is a graph, then $E(R) = \{e_1, e_2, \dots, e_m\}$ and $V(R) = \{1, 2, \dots, n\}$. The adjacency matrix of R is the $n \times n$ matrix with the following definition, indicated by $A(R)$: $V(R)$ indexes both the rows and the columns of $A(R)$. When i is not equal to j, the (i, j)-entry of $A(R)$ is 0 for vertices i and j that are not adjacent, and it is 1 for vertices i and j that are adjacent. For $i = 1, 2, \dots, n$, the (i, i)-entry of $A(R)$ is 0.

Definition 5 (Bapat, 2010) Eigenvalues of a Matrix
The roots of the characteristic equation $det(A - \lambda I) = 0$ of A are called the eigenvalues of A.

Definition 6 (Bapat, 2010) Energy of a Graph
Consider R to be a graph and $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of R. The energy of R, $\varepsilon(R)$, is defined as follows:

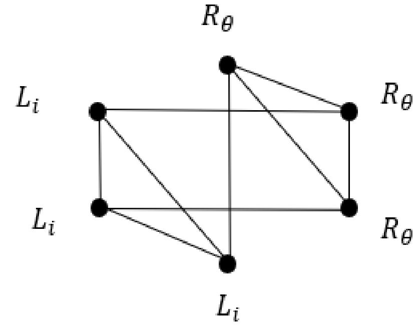
$$\varepsilon(R) = \sum_{i=1}^{n} |\lambda_i|.$$

RESULTS AND DISCUSSION

In this section, the primary results are presented through various theorems. The Cayley graphs associated with the dihedral groups $D_6$and subsets S of order three are constructed, followed by the calculation of their energy.

The Cayley Graph Associated to the Dihedral Group of Order Six with Subsets of Order Three
In this section, Cayley graphs associated with the dihedral group of order six and subsets SSS of order three are constructed. From Definition 1, $D_6 = \langle R_0, R_{120}, R_{240}, L_1, L_2, L_3 \rangle$. By Definition 2, the subsets of order three of D_6 are $\{L_1, R_{120}, R_{240}\}, \{L_2, R_{120}, R_{240}\}, \{L_3, R_{120}, R_{240}\}$ and $\{L_1, L_2, L_3\}$. The following two theorems give the outcomes for these Cayley graphs.

Theorem 1 Let D_6 be the dihedral group of order six. Then the Cayley graph of D_6 with subsets of order 3 consisting of one reflection and two rotations $S = \{L_i, R_{120}, R_{240}\}$, $i \in \{1,2,3\}$, $Cay(D_6, S)$ is as shown in Figure 1.



where $i \in \{1,2,3\}$ and $\theta \in \{0, 120, 240\}$.
Figure 1: The Cayley graph of D_6 with the subset $\{L_i, R_{120}, R_{240}\}$

Proof Let D_6 be the dihedral group of order six, $D_6 = \langle R_0, R_{120}, R_{240}, L_1, L_2, L_3 \rangle$, and $Cay(D_6, S)$ be the Cayley graph of D_6 with subsets S of order three, namely $\{L_1, R_{120}, R_{240}\}, \{L_2, R_{120}, R_{240}\}$ and $\{L_3, R_{120}, R_{240}\}$. According to Definition 2, $V(Cay(D_6, \{L_i, R_{120}, R_{240}\})) = D_6 = \langle R_0, R_{120}, R_{240}, L_1, L_2, L_3 \rangle$ is the vertex set of the Cayley graph. Next, to determine the edges of the graph, the Cayley table of D_6 (Table 1) is used. The vertices v_1 and v_2 are connected by an edge according to Definition 2 if and only if $v_2 = sv_1$ for $s \in \{L_i, R_{120}, R_{240}\}$, and v_1, v_2 in D_6, or in short $v_2 = L_1 v_1$.

Table 1: The Cayley table of D_6

	R_0	R_{120}	R_{240}	L_1	L_2	L_3
R_0	R_0	R_{120}	R_{240}	L_1	L_2	L_3
R_{120}	R_{120}	R_{240}	R_0	L_3	L_1	L_2
R_{240}	R_{240}	R_0	R_{120}	L_2	L_3	L_1
L_1	L_1	L_2	L_3	R_0	R_{120}	R_{240}
L_2	L_2	L_3	L_1	R_{240}	R_0	R_{120}
L_3	L_3	L_1	L_2	R_{120}	R_{240}	R_0

The edge set of the Cayley graph $E(Cay(D_6, \{L_i, R_{120}, R_{240}\}))$ is then obtained. Hence, by Definition 2, the Cayley graph of D_6 with the subset $\{L_i, R_{120}, R_{240}\}$ can be drawn as in Figure 1. □

Theorem 2 Let D_6 be the dihedral group of order six and $Cay(D_6, \{L_1, L_2, L_3\})$ be the Cayley graph of D_6 with the subset $\{L_1, L_2, L_3\}$. Then, $Cay(D_6, \{L_1, L_2, L_3\}) = K_{3,3}$, where $K_{3,3}$ is the complete bipartite graph.

Proof Let D_6 be the dihedral group of order six, $D_6 = \langle R_0, R_{120}, R_{240}, L_1, L_2, L_3 \rangle$, and $Cay(D_6, S)$ be the Cayley graph of D_6 with subsets S of order three, namely $\{L_1, L_2, L_3\}$. According to Definition 2, $V(Cay(D_6, \{L_1, L_2, L_3\})) = D_6 = \langle R_0, R_{120}, R_{240}, L_1, L_2, L_3 \rangle$ is the vertex set of the Cayley graph. Next, to determine the edges of the graph, the Cayley table of D_6 (Table 1) is used. The vertices v_1 and v_2 are connected by an edge according to Definition 2 if and only if $v_2 = sv_1$ for $s \in \{L_1, L_2, L_3\}$, and v_1, v_2 in D_6, or in short $v_2 = L_1 v_1$. Thus, the edge set of the Cayley graph, $E(Cay(D_6, \{L_1, L_2, L_3\})) = \{\{L_1, R_0\}, \{L_2, R_{120}\}, \{L_3, R_{240}\}, \{L_2, R_0\}, \{L_3, R_{120}\}, \{L_1, R_{240}\}, \{L_3, R_0\}, \{L_1, R_{120}\}, \{L_2, R_{240}\}\}$. Hence, by Definition 2, the Cayley graph of D_6 with the subset $\{L_1, L_2, L_3\}$ can be drawn as in Figure 2.

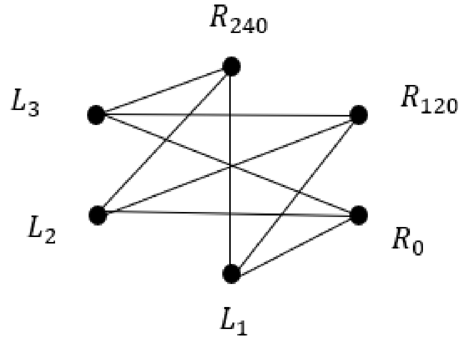


Figure 2: The Cayley graph of D_6 with the subset $\{L_1, L_2, L_3\}$. □

The Energy of the Cayley Graph Associated to the Dihedral Group of Order Six with Subsets of Order Three

This section focuses on computing and presenting the energy of the Cayley graph related to the dihedral group of order six, using subsets of order three.

Theorem 3 Let D_6 be the dihedral group of order six. Then, the energy of the Cayley graph of D_6 with the subsets S of order three for $\{L_1, R_{120}, R_{240}\}$, $\{L_2, R_{120}, R_{240}\}$ and $\{L_3, R_{120}, R_{240}\}$, $\varepsilon(Cay(D_6, S)) = 8$.

Proof Let R be a graph, D_6 be the order six dihedral group and $Cay(D_6, S)$ be the Cayley graph of D_6 with the subset S of order three. First, let $S = \{L_1, R_{120}, R_{240}\}$. The adjacency matrix's Definition 4 states that the rows and columns of $A(R)$ are indexed by $V(R)$, specifically $v_1, v_2, v_3, v_4, v_5, v_6$ where $v_1 = R_0, v_2 = R_{120}, v_3 = R_{240}, v_4 = L_1, v_5 = L_2, v_6 = L_3$. The corresponding adjacent vertices have the entry 1, otherwise, the entries are 0. Thus, the adjacency matrix of $Cay(D_6, \{L_1\})$ is obtained as follows:

$$A(R) = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \end{array} \begin{array}{c} \begin{array}{cccccc} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 \end{array} \\ \begin{bmatrix} 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \end{bmatrix} \end{array}.$$

Next, $A(R)$'s characteristic polynomial,

$$f(A(R), \lambda I) = det(A(R) - \lambda I) = \begin{vmatrix} -\lambda & 1 & 1 & 1 & 0 & 0 \\ 1 & -\lambda & 1 & 0 & 1 & 0 \\ 1 & 1 & -\lambda & 0 & 0 & 1 \\ 1 & 0 & 0 & -\lambda & 1 & 1 \\ 0 & 1 & 0 & 1 & -\lambda & 1 \\ 0 & 0 & 1 & 1 & 1 & -\lambda \end{vmatrix} = \lambda^2(\lambda - 1)(\lambda + 2)^2(\lambda - 3).$$

By Definition 5, the eigenvalues are $\lambda_1 = 0$ with multiplicity 2, $\lambda_2 = 1$ with multiplicity 1, $\lambda_3 = -2$ with multiplicity 2 and $\lambda_4 = 3$ with multiplicity 1. By Definition 6, the energy of $Cay(D_6, \{L_1\})$, $\varepsilon(Cay(D_6, \{L_1, R_{120}, R_{240}\})) = 2|0| + |1| + 2|-2| + |3| = 8$. The proof for $\varepsilon(Cay(D_6, \{L_2, R_{120}, R_{240}\}))$ and $\varepsilon(Cay(D_6, \{L_3, R_{120}, R_{240}\}))$ is similar as $\varepsilon(Cay(D_6, \{L_1, R_{120}, R_{240}\}))$. Hence, the energy of the Cayley graph of D_6 with subset S of order three, $\varepsilon(Cay(D_6, S)) = 8$. □

Theorem 4 Let D_6 be the dihedral group of order six and $Cay(D_6, \{L_1, L_2, L_3\})$ be the Cayley graph of D_6 with the subset $\{L_1, L_2, L_3\}$. Then, the energy of $Cay(D_6, \{L_1, L_2, L_3\})$, $\varepsilon(Cay(D_6, \{L_1, L_2, L_3\})) = 6$.

Proof Let R be a graph, D_6 be the dihedral group of order six and $Cay(D_6, S)$ be the Cayley graph of D_6 with the subset $S = \{L_1, L_2, L_3\}$. The adjacency matrix's Definition 4 states that the rows and columns of $A(R)$ are indexed by $V(R)$, specifically $v_1, v_2, v_3, v_4, v_5, v_6$ where $v_1 = R_0, v_2 = R_{120}, v_3 = R_{240}, v_4 = L_1, v_5 = L_2, v_6 = L_3$. The corresponding adjacent vertices have the entry 1, otherwise, the entries are 0. Thus, the adjacency matrix of $Cay(D_6, \{L_1, L_2, L_3\})$ is obtained as follows:

$$A(R) = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \end{array} \begin{array}{c} \begin{array}{cccccc} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 \end{array} \\ \begin{bmatrix} 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \end{bmatrix} \end{array}.$$

Next, $A(R)$'s characteristic polynomial,

$$f(A(R),\lambda I) = det(A(R) - \lambda I) = \begin{vmatrix} -\lambda & 0 & 0 & 1 & 1 & 1 \\ 0 & -\lambda & 0 & 1 & 1 & 1 \\ 0 & 0 & -\lambda & 1 & 1 & 1 \\ 1 & 1 & 1 & -\lambda & 0 & 0 \\ 1 & 1 & 1 & 0 & -\lambda & 0 \\ 1 & 1 & 1 & 0 & 0 & -\lambda \end{vmatrix} = \lambda^4(\lambda - 3)(\lambda + 3).$$

By Definition 5, the eigenvalues are $\lambda_1 = 0$ with multiplicity 4, $\lambda_2 = 3$ with multiplicity 1 and $\lambda_3 = -3$ with multiplicity 1. By Definition 6, the energy of $Cay(D_6, \{L_1, L_2, L_3\})$, $\varepsilon\big(Cay(D_6, \{L_1, L_2, L_3\})\big) = 4|0| + |3| + |-3| = 6.$ □

CONCLUSION

As a conclusion, the results show that two types of Cayley graphs are identified within the dihedral group of order six, using subsets of order three. The energies calculated for these two graphs are 8 and 6, respectively.

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