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Research Article

Permanents of Hexagonal and Armchair Chains

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The permanent is important invariants of a graph with some applications in physics. If G is a graph with adjacency matrix $A = [a_{ij}]$, then the permanent of A is defined as $\operatorname{perm}(A) = \sum_{\sigma \in S_n} \prod_{i=1}^n a_{i\sigma(i)}$, where S_n denotes the symmetric group on n symbols. In this paper, the general form of the adjacency matrices of hexagonal and armchair chains will be computed. As a consequence of our work, it is proved that if G[k] and H[k] denote the hexagonal and armchair chains, respectively, then $\operatorname{perm}(A(G[1])) = 4$, $\operatorname{perm}(A(G[k])) = (k+1)^2$, $k \ge 2$, and $\operatorname{perm}(A(H[k])) = 4^k$ with $k \ge 1$. One question about the permanent of a hexagonal zig-zag chain is also presented.

1. Introduction

Throughout this paper, all graphs are simple and finite. Suppose X is such a graph and $V(X) = \{u_1, u_2, \ldots, u_n\}$ is the set of all vertices of X. Two vertices of X are assumed to be adjacent, if there is an edge connecting them. Define a zero-one matrix $A = A(G) = [a_{ij}]$ in such a way that $a_{ij} = 1$ if and only if there is an edge connecting v_i and v_j . The adjacency matrix is a very important tool for introducing a graph to a computer. It records all information regarding the graph under consideration. We refer to the famous book of Biggs [1] for important properties of this matrix.

A perfect matching of a simple graph X is a subset $L \subseteq E(X)$ such that end vertices of all edges in L are different, and they coincide with the vertex set of X [2].

Suppose G is a graph with an adjacency matrix $A = [a_{ij}]$. The permanent of A is defined as perm $(A) = \sum_{\sigma \in S_n} \prod_{i=1}^n a_{i\sigma(i)}$, where S_n denotes the symmetric group on n symbols. In a recent interesting paper, Bohra and Reddy [3] computed the number of matrices M for which perm $(M) \equiv x \pmod{n}$, where x is a given integer. By permanent of a graph, we consider the permanent of its adjacency matrix.

A 2-connected graph is a connected graph with this property that at least two vertices must be removed to make it

disconnected. Following Xu and Zhang [4], a hexagonal chain is a connected plane graph with no cut vertices in which every interior region is bounded by a regular hexagon such that two hexagons are either disjoint or have exactly one common edge, no three hexagons share a common vertex, and each hexagon is adjacent to two other hexagons, with the exception of exactly two terminal hexagons to which a single hexagon is an adjacent. For more information about hexagonal systems and its applications in chemistry, we refer interested readers to consult the famous book of Cyvin and Gutman [5].

In this paper, we consider the hexagonal chain G[k], Figure 1, the armchair chain H[k], Figure 2, and a zig-zag hexagonal chain I[2k+1], Figure 3, where G[k] and H[k] have exactly k hexagons and the zig-zag hexagonal chain I[2k+1] has exactly 2k+1 hexagons. The adjacency matrices and permanents of G[k] and H[k] are computed, but we obtained a recurrence relation of order 2 for the zig-zag hexagonal chain I[2k+1] which is not solvable. We refer our interested readers to consult the paper [6] for more information about hexagonal chains.

Our notations here are standard, and the readers can consult the famous book of Biggs [1] for more information on this topic. We refer the interested readers to study [7, 8] for counting perfect matchings of hexagonal systems.

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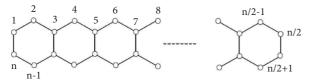


FIGURE 1: The hexagonal chain G[k].

FIGURE 2: The armchair chain H[k].

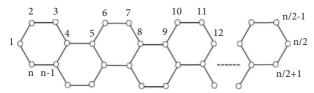


Figure 3: The zig-zag hexagonal chain I[2k+1].

2. Adjacency Matrix and Permanent of G[k]

It is easy to see that G[k] has exactly n = 6 + 4(k - 1) vertices. Suppose $A(G[k]) = [a_{ij}]$ is the adjacency matrix of the graph G[k]. In our labeling of G[k], the vertex i is adjacent with the vertex i + 1, $1 \le i \le n - 1$, and the vertex 1 is adjacent to the vertex n. Moreover, the vertices i and j such that i + j = n + 1 will be adjacent. In a simple form, the vertices i and j are adjacent if and only if |i - j| = 1 or i + j = n + 1. Note that by adding one hexagon to G[k], the number of vertices will be increased by 4. The form of the adjacency matrix of G[k] is as follows:

To compute the permanent of this matrix, we need to calculate the permanent of two matrices $E_{n\times n}$, $n\ge 3$, and $F_{n\times n}$, $n\ge 5$. In both of these matrices, n is assumed to be an odd number. In the matrix $E_{n\times n}$, the entries in the positions (i,i) for $1\le i\le n$, (i+1,i) for $1\le i\le n-1$, and (i,n+1-i) for $1\le i\le n+1/2$ are equal to one, and other entries are 0. In the

matrix $F_{n\times n}$, the entries in the positions (i,i) for $1 \le i \le n$, (i,i+1) for $1 \le i \le n-1$, and (n+1-i,i) for $(n+1)/2 \le i \le n$ are equal to one, and other entries are 0. These matrices have the following forms:

$$E_{n\times n} = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 & 1 \\ 1 & 1 & 0 & \dots & 1 & 0 \\ 0 & 1 & \dots & 1 & 0 & 0 \\ \vdots & & & & & \\ 0 & 0 & \dots & 1 & 1 & 0 \\ 0 & 0 & 0 & \dots & 1 & 1 \end{bmatrix},$$

$$F_{n\times n} = \begin{bmatrix} 1 & 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & 1 & \dots & 0 & 0 \\ 0 & 0 & \dots & 1 & 0 & 0 \\ \vdots & & & & & \\ 0 & 1 & 0 \dots & 0 & 1 & 1 \\ 1 & 0 & 0 & \dots & 0 & 1 \end{bmatrix}.$$

$$(2)$$

Lemma 1. $perm(E_{n \times n}) = (n+1)/2$, *n* is odd.

Proof. We proceed by induction on n with step 2. If n = 3, then a simple calculation shows that $\operatorname{perm}(E_{3\times 3}) = 2$. By our inductive assumption, $\operatorname{perm}(E_{(n-2)\times (n-2)}) = (n-1)/2$, when $n \ge 5$. We now expand the matrix $E_{n\times n}$ through the first row to obtain two matrices A and B as follows:

$$A = \begin{bmatrix} 1 & 0 & \dots & 1 & 0 \\ 1 & 1 & \dots & 1 & 0 & 0 \\ \vdots & & & & & \\ 0 & \dots & 1 & 1 & 0 \\ 0 & 0 & \dots & 1 & 1 \end{bmatrix},$$

$$B = \begin{bmatrix} 1 & 1 & 0 & \dots & 1 \\ 0 & 1 & \dots & 1 & 0 \\ \vdots & & & & & \\ 0 & 0 & \dots & 1 & 1 \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix}.$$
(3)

Since n is odd, perm $(E_{n\times n})=$ perm (A)+ perm (B). The matrix B is unitriangular, and so its permanent is 1. We now expand the matrix A through the last column to obtain another matrix A' with the same permanent. Therefore, $A'=E_{(n-2)\times(n-2)}$, and by inductive assumption, perm $(E_{n\times n})=(n-1)/2+1=(n+1)/2$, proving the lemma.

Lemma 2. $perm(F_{n \times n}) = (n+1)/2$, *n* is odd.

Proof. Similar to the proof of Lemma 1, we proceed by induction with step 2. By an easy calculation, $\operatorname{perm}(F_{5\times 5}) = 3$. By our inductive assumption, $\operatorname{perm}(F_{(n-2)\times (n-2)}) = ((n-2)+1)/2 = (n-1)/2, n \ge 7$. We now expand the matrix $F_{n\times n}$ through the first row to obtain two matrices C and D as follows:

$$C = \begin{bmatrix} 1 & 1 & \dots & 0 & 0 \\ 0 & \dots & 1 & 0 & 0 \\ \vdots & & & & \\ 1 & 0 & \dots & 0 & 1 & 1 \\ 0 & 0 & \dots & 0 & 1 \end{bmatrix},$$

$$D = \begin{bmatrix} 0 & 1 & \dots & 0 & 0 \\ 0 & 1 & 1 & \dots & 0 & 0 \\ \vdots & & & & & \\ 0 & 0 & \dots & 0 & 1 & 1 \\ 1 & 0 & & & 0 & 1 \end{bmatrix}.$$

$$(4)$$

If we expand the matrix D through its first column, we will have a triangular matrix with permanent one, and if expand the matrix C through its last row, then we will have another matrix C' which is equal to $F_{(n-2)\times(n-2)}$. Therefore, perm $(F_{n\times n}) = \text{perm}(C) + \text{perm}(D) = (n-1)/(2) + 1 = (n+1)/(2)$, proving the lemma.

Lemma 3. Suppose $n \equiv 2 \pmod{4}$ is a positive integer greater than or equal to 10. Then, perm(A(G[k])) = perm(A(G[k-1])) - n/2 - 4.

Proof. Expand the matrix A(G[k]) through the first row to obtain two matrices in which the first matrix is related to the second column, and another one is related to the n-th column. These matrices have the following form:

$$M = \begin{bmatrix} 1 & 1 & 0 & 0 & . & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & . & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & . & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & . & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & . & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & . & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & . & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & . & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & . & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & . & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & . & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & . & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & . & . & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & . & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & . & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & . & 0 & 0 & 1 & 0 \end{bmatrix}.$$

$$(5)$$

L 1 0 0 0 0 . 0 0 0 1 .

Our main proof will consider the methods for computing the permanent of L and M.

2.1. Computing the Permanent of L. To compute perm (L), we expand the matrix L through its first row to construct matrices B and C as follows:

$$B = \begin{bmatrix} 0 & 1 & 0 & . & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & . & 0 & 0 & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & . & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & . & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & . & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & . & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & . & 1 & 0 & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & . & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & . & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

$$(6)$$

Since B has a unique nonzero entry in the last row, we expand B through its last row to obtain a new matrix B'. The matrix B' has a unique nonzero entry in its last column, and by expanding it through this column, the matrix A(G[k-1]) will be obtained. For the matrix C, we first expand it through the first column and next expand the new matrix through its last column to find the matrix C' as follows:

$$C' = \begin{bmatrix} 1 & 0 & . & 0 & 0 & 1 & 0 \\ 0 & 1 & . & 0 & 0 & 0 & 0 \\ 1 & 0 & . & 1 & 0 & 0 & 0 \\ . & . & . & . & . & . & . \\ 0 & 1 & . & 0 & 1 & 0 & 0 \\ 0 & 0 & . & 1 & 0 & 1 & 0 \\ 0 & 0 & . & 0 & 1 & 0 & 1 \end{bmatrix}$$
 (7)

Note that C' is a matrix of size $(n-4) \times (n-4)$, and by our assumption, it can be assumed that n=4k-2. We now prove that $\operatorname{perm}(C')=\operatorname{perm}(E_{(2k-1)\times(2k-1)}), \quad k\geq 2$. To do this, we proceed by induction with step 4. We start by n=10. By our algorithm for constructing the matrix C', it can be easily seen that

$$C' = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \end{bmatrix}.$$
 (8)

We now expand C' through its second row, the new matrix through its third row, and the resulting matrix through its fourth row to construct the matrix.

$$C'' = E_{3\times 3} = \begin{bmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}. \tag{9}$$

With permanent 2 = perm(C'). Suppose that n = 4k - 2. By our discussion above, C' has the size $(4k-6) \times (4k-6)$. We do the following operations on C' to construct $E_{(2k-1)\times(2k-1)}, k \ge 2.$

- (a) Expand the matrix C' through its second row to construct the matrix C_2
- (b) Expand the matrix C_2 through its third row to construct the matrix C_3
- (c) Expand the matrix C_{4k-7} through its 4k-8-th row to construct the matrix C_{4k-6}

algorithm $C_{4k-6}=E_{(2k-1)\times(2k-1)}.$ We now apply Lemma 1 to deduce that perm $(C)=\operatorname{perm}\left(E_{2k-1\times2k-1}\right)=k,k\geq2.$

- 2.2. Computing the Permanent of M. In a similar argument as (1), we expand the matrix M and its resulting matrices are as follows:
 - (a) Expand the matrix M through its second column to construct the matrix D_2
 - (b) Expand the matrix D_2 through its third column to construct the matrix D_3
 - (c) Expand the matrix D_{2k-1} through its 2k-2-th column to construct the matrix D_{2k}

It can be seen that $D_{2k} = F_{(2k+3)\times(2k+3)}$, and by Lemma 2,

perm
$$(M) = \text{perm}(F_{(2k+1)\times(2k+1)}) = k+1, \quad k \ge 2.$$
 (10)

 $\operatorname{perm}\left(A(G[k])\right) = \operatorname{perm}\left(A(G[k-1])\right) +$ Therefore, perm(L) + perm(M) = perm(A(G[k])) + (n/2) + 4.completes the proof.

Theorem 1. perm(A(G[1])) = 4 and perm(A(G[k])) = $(k+1)^2$, where $k \ge 2$.

Proof. By a simple calculation, one can see that perm(A(G[1])) = 4. By Lemma 3, perm(A(G[k])) =perm (A(G[k-1])) + 2k + 1, and by solving this recursive equation, perm $(A(G[k])) = (k+1)^2$, where $k \ge 2$.

3. Adjacency Matrix and Permanent of H[k]

The aim of this section is to calculate the adjacency matrix and permanent of H[k], Figure 2. It is easy to see that this graph has exactly n = 6k vertices. The adjacency matrix of H[k] is denoted by $A(H[k]) = [b_{ij}]$.

We first calculate the general term of the adjacency matrix. From Figure 2, one can see that $b_{n(n+1)} = 1$, $1 \le i \le n - 1$ 1, other than all values of *i* with $i \neq 6t - 3$ with $1 \leq t \leq k$. Furthermore, $b_{(6t-3)(6t)} = 1$ and $b_{(6t-5)(6t-2)} = 1$, where $1 \le t \le k$. Since the adjacency matrix is symmetric, if $b_{ij} = 1$, then $b_{ji} = 1$. In other cases, $b_{ij} = 0$. Therefore, the adjacency matrix of H[k] is as follows:

Lemma 4. Suppose A(H[k]) is the adjacency matrix of H[k]with n = 6k vertices. Then, perm(A(H[1])) = 4 and $perm(A(H[k])) = 4perm(A(H[k-1])), where k \ge 2.$

Proof. Our proof is by induction on k. The case of k = 1, 2 are we have perm(A(H[1])) = 4 and perm(A(H[2])) = 16. So, we proceed by induction and assume that $k \ge 3$ is a natural number. Suppose perm (A(H[k -1])) = 4perm(A(H[k-2])). In the first row of the matrix A(H[k]), there are two nonzero entries which are b_{12} and b_{14} . To calculate the permanent, we expand the matrix through the first row. Then, we will have two new matrices B_1 and B_2 such that $perm(A(H[k])) = perm(B_1) + perm(B_2)$. We first calculate perm (B_1) . Note that B_1 has a unique nonzero entry on its second row and so by expanding it through this row, it is enough to calculate the permanent of this new matrix. The new matrix has a unique nonzero entry on the third row that

to simplify our calculations, we expand again this new matrix through this row. The resulting matrix D is as follows:

$$D = \begin{bmatrix} 1 & 1 & 0 & 0 & . & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & . & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & . & 0 & 0 & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & . & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & . & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & . & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & . & 0 & 0 & 1 & 0 & 1 & 0 \end{bmatrix}.$$
 (12)

If we expand D through the first row, then we will find two matrices B and C. These matrices can be written as follows:

$$B = \begin{bmatrix} 0 & 1 & 0 & . & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & . & 0 & 0 & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & . & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & . & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & . & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & . & 0 & 1 & 0 & 1 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 & 0 & . & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & . & 0 & 0 & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & . & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & . & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & . & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & . & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & . & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & . & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & . & 0 & 0$$

By expanding B through its first row and expanding the new matrix through its first column, the resulting matrix will be A(H[k-1]). On the other hand, by expanding the matrix C through its first column and expanding the new matrix through its first column, the resulting matrix will be again A(H[k-1]). Therefore, perm (D) = perm(B) + perm(C) = perm(A(H[k-1])) + perm(A(H[k-1])).

We are now ready to calculate perm (B_2) . The second column of B_2 has a unique nonzero entry, and by expanding

it through this column and then expanding this new matrix through its third row, we obtain again the matrix D. This proves that perm(A(H[k])) = 4perm(A(H[k-1])).

Theorem 2. $perm(A(H[k])) = 4^k$, where $k \ge 1$.

Proof. Induct on *k*.

4. Concluding Remarks

In this paper, the adjacency matrices and permanents of a hexagonal and armchair chain were computed. At the end of this section, a zig-zag hexagonal chain I[2k+1], $k \ge 1$, with exact 2k+1 hexagons and n=8k+6 vertices, is investigated.

To calculate the form of the adjacency matrix $A(I[2k+1]) = [c_{ij}]$, we will determine all unit entries c_{ij} such that $i \le j$, and then, all entries will be calculated based on the condition that $c_{ij} = c_{ji}$. Suppose that t = [n/8] + 1. By the labeling of this graph given in Figure 3, one can see that $c_{i(i+1)} = 1$, where $1 \le i \le n - 1$. Furthermore, $c_{1n} = 1$. It is also clear from our figure that $c_{(4i)(n-(4i-3))} = 1$, $i = 1, 2, \ldots, t - 1$. The final set of our unit entries is corresponding to the pairs (4i - 3, n - (4i - 4)), where $i = 2, 3, \ldots, t$. Based on these calculations, the form of the adjacency matrix of I[2k+1] is as follows:

Our calculations with Mathematica [9] and some arguments as Theorems 1 and 2 suggest the following conjecture:

Conjecture 1.
$$perm(A(I[2k+1])) = (3\sqrt{perm(A(I([2k-1])))} - \sqrt{perm(A(I[2k-3]))})^2$$
, where $n \ge 22$.

Moreover, by our calculations with Mathematica on adjacency matrices of small dimensions, we calculate that perm (A(I[3])) = 25, perm (A(I[5])) = 169, perm (A(I[7])) = 1156, perm (A(I[9])) = 7921, perm (A(I[11])) = 54289, and perm (A(I[13])) = 372100. We could not solve the equation of Conjecture 1, but it is possible to apply some techniques in numerical analysis to obtain approximately the permanent. We end this section with the following question:

Question 1. What is the exact value of perm (A(I [2k + 1])).

Data Availability

No data were used in this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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