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Wiener Polynomial for Tensor Product of Graphs

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Abstract: Wiener Index is a graph invariant introduced originally for molecular graphs of alkanes. All structural formulas of chemical compounds are molecular graphs where vertices represent the set of atoms and edges represent chemical bonds. The construction and investigation of topological indices that could be used to describe molecular structures is one of the important directions of mathematical chemistry. The Wiener Index $W(G)$ of a graph G is defined as the half of the minimum distances between every pair of vertices of G. As such there is no exact formula to determine the value of $W(G)$ though there are some for particular classes of graphs. In this paper we determine Wiener index and polynomial for some Tensor product graphs.

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Keywords: Graph, Tensor Product, Wiener Index, Wiener Polynomial.

1. Introduction

The Wiener number or Wiener Index $W(G)$ is originated from the work of *H.* Wiener [4] as a topological index to study the relation between molecular structure and physical and chemical properties of certain hydrocarbon compounds. It is employed to predict boiling point, molar volumes and large number of physico-chemical properties of alkanes. It is defined as the half-sum of the distances between all ordered pairs of vertices of the graph G.

$$W(G) = \frac{1}{2} \sum_{u,v \varepsilon V(G)} d(u, v)$$

Where $d(u, v)$ is the number of edges in a shortest path connecting the vertices u and v in G.

This number is widely used in computational chemistry to measure some topological properties and in the study of Quantitative Structure Property Relationship (*QSPR*). When G is a path graph P_n, $W(G) = (n^3 - n)/6$ where n denotes the number of vertices of graph G.

Definition 1.1: Tensor product of two graphs G_1 and G_2 is a graph $G(V, E)$ with vertex set $V = \{v_1, v_2, ..., v_n, u_1, u_2, ..., u_m\}$ and edge set $E = \{w_1w_2/u_1u_2 \varepsilon E_1, \& v_1v_2, \varepsilon E_2\}$ where $w_1 = (u_1, v_1)$ and $w_2 = (u_2, v_2)$.

Tensor product of P_m and C_n is (2, 4) biregular graph, tensor product of C_m and C_n is 4-regular and tensor product of P_2 and K_n is a $n - 1$ regular graph. In this paper we consider some tensor product graphs such as $P_3 \wedge C_n$, $C_3 \wedge C_n$ and $P_2 \wedge K_n$ and find Wiener index for them.

2. Construction of Graphs

$P_3 \wedge C_n$ graph is a (2, 4) biregular connected graph when n is odd and a disconnected graph with two components when n is even and each component is a (2, 4) biregular graph. The biregular graph $P_3 \wedge C_n$ is a connection of n cycles with 4 vertices and each cycle has one common vertex with the other cycle.

Algorithm 2.1:

Input: The path graph with 3 vertices and cycle graph with odd number of vertices.

Output: A (2, 4) biregular graph with $3n$ vertices.

Begin

for $i = 1$ to n

$V_1 = \{v_i\}$

for $j = 1$ to $2n$

$V_2 = \{u_j\}$

for $(i = 1, j = 1, i{+}{+}, j = 2)$

$E_1 = \{(v_i, u_j) \cup (v_i, u_{j+1}) \cup (u_j, v_{i+1}) \cup (u_{j+1}, v_{i+1})\}$

$E = E_1 \cup \{(v_1, u_{2n-1}) \cup (v_1, u_{2n})\}$

End

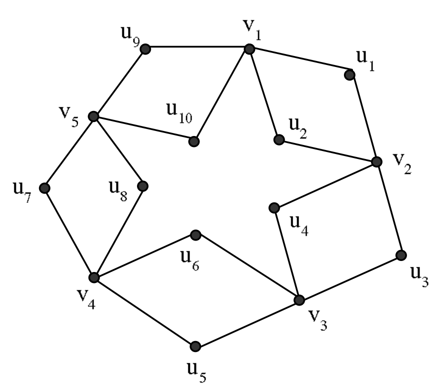

Figure 2.1: $P_3 \wedge C_5$

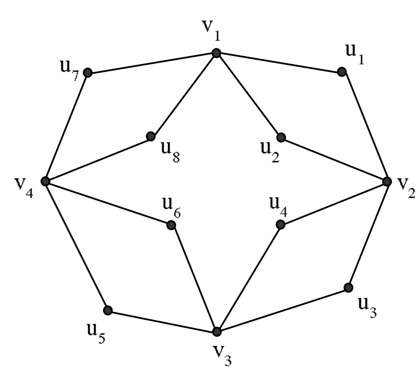

Figure 2.2: One Component of $P_3 \wedge C_8$

The construction of a tensor product of C_3 and C_n contains two parts

(i) Construction of a cycle with $3n$ vertices

(ii) Drawing lines with in the cycle.

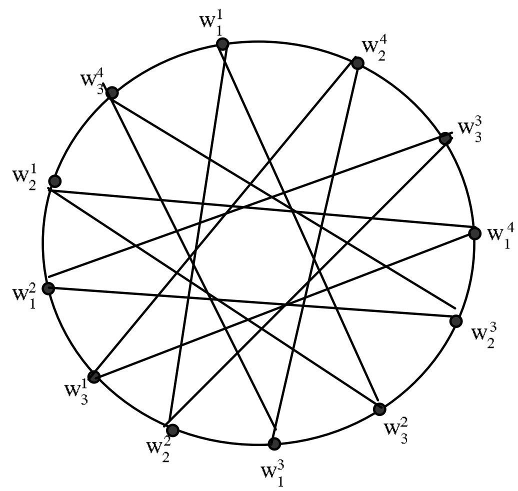

Figure 2.3: $C_3 \wedge C_4$

Algorithm 2.2:

Input: Cycle graph with 3 vertices and Cycle graph with n vertices.

Output: A (2, 4)biregular graph with $3n$ vertices.

Begin

for $i = 1$ to 3

for $j = 1$ to n

$V = \{w_i^j\}$

$E_1 = \{(w_1^1, w_2^n) \cup (w_2^n, w_3^{n-1}) \cup (w_3^{n-1}, w_1^n)\}$

for $k = n$ to 3

$E_2 = \{(w_i^k, w_{i+1}^{k-1}) \cup (w_2^n, w_{i+2}^{k-2}) \cup (w_{i+2}^{k-2}, w_i^{k-1})\}$

$E_3 = \{(w_1^2, w_2^1) \cup (w_3^n, w_1^1)\}$

$E_4 = \{(w_1^1, w_2^2) \cup (w_2^2, w_3^3)\}$

for $k = 2$ to $n - 2$

$E_5 = \{(w_i^k, w_{i+1}^{k+1}) \cup (w_{i+1}^{k+1}, w_{i+2}^{k+2}) \cup (w_{i+2}^{k+2}, w_i^{k+1})\}$

$$E_6 = \{(w_2^n, w_3^1) \cup (w_3^1, w_1^n) \cup (w_1^n, w_2^1) \cup (w_2^1, w_3^2) \cup (w_3^2, w_1^1)\}$$

$$E = E_1 \cup E_2 \cup E_3 \cup E_4 \cup E_5 \cup E_6$$

End

3. Calculation of Wiener Index and Wiener Polynomial

Theorem 3.1: The Wiener Index of a graph $P_3 \wedge C_n$ is $\frac{n}{4}(9n^2 + 7)$, n is odd.

Proof: The vertices of $P_3 \wedge C_n$ can be divided into three categories

(i) Vertices of degree four

(ii) Inner vertices of degree two

(iii) Outer vertices of degree two

The general term of distances between vertices of degree four and all the vertices is

$$n\,[4\,(1 + 3 + 5 + \dots + (n - 2)) + 2\,(2 + 4 + \dots + (n - 1)) + 2n] = \frac{n}{2}\,[3n^2 + 1]$$

The general term of distances between outer vertices of degree two and inner vertices is

$$n\,[2\,(1 + 2 + 3 + \dots + (n - 1) + n] = n^3$$

The general term of distances between inner vertices and outer vertices is

$$n\left[3(2) + 4\left(2 + 3 + \dots + \frac{n-1}{2}\right)\right] = \frac{n(n^2 + 3)}{2}$$

The general term of distances between inner vertices and inner vertices is

$$n\,[4 + 2\,(2 + 3 + \dots + (n - 1) + n] = n\,(n^2 + 2)$$

The general term of distances between outer vertices of degree two and outer vertices of degree two is $n\left[4\left(1 + 2 + \dots + \frac{n-1}{2}\right)\right] = \frac{n(n^2 - 1)}{2}$

$$W(P_3 \wedge C_n) = \frac{1}{2}\left[\frac{n}{2}(3n^2 + 1) + n^3 + \frac{n(n^2 + 3)}{2} + n(n^2 + 2) + \frac{n(n^2 - 1)}{2}\right]$$

$$W(P_3 \wedge C_n) = \frac{n}{4}(9n^2 + 7)$$

Theorem 3.2: The Wiener polynomial for tensor product of P_3 and C_n is

$$W(P_3 \wedge C_n) = 4n(q + q^3 + \ldots + q^{n-2}) + 6nq^2 + 5n(q^4 + q^6 + \ldots + q^{n-1}) + 2nq^n$$

Proof: Since $P_3 \wedge C_n$ (2, 4)biregular graph with n vertices of degree 4 and $2n$ vertices are of degree 2. A vertex of degree 4 gives 4 pair of vertices of distance one and a vertex of degree two gives 2 pair of vertices of distance one, hence the coefficient of q is $\frac{1}{2}$ $[4n + 2(2n)] = 4n$.

A vertex of degree 4 gives 2 pair of vertices of distance two and a vertex of degree 2 gives five pair vertices of distance two including opposite vertices of degree two, hence the coefficient of q^2 is $\frac{1}{2}$ $[2n + 5(2n)] = 6n$.

A vertex of degree 4 gives 4 pair of vertices of distance three and a vertex of degree two gives 2 pair of vertices of distance three, hence the coefficient of q^3 is $\frac{1}{2}$ $[4n + 2(2n)] = 4n$.

A vertex of degree 4 gives 2 pair of vertices of distance four and a vertex of degree 2 gives four pair vertices of distance four, hence the coefficient of q^4 is $\frac{1}{2}$ $[2n + 4(2n)] = 5n$.

Similarly the odd powers of q have coefficient $4n$ and even powers of q have coefficient $5n$ except the coefficient of q^2 and the coefficient of q^n.

In $P_3 \wedge C_n$ the maximum distance between vertices is n, hence the highest degree in the Wiener polynomial is n.

A vertex of degree 4 gives 2 pair of vertices of distance n and a vertex of degree two have exactly one vertex of distance n, hence $\frac{1}{2}$ $[2n + 2n(1)] = 2n$.

Hence $W(P_3 \wedge C_n), q) = 4n(q + q^3 + \ldots + q^{n-2}) + 6nq^2 + 5n(q^4 + q^6 + \ldots + q^{n-1}) + 2nq^n$

Corollary 3.1: Since $W[G] = W'[G; 1]$, where W' denotes the derivative of Wiener polynomial

$$W(P_3 \wedge C_n) = 4n(1 + 3 + \ldots + (n-2)) + 12n + 5n(4 + 6 + \ldots + (n-1)) + 2n^2$$

$$= n(n-1)^2 + 5n\left[\frac{n^2-1}{4} - 2\right] + 12n + 2n^2$$

$$= \frac{4n^3 + 52n + 5n^3 - 45n}{4} = \frac{n(9n^2+7)}{4}$$

Theorem 3.3: The Wiener Index for a tensor product of cycle graphs C_3 and C_n is

$$W(C_3 \wedge C_n) = \frac{3n}{2}\left[n^2 - 2n - 4 + \frac{n}{2} \bmod (3n-5, 8)\right], \quad n > 4 \text{ and } n \text{ is even}$$

$$W(C_3 \wedge C_n) = \frac{3n}{2}\left[n^2 - 4n - 1 + \frac{n-1}{2} \bmod (3n-5, 8)\right],$$

$n > 5$ and n is odd & mod $(3n - 5, 8) \neq 0$

$$W(C_3 \wedge C_n) = \frac{3n(n^2-5)}{2}, \quad 3n - 5 \text{ is a multiple of } 8.$$

Proof: Since $C_3 \wedge C_n$ is a 4-regular graph, each vertex of $C_3 \wedge C_n$ is connected directly to four different vertices. The four different vertices are connected to eight different vertices and these eight vertices are connected to other 8 vertices and so on. In this way we can go from starting vertex to all other vertices of $C_3 \wedge C_n$. Except the first five vertices all the other vertices are divided into group of eight vertices and each group of distances

(i) 2, 3, $(n - 2)/2$ if n is even and $n > 4$,

(ii) 2, 3, …, $(n - 3)/2$ if n is odd and mod $(3n - 5, 8)$ is not equal to zero and

(iii) 2, 3, … , $(n - 1)/2$ if $3n - 5$ is a multiple of 8.

$$W(C_3 \wedge C_n) = \frac{3n}{2}\left[4 + 8\left(2 + 3 + \ldots + \frac{(n-2)}{2}\right) + \bmod (3n-5, 8)\frac{n}{2}\right]$$

$$W(C_3 \wedge C_n) = \frac{3n}{2}\left[n^2 - 2n - 4 + \frac{n}{2} \bmod (3n-5, 8)\right], \ n > 4 \text{ and } n \text{ is even}$$

If n is odd and $n > 5$ then

$$W(C_3 \wedge C_n) = \frac{3n}{2}\left[4 + 8\left(2 + 3 + \ldots + \frac{n-3}{2}\right) + \frac{n-1}{2} \bmod (3n-5, 8)\right]$$

$$W(C_3 \wedge C_n) = \frac{3n}{2}\left[n^2 - 4n - 1 + \frac{n-1}{2} \bmod (3n-5, 8)\right],$$

$n > 5$ and n is odd & mod $(3n - 5, 8) \neq 0$ or

$$W(C_3 \wedge C_n) = \frac{3n}{2}\left[4 + 8\left(2 + 3 + \ldots + \frac{n-1}{2}\right)\right]$$

$$W(C_3 \wedge C_n) = \frac{3n(n^2-5)}{2}, \quad 3n - 5 \text{ is a multiple of } 8.$$

Corollary 3.2: From Wiener index can get Wiener polynomial

$$W(C_3 \wedge C_n) = \frac{3n}{2}\left[4 + 8\left(2 + 3 + \ldots + \frac{(n-2)}{2}\right) + \text{mod}\,(3n-5, 8)\,\frac{n}{2}\right]$$

$$W((C_3 \wedge C_n), q) = \frac{3n}{2}\left[4q + 8\left(q^2 + q^3 + \ldots + q^{\frac{n-2}{2}}\right) + \text{mod}\,(3n-5, 8)\, q^{\frac{n}{2}}\right],$$

$n > 4$ and n is even

$$W(C_3 \wedge C_n) = \frac{3n}{2}\left[4 + 8\left(2 + 3 + \ldots + \frac{n-3}{2}\right) + \frac{n-1}{2}\,\text{mod}\,(3n-5, 8)\right],$$

$n > 5$ and n is odd & mod $(3n - 5, 8) \neq 0$

$$W((C_3 \wedge C_n), q) = \frac{3n}{2}\left[4q + 8\left(q^2 + q^3 + \ldots + q^{\frac{n-3}{2}}\right) + \text{mod}\,(3n-5, 8)\, q^{\frac{n-1}{2}}\right]$$

$$W(C_3 \wedge C_n) = \frac{3n}{2}\left[4 + 8\left(2 + 3 + \ldots + \frac{n-1}{2}\right)\right], \quad 3n - 5 \text{ is a multiple of } 8$$

$$W((C_3 \wedge C_n), q) = \frac{3n}{2}\left[4q + 8\left(q^2 + q^3 + \ldots + q^{\frac{n-1}{2}}\right)\right]$$

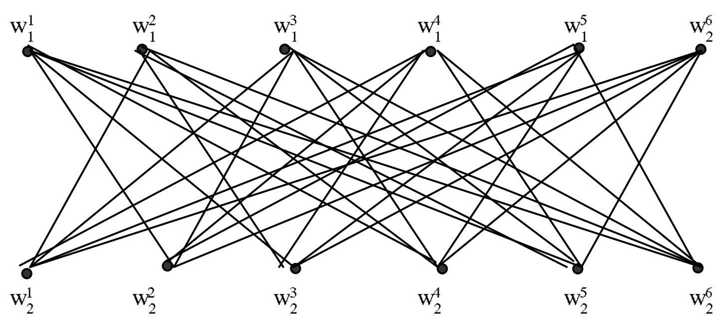

Figure 3.1: $P_2 \wedge K_6$

Theorem 3.4: The Wiener Index of a tensor product of path graph P_2 and the complete graph K_n is $3n^2$**.**

Proof: The tensor product of P_2 and K_n is a $n - 1$ regular graph. Any vertex of $(P_2 \wedge K_n)$ can reach $n - 1$ vertices with distance one. These $n - 1$ vertices can reach other $n-1$ vertices with distances two. Hence from a starting vertex one can cover $2n-2$ vertices. The remaining one vertex can reach by three edges from the starting vertex. Therefore, $W(P_2 \wedge K_n) = \frac{1}{2}[2n((n-1)+(n-1)2+3)] = 3n^2$.

Theorem 3.5: The Wiener polynomial of tensor product of path graph P_2 and complete graph K_n is $W[(P_2 \wedge K_n), q] = n(n-1)q + n(n-1)q^2 + nq^3$.

Proof: Since $(P_2 \wedge K_n)$ is a $(n-1)$-regular graph and it is a bipartite graph with vertex sets V_1 and V_2 with n vertices each.

Each vertex W_1^i in V_1 is connected to $n-1$ vertices W_2^j, in V_2 by an edge and when $i = j$ the distance between W_1^i and W_2^i is 3. The distance between vertices in V_1 is two, similarly in V_2.

Hence $W[(P_2 \wedge K_n), q] = n(n-1)q + n(n-1)q^2 + nq^3$.

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