

Wiener Polynomial of Splitting Graph of Comb Graph

Latha Devi Puli


Associate Professor Government First Grade College, Yelahanka Bangalore, Karnataka, India

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ABSTRACT

The sum of distances between all unordered pairs of vertices in a connected graph is called the Wiener index. In this work, we found the Wiener polynomial and index of splitting graph of comb graph .

Keywords: Graph theory, Wiener index, Wiener polynomial

1. INTRODUCTION

It is well established that the Wiener index W exhibits strong correlations with various physicochemical properties of organic compounds, including boiling point, heat of vaporization, heat of formation, chromatographic retention times, surface tension, and vapor pressure. This relationship can be explained by the observation that the Wiener index is approximately proportional to the van der Waals surface area of a molecule.

Since the biological activity of organic compounds is closely related to their molecular structure, it becomes essential to develop suitable mathematical representations of these structures. Such representations are commonly expressed through molecular descriptors, which quantify specific structural features of molecules. Among these, the Wiener index is one of the earliest and most extensively studied topological descriptors, with significant applications in chemistry.

A representation that captures only the number of elements and their connectivity is referred to as a topological representation. In chemistry, this is often modelled using a molecular graph, where atoms are represented as vertices and covalent bonds as edges.

Let G be a graph, and let u and v be two vertices of G . If $d(u, v)$ denotes the length of the shortest path between u and v , then the Wiener index of G is defined as: $W(G) = \sum_{u, v \in V(G)} d(u, v)$,

where the summation is taken over all unordered pairs of vertices in G .

The Wiener polynomial is a related generating function which was first defined by Haruo Hosoya [7] with this name, in honor of Harry Wiener but also known today as Hosoya polynomial, extends this concept to capture the complete distribution of distances in graph. If q is a parameter, then the Wiener polynomial of G is $W(G; q) = \sum_{\{u, v\} \subseteq V(G)} q^{d(u, v)}$

This paper gives the expressions for Wiener polynomial of Splitting graph of Comb graph.

2 Splitting graph of a graph: The splitting graph is introduced by Prof . E. Sampath Kumar, Prof. H.B. Walikar in [8]. For a graph G , Splitting graph is denoted by $S(G)$. For each vertex v of a graph G , take a new vertex v' . Join v'

to all the vertices of G adjacent to v . The graph $S(G)$ thus obtained is called Splitting graph or Duplicate graph of G . In [8], they have studied some properties of $S(G)$ and obtained the characterization of $S(G)$. Prof. Jan Mycielski, in his work in sets and logic used a graph called shadow graph $S(G)$. For a graph G , the shadow graph $S(G)$ is obtained from G by adding for each vertex v of G , a new vertex v' called shadow vertex of v , and joining v' to the neighbour of v in G .

2.1 Observations on $S(G)$:

1. A vertex of G and its duplicate vertices are not adjacent in $S(G)$.
2. All duplicate vertices induces a null graph.
3. $d(v_i)$ in $G = d(v_i')$ in $S(G)$.
4. $d(v_i)$ in $S(G) = 2d(v_i')$ in $S(G)$
5. By definition of splitting graph, $d(v_i, v_j / G) = d(v_i, v_j / S(G))$

2.2 Note[9]: As the splitting graph consists of the vertices of given graph and its duplicate vertices, for convenience

sake ,partition the vertex set of $S(G)$ into the sets A, B as below.

$$A = \{v_i / v_i \in V(G)\}$$

$$B = \{v_i' / v_i' \in V(S(G)) - V(G)\}$$

In order to demonstrate the validity of the theorem, we adopt the following notation:

$d_A(G, i) =$ number of pairs of vertices in the set A , at a distance i

$d_B(G, i) =$ number of pairs of vertices in the set B , at a distance i

$d_{AB}(G, i) =$ number of pairs of vertices of which one is in the set A and the other is in the set B , that are at a distance i

$d_A(v_i, v_j) =$ distance between the vertices v_i, v_j among the vertices of the set A

$d_B(v_i, v_j) =$ distance between the vertices v_i, v_j among the vertices of the set B

$d_{AB}(v_i, v_j) =$ distance between the vertices v_i, v_j among the vertices of the set A, B

With the above notation, the Wiener polynomial of Splitting graph is given as

$$W(S(G, q)) = a_1q + a_2q^2 + a_3q^3 + \dots + a_iq^i$$

It can be easily observed that $a_i = d_A(G, i) + d_B(G, i) + d_{AB}(G, i)$

By computing these three terms we found the coefficients of wiener polynomial.

Note: In the following proofs consider j as n whenever $j \equiv 0 \pmod{n}$.

2.3 Theorem : The wiener polynomial of $S(P_n \otimes K_1)$ is

$$W(S(P_n \otimes K_1)) = 4W(P_n \otimes K_1) + (1 - 3n)q + 2nq^2 + (3n - 1)q^3, n \geq 4$$

Proof: Let $v_1, v_2, \dots, v_n \in V(C_n), a_1, a_2, \dots, a_n$ be the pendent vertices that are adjacent to v_i in $(P_n \otimes K_2)$
 $v'_1, v'_2, \dots, v'_n \in V(C_n), a'_1, a'_2, \dots, a'_n$ be the corresponding duplicate vertices. For convenience sake we partition the vertex set into the following subsets and found the distances between them.

$A =$ Set of vertices of comb graph

$B =$ Set of duplicate vertices of comb graph

Further the sets A, B are partitioned as

$A1 =$ Set of vertices of path of comb graph $B1 =$ Set of duplicate vertices of path.

$A2 =$ Set of pendent vertices of comb graph $B2 =$ Set of duplicate vertices of degree one

The distances between the vertices from the above sets are given in ten combinations as follows.

Case1: Wiener polynomial of set of vertices of A1 is given in theorem1 as

$$\sum_{\{v_i, v_j\} \in V(A1)} q^{(v_i, v_j)} = (n-1)q^1 + (n-2)q^2 + (n-3)q^3 + \dots + 1q^{n-1} = \sum_{i=1}^{n-1} (n-i)q^i$$

Case2: Wiener polynomial of set of vertices of A1, A2 is given in theorem1 as

$$\sum_{\{v_i, a_j\} \in V(A1, A2)} q^{(v_i, a_j)} = nq + 2((n-1)q^2 + (n-2)q^3 + \dots + 1.q^n) = nq + 2 \sum_{i=1}^{n-1} (n-i)q^{i+1}$$

Case3: Distance between the vertices of A2 is given as

$$d(a_i, a_j) = j - i + 2 \text{ for } 1 \leq i < j \leq n,$$

$$d_{A2}(G, i) = n - i + 2 \text{ for } 3 \leq i \leq n + 1$$

$$\sum_{\{a_i, a_j\} \in V(A2)} q^{(a_i, a_j)} = (n-1)q^3 + (n-2)q^4 + \dots + 1.q^{n+1} = \sum_{i=1}^{n-1} (n-i)q^{i+2}$$

Case4: Distance between the vertices of B1 is given as in theorem1.

Case5: Distance between the vertices of B1, B2 is given as

$$d(v'_i, a'_j) = \begin{cases} 3, & \text{for } i = j \\ |j - i| + 1 & \text{for } i \neq j, 1 \leq i, j \leq n, \end{cases}$$

$$d_{B1B2}(G, i) = \begin{cases} 3n - 4 & \text{for } i = 3 \\ 2(n - i + 1), & 2 \leq i \leq n \end{cases}$$

The corresponding wiener polynomial is given as

$$\sum_{\{v_i', a_j'\} \in V(B1B2)} q(v_i', a_j') = nq^3 + 2((n-1)q^2 + (n-2)q^3 + \dots + 1 \cdot q^n) = nq^3 + 2 \sum_{i=1}^{n-1} (n-i)q^{i+1}$$

Case6: Distance between the vertices of B2 is given as

$$d_{B2}(a_i', a_j') = j - i + 2 \text{ for } 1 \leq i < j \leq n$$

$$d_{B2}(G, i) = (n - i + 2), 3 \leq i \leq n + 1$$

$$\sum_{\{a_i', a_j'\} \in V(B2)} q(a_i', a_j') = (n-1)q^3 + (n-2)q^4 + (n-3)q^5 + \dots + 1 \cdot q^{n+1} = \sum_{i=1}^{n-1} (n-i)q^{i+2}$$

Case7: The distance between the vertices of A1, B1 is given as in case – of theorem 1

Case8: Distance between the vertices of A1, B2 is given as

$$d(v_i, a_j') = |j - i| + 1 \text{ for } i \neq j, 1 \leq i, j \leq n,$$

$$d_{A2B1}(G, i) = \begin{cases} n & \text{for } i = 1 \\ 2(n - i + 1), & 2 \leq i \leq n \end{cases}$$

$$\sum_{\{v_i, a_j'\} \in V(A2B1)} q(v_i, a_j') = nq^1 + 2((n-1)q^2 + (n-2)q^3 + \dots + 1 \cdot q^n) = nq^1 + 2 \sum_{i=1}^{n-1} (n-i)q^{i+1}$$

Case9: Distance between the vertices of A2, B1 is given as in case5

Case10: Distance between the vertices of A2, B2 is given as

$$d(a_i, a_j') = |j - i| + 2 \text{ for } 1 \leq i, j \leq n,$$

$$d_{A2B2}(G, i) = \begin{cases} n & \text{for } i = 2 \\ 2(n - i + 2), & 3 \leq i \leq n + 1 \end{cases}$$

$$\sum_{\{a_i, a_j'\} \in V(A2B2)} q(a_i, a_j') = nq^2 + 2((n-1)q^3 + (n-2)q^4 + \dots + 1 \cdot q^{n+1}) = nq^2 + 2 \sum_{i=1}^{n-1} (n-i)q^{i+2}$$

By adding all the above wiener polynomials, we get

$$W(S(P_n \otimes K_1)) = 4W(P_n \otimes K_1) + (1 - 3n)q + 2nq^2 + (3n - 1)q^3, n \geq 4$$

$$W(S(T_{n,k})) = 4W(T_{n,k}) + (n + k)(q^3 + q^2 - q), n \geq 5$$

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