

WIENER INDEX OF DEGREE SPILTTING GRAPH OF mC_n AND mK_n

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ABSTRACT

The Wiener index $W(G)$ is a distance-based topological invariant much used in the study of the structure-property and the structure-activity relationships of various classes of biochemically interesting compounds introduced by Harold Wiener in 1947. It is defined by the sum of the distances between all (ordered) pairs of vertices of G . In this paper, we obtain Wiener index of degree splitting graph of cyclic snakes mC_n and also complete snakes mK_n obtained from the path using MATLAB.

KEYWORDS: Distance Sum, Path, Cycle, MATLAB

2010 Mathematics Subject Classification: 05C12, 05C85

1. INTRODUCTION

The concept of Wiener index was first proposed by Harold Wiener 50 years ago as an aid to determine the boiling point of paraffin [12]. It is defined as the half sum of the distances between all pairs of vertices of G .

$W(G) = \frac{1}{2} \sum_{u,v} d(u,v)$ Where $d(u,v)$ is the number of edges in a shortest path connecting the vertices u & v in G

$$\text{Notation: } W(G) = \frac{1}{2} \sum_{u,v} d(u,v) = \sum_{u<v} d(u,v)$$

Basic Results

$$1. W(P_n) = \frac{n(n^2 - 1)}{6}$$

$$2. W(C_n) = \begin{cases} \frac{1}{8} n^3 & \text{for } n \text{ even} \\ \frac{1}{8} (n-1)n(n+1) & \text{for } n \text{ odd} \end{cases}$$

$$3. W(K_n) = \frac{n(n-1)}{2}$$

2. DEFINITIONS AND PRELIMINARIES

Our notation is standard and mainly taken from standard books of graph theory [1], [3]. In this paper, we consider finite, nontrivial, simple and undirected graphs. For a graph G , we denote by $V(G)$ and $E(G)$, its vertex and edge sets, respectively.

The **Path** P_n is a tree with two vertices of degree 1 and $(n-2)$ vertices of degree 2. The **distance** $d(u,v)$ between the vertices u and v of the graph G is equal to length of the shortest path that connects u and v .

In 1966 **A. Rosa** has defined mC_n is the connected graph in which m -copies are isomorphic to the cycle C_n [2],[5]. Similarly, mK_n is the connected graph in which m -copies are isomorphic to the complete graph K_n . Recently we have determined the Wiener indices of mC_n and mK_n without using MATLAB [11]

Suppose chemical reaction is represented as the transformation of the chemical graph representing the reaction's substrate into another chemical graph representing the degree splitting, the graph obtained in this manner may or may not exist in reality, but it is in the interest of the chemist to check the characterization of the so obtained new molecular structure. In this paper, we have given program for finding $W(mC_n)$, $W(DS(mC_n))$ and $W(mK_n)$, $W(DS(mK_n))$ with respect to the Adjacency matrix using MATLAB.

Splitting Graph $S(G)$ was introduced by **Sampath Kumar and Walikar**. For each vertex v of a graph G , take a new vertex v' and join v' to all vertices of G adjacent to v : The graph $S(G)$ thus obtained is called the splitting graph of G [6]. In the similar way, **degree splitting graph** $DS(G)$ was introduced by **R. Ponraj and S. Somasundaram**. Let $G = (V; E)$ be a graph with $V = S_1 \cup S_2 \cup \dots \cup S_t \cup T$, where each S_i is a set of vertices having at least two vertices and having the same degree and $T = V - \cup S_i$. The **degree splitting graph of** G denoted by $DS(G)$ is obtained from G by adding vertices w_1, w_2, \dots, w_t and joining w_i to each vertex of S_i ($1 \leq i \leq t$) [4],[7].

Example

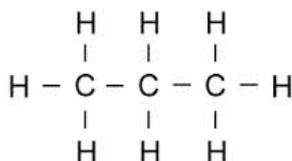


Figure 2.1: Propane $-C_3H_8$



Figure 2.2: P_3

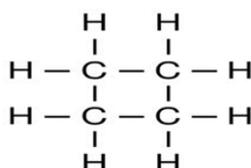


Figure 2.3: Cyclobutane $-C_4H_8$

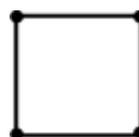


Figure 2.4: C_4

3. WIENER INDEX OF DEGREE SPLITTING GRAPH OF mC_n

Definition: 3.1[9]

A **Triangular Snake** is a graph which is obtained from a path $P_{m+1}:\{v_1,v_2,\dots,v_{m+1}\}$ by joining v_i and v_{i+1} to a new vertex w_i for $i=\{1,2,\dots,m\}$. It is denoted by TS_m , where ‘ m ’ denotes number of blocks in a graph.

Definition: 3.2[8]

A **Quadrilateral Snake Graph QS_m** is obtained from a path $P_{m+1}:\{u_1,u_2,\dots,u_{m+1}\}$ by joining u_i and u_{i+1} to two new vertices a_i and b_i and also joining a_i and b_i for $i=1$ to m



Figure 2.5: - 5C4

Definition: 3.3[11]

Cyclic snake is a graph which is obtained from a path $P_{m+1}:\{u_1,u_2,\dots,u_{m+1}\}$ by joining u_i and u_{i+1} to the initial and terminal vertices of the path of length $n-2$ respectively. It is denoted by mC_n , where ‘ m ’ denotes number of copies in a graph. In other words, each cycle shares two vertices in the chain with an exception of the initial and terminal cycles. i.e. the number of copies in a chain is denoted by m and each cycle of length is n .

Theorem: 3.1[11]

$$\begin{aligned}
 W(mC_n) &= (2n - 3)W(P_{m+1}) + (n - 2)^2 W(P_m) + \frac{1}{2}(n - 2)(n^2 - 2n - 1) \binom{m}{2} + \\
 &2(n^2 - 10n + 27) \binom{m+1}{2} + \left(\frac{1}{8}(n - 4)(n^2 - 1) + 1\right)m \quad \text{when } n \text{ be odd and } n \neq 3 \\
 &= (2n - 3)W(P_{m+1}) + (n - 2)^2 W(P_m) + \frac{n}{2}(n^2 - 4n + 4) \binom{m}{2} + \\
 &\frac{1}{2}(n - 2)^2 \binom{m+1}{2} + \frac{1}{8}(n^3 - 4n^2 + 8) + 1)m \quad \text{When } n \text{ be even}
 \end{aligned}$$

The following MATLAB program illustrates finding Adjacency matrix of degree splitting graph of mC_n with the extension of the earlier finding [11].

```

%%Program for finding Adjacency matrix of degree splitting graph of  $mC_n$ 

m= input ('No.of Copies m=');

n= input ('Cycle with vertices n=');

A= [];

for i=1:(m*n)-m

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A (i, i+1) =1; A (i+1, i) =1;

end

for i=1:n-1:(m*n)-m-n+2

A (i, i+n-1) =1; A (i+n-1, i) =1;

end

for i=1:(m*n)-m+1

A (i, (m*n)-m+2) =1; A ((m*n)-m+2, i) =1;

end

if m>=3&&n>=3

for i=n:n-1:(m*n)-m-n+2

A(i,(m*n)-m+3)=1;A((m*n)-m+3,i)=1;

end

elseif m<3&&n>=3

for i=n:n-1:(m*n)-m-n+2

A(i,(m*n)-m+2)=0;A((m*n)-m+2,i)=0;

end

end

end

A;
    
```

Table 3.1: Values of W (mCn) for 1 ≤ M ≤ 10, 3 ≤ N ≤ 10

W(mCn)		n							
		3	4	5	6	7	8	9	10
m	1	3	8	15	27	42	64	90	125
	2	14	40	78	144	228	352	500	700
	3	37	105	205	376	594	913	1294	1806
	4	76	212	415	748	1176	1796	2536	3524
	5	135	370	715	1285	2010	3050	4290	5935
	6	218	588	1130	2012	3132	4724	6620	9120
	7	329	875	1673	2954	4578	6867	9590	13160
	8	472	1240	2360	4136	6384	9528	13264	18136
	9	651	1692	3207	5583	8586	12756	17706	24126
	10	870	2240	4230	7320	11220	16600	22980	31220

Table 3.2: Values of W (DS (mCn)) for 1 ≤ m ≤ 10, 3 ≤ n ≤ 10

W(DS(mCn))		n							
		3	4	5	6	7	8	9	10
m	1	6	12	20	30	42	56	72	90
	2	20	42	72	112	160	216	280	352
	3	57	115	192	293	413	551	707	881

	4	94	194	328	502	710	950	1222	1526
	5	141	295	502	769	1089	1459	1879	2349
	6	198	418	714	1094	1550	2078	2678	3350
	7	265	563	964	1477	2093	2807	3619	4529
	8	342	730	1252	1918	2718	3646	4702	5886
	9	429	919	1578	2417	3425	4595	5927	7421
	10	526	1130	1942	2974	4214	5654	7294	9134

4. WIENER INDEX OF DEGREE SPLITTING GRAPH OF mK_n

Definition: 4.1[8]

mK_4 snake is a graph obtained from quadrilateral snake graph (QS_m) by joining each u_i to b_i and u_{i+1} to a_i , where $i=1$ to m .

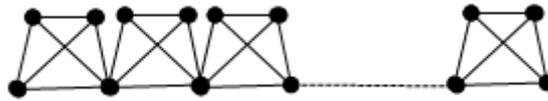


Figure 5: mK_4

Definition: 4.2 [8]

mK_n snake is a graph obtained from mC_n in which all the vertices in a copy are adjacent to each other.

Theorem: 4.1[8]

$$W(mK_n) = \frac{n(n-1)}{2} W(P_{m+1}) + \frac{n^2 - 3n + 2}{2} (W(P_m) + \binom{m}{2})$$

The following MATLAB program illustrates finding Adjacency matrix of degree splitting graph of mK_n with the extension of the earlier finding [10].

```

%%Program for finding Adjacency matrix of degree splitting graph of  $mK_n$ 

m= input ('No.of Copies m=');
n= input ('complete graph with vertices n=');

A= [];

for i=1:(m*n)-m+1

for k=1:m

for i=((k-1)*n)-(k-1)+1:(k*n)-k+1

For j= ((k-1)*n)-(k-1) + 1 :( k*n)-k+1

if i==j

A(i,j)=0;A(j,i)=0;

else
    
```

```

A(i,j)=1;A(j,i)=1;

end

end

end

end

end

for i=1:(m*n)-m+1

A(i,(m*n)-m+2)=1;A((m*n)-m+2,i)=1;

for i=n:n-1:(m*n)-m-n+2

A(i,(m*n)-m+2)=0;A((m*n)-m+2,i)=0;

end

end

if m>=3&&n>=3

for i=n:n-1:(m*n)-m-n+2

A(i,(m*n)-m+3)=1;A((m*n)-m+3,i)=1;

end

elseif m<3&&n>=3

For i=n: n-1:(m*n)-m-n+2

A (i, (m*n)-m+2) =0; A((m*n)-m+2,i)=0;

end

end

end

A;

```

Table 4.1: Values of W (mKn) for $1 \leq m \leq 10$, $3 \leq n \leq 10$

W(mKn)	n							
	3	4	5	6	7	8	9	10
1	3	6	10	15	21	28	36	45
2	14	30	52	80	114	154	200	252
3	37	81	142	220	315	427	556	702
4	76	168	296	460	660	896	1168	1476
5	135	330	530	825	1185	1610	2100	2655
6	218	486	860	1340	1926	2618	3416	4320
7	329	735	1302	2030	2919	3969	5180	6552
8	472	1056	1872	2920	4200	5712	7456	9432
9	651	1458	2586	4035	5805	7896	10308	13041
10	870	1950	3460	5400	7770	10570	13800	17460

Table 4.2: Values of W (DS (mKn)) for $1 \leq m \leq 10, 3 \leq n \leq 10$

W(DS(mKn))		n							
		3	4	5	6	7	8	9	10
m	1	6	10	15	21	28	36	45	55
	2	20	38	62	92	128	170	218	272
	3	57	105	168	246	339	447	570	708
	4	94	180	284	436	606	804	1030	1284
	5	141	277	458	684	955	1271	1632	2038
	6	198	396	660	990	1386	1848	2376	2970
	7	265	537	900	1354	1899	2535	3262	4080
	8	342	700	1178	1776	2494	3332	4290	5368
	9	429	885	1494	2256	3171	4239	5460	6834
	10	526	1092	1848	2794	3930	5256	6772	8478

5. CONCLUSIONS

In this paper, Wiener Index of certain classes of cyclic chain mC_n and mK_n ,

$W (DS (mC_n)), W (DS (mK_n))$ is formulated using MATLAB.

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