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WIENER POLYNOMIAL AND WIENER INDEX FOR GRAPHS DERIVED FROM PATH GRAPHS

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ABSTRACT: The sum of distances between all the pairs of vertices in a connected graph is known as WIENER INDEX. We introduce a new class of graphs $G_2(P_n)$ derived from path graphs P_n and study wiener index and wiener polynomial for these graphs.

AMS CLASSICATION: 05C12, 92E10.

KEYWORDS: Graph, Wiener Index, Wiener Polynomial.

1. INTRODUCTION

The fact that there are good correlations between W and a variety of physico-chemical properties of organic compounds (boiling point, heat of evaporation, heat of formation, chromatographic retention times, surface tension, vapor pressure, etc.) could be rationalized by the assumption that W is roughly proportional to the Van der Waals surface area of the respective molecule. The biological activity of organic compounds also depends on their molecular structure, it is necessary to find appropriate representations of the molecular structure of organic compounds. These representations are realized through the molecular descriptors. Molecular descriptors are terms that characterize specic aspect of molecule. The Wiener Index W is one of the oldest molecular-graph based structure-descriptors and its chemical applications are well documented.

A representation of an object giving information only about the number of elements composing it and their connectivity is named a topological representation of this object. A topological representation of molecule can be carried through the molecular graph. A molecular graph is a collection of points representing the atoms in the molecule and set of lines representing the covalent bonds. These points are named vertices and the lines are named edges in graph theory language.

If G is graph, u and v are two vertices of G, and $d(u, v)$ is the length of the shortest path connecting u and v, then the Wiener Index is defined as:

$$W(G) = \sum_{u<v} d(u, v)$$

with the summation going over all pairs of vertices of G.

For any graph G we have $W(Kn) \leq W(G) \leq W(P_n)$.

Definition 1.1: Consider a path graph P_n with n vertices. The graph $G_2^1(P_n)$ is obtained from P_n by connecting vertices of distance two by an edge. The resultant graph is concatenation of $(n-2)$ 3-cycles.

Consider a path graph P_6 then is concatenation of four 3-cycles.

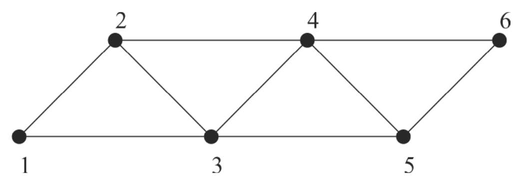

Figure 1: $G_2^1(P_6)$

Definition 1.2: The graph $G_2^k(P_n)$ is obtained from $G_2^{k-1}(P_n)$ by introducing an edge between vertices of distance two.

In this paper, we obtain generalized Wiener Index for $G_2^k(P_n)$.

Consider the graph $G_2^1(P_6)$ then $G_2^2(P_6)$ is

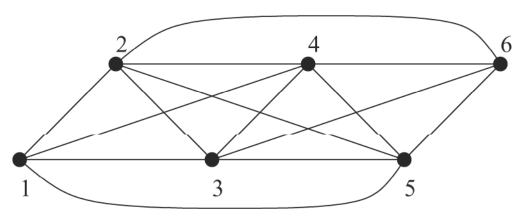

Figure 2: $G_2^2(P_6)$

Definition 1.3: The Wiener polynomial of G is

$$W(G;q) = \sum_{i=1}^{n} a_i q^i \quad \text{and} \quad W(G) = W'(G; q=1)$$

Result 1.1:

$$W(P_n;q) = (n-1)q + (n-2)q^2 + \ldots + q^{n-1} = \sum_{j=1}^{n-1} jq^{n-j}$$

In this paper, we try to reduce the distance between the vertices of distance two to distance 1 by adding a new edge. The interesting case will be reducing the path graph to complete graph in finite number of steps. In this process, path graph reduces to $G_2^k(P_n)$ thereby the Wiener number of the resultant graph gradually decreases.

2. MAIN RESULTS

In $K = \left[\frac{n}{2}\right]$ number of steps path graph P_n will reach the complete graph.

Classification of $G_2^k(P_n)$

K	Complete Graph	Possible graphs with Maximum Deg
1	$G_2^1(P_2)$, $G_2^1(P_3)$	$G_2^1(P_5)$ ...
2	$G_2^2(P_4)$, $G_2^2(P_5)$	$G_2^2(P_9)$ ...
3	$G_3^2(P_6)$, $G_2^3(P_7)$	$G_2^3(P_{13})$ ...
...		
K	$G_2^k(P_{2k})$, $G_2^k(P_{2k+1})$	$G_2^k(P_{4k+1})$ ...

From the above classification we have following two types of graphs

- Graphs from $G_2^k(P_{2k+2})$ to $G_2^k(P_{4k})$ have no vertex of maximum degree $4k$.
- Graphs $G_2^k(P_{4k+1})$ onwards have vertices with maximum degree $4k$.

Theorem 2.1: If P_n is a path graph with n vertices, then the Wiener polynomial of $G_2^k(P_n)$ is $W(G_2^1(P_n); q) = \sum_{i=1}^{\left[\frac{n}{2}\right]} ((2n+1) - 4\mathrm{i})q^i$ and $W(G_2^1(P_n)) = \sum_{i=1}^{\left[\frac{n}{2}\right]} ((2n+1)\ 4i)$.

Proof: The Wiener polynomials of $G_2^1(P_4)$, $G_2^1(P_5)$, ..., $G_2^1(P_n)$ are obtained by their distance matrix D_i, $i = 4, 5, ..., n$.

$$D_4 = \begin{pmatrix} 0 & 1 & 1 & 2 \\ - & 0 & 1 & 1 \\ - & - & 0 & 1 \\ - & - & - & 0 \end{pmatrix}, \quad D_5 = \begin{pmatrix} 0 & 1 & 1 & 2 & 2 \\ - & 0 & 1 & 1 & 2 \\ - & - & 0 & 1 & 1 \\ - & - & - & 0 & 1 \\ - & - & - & - & 0 \end{pmatrix}, \quad D_6 = \begin{pmatrix} 0 & 1 & 1 & 2 & 2 & 3 \\ - & 0 & 1 & 1 & 2 & 2 \\ - & - & 0 & 1 & 1 & 2 \\ - & - & - & 0 & 1 & 1 \\ - & - & - & - & 0 & 1 \\ - & - & - & - & - & 0 \end{pmatrix}$$

and so on.

Wiener polynomials of $G_2^1(P_n)$ for dierent values of n are as follows:

n	Wiener polynomial
4	$5q + q^2$
5	$7q + 3q^2$
6	$9q + 5q^2 + q^3$
7	$11q + 7q^2 + 3q^3$
8	$13q + 9q^2 + 5q^3 + q^4$
9	$15q + 9q^2 + 5q^3 + 3q^4$
10	$17q + 13q^2 + 7q^3 + 5q^4 + q^5$
11	$19q + 15q^2 + 11q^3 + 7q^4 + 3q^5$
12	$21q + 17q^2 + 13q^3 + 9q^4 + 5q^5 + q^6$

From the above table the highest degree of the polynomial is $\left[\frac{n}{2}\right]$ and from the matrices we have $(n - 1 + n - 2)$ pair of vertices are of distance one, $(n - 3 + n - 4)$ pair of vertices are of distance two, ..., one pair of vertices of distance $\left[\frac{n}{2}\right]$.

$$W(G_2^1(P_n); q) = \{2n - 3\}q + \{2n - 7\}q^2 + \{2n - 11\}q^3 + \{2n - 15\}q^4$$

$$+ \ldots + \left[\frac{n}{2}\right] q^{\left[\frac{n}{2}\right]}, \quad \text{if} \quad n \equiv 0 \bmod 2$$

$$W(G_2^1(P_n); q) = \{2n - 3\}q + \{2n - 7\}q^2 + \{2n - 11\}q^3 + \{2n - 15\}q^4$$

$$+ \ldots + 3\left[\frac{n}{2}\right] q^{\left[\frac{n}{2}\right]}, \quad \text{if} \quad n \equiv 1 \bmod 2$$

$$= \{2n - (4.1 - 1)\}q + \{2n - (4.2 - 1)\}q^2 + \{2n - (4.3 - 1)\}q^3$$

$$+ \{2n - (4.4 - 1)\}q^4 + \ldots + \left\{2n - \left(4\left[\frac{n}{2}\right] - 1\right)\right\} 2q^{\left[\frac{n}{2}\right]}$$

$$W(G_2^1(P_n); q) = \sum_{i=1}^{\left[\frac{n}{2}\right]} ((2n + 1) - 4i)q^i$$

Hence, $W(G_2^1(P_n); q) = \sum_{i=1}^{\left[\frac{n}{2}\right]} i((2n + 1) - 4i)$.

Theorem 2.2: The Wiener polynomial of $G_2^2(P_n)$ is

$$W(G_2^2(P_n); q) = \sum_{i=1}^{\left[\frac{n}{4}\right]} \{(4n+2) - 4(4i-1)\}q^i, \quad n \equiv 0, 1, \bmod 4$$

$$= \sum_{i=1}^{\left[\frac{n}{4}\right]} \{(4n+2) - 4(4i-1)\}q^i + \left(\sum_{j=1}^{\ell-1} j\right) q^{\left[\frac{n}{4}\right]+1},$$

$$n \equiv \ell \bmod 4 \ \& \ \ell = 2, 3.$$

Proof: The Wiener polynomials of $G_2^2(P_4)$. $G_2^2(P_5)$. ..., $G_2^2(P_n)$ are obtained by their distance matrix D_i; $i = 4, 5, ..., n$.

$$D_4 = \begin{pmatrix} 0 & 1 & 1 & 1 \\ - & 0 & 1 & 1 \\ - & - & 0 & 1 \\ - & - & - & 0 \end{pmatrix}, \quad D_5 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ - & 0 & 1 & 1 & 1 \\ - & - & 0 & 1 & 1 \\ - & - & - & 0 & 1 \\ - & - & - & - & 0 \end{pmatrix}, \quad D_6 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 2 \\ - & 0 & 1 & 1 & 1 & 1 \\ - & - & 0 & 1 & 1 & 1 \\ - & - & - & 0 & 1 & 1 \\ - & - & - & - & 0 & 1 \\ - & - & - & - & - & 0 \end{pmatrix}$$

and so on.

Wiener polynomials of $G_2^2(P_n)$ for different values of n are as follows:

n	Wiener polynomial
4	$6q$
5	$10q$
6	$14q + q^2$
7	$18q + 3q^2$
8	$22q + 6q^2$
9	$26q + 10q^2$
10	$30q + 14q^2 + q^3$
11	$34q + 18q^2 + 3q^3$
12	$38q + 22q^2 + 6q^3$
13	$42q + 26q^2 + 10q^3$
14	$46q + 30q^2 + 14q^3 + q^4$
15	$50q + 34q^2 + 18q^3 + 3q^4$

From the above table the highest degree of the polynomial is

$$\left[\frac{n}{4}\right] \text{ if } n \equiv 0, 1 \bmod 4 \quad \text{and} \quad \left[\frac{n}{4}\right] + 1 \text{ if } n \equiv 2, 3 \bmod 4.$$

The minimum degree in $G_2^2(P_n)$ is 4 and from the matrices

$(n-1)+(n-2)+(n-3)+(n-4)$ pair of vertices are of distance one

$(n-5)+(n-6)+(n-7)+(n-8)$ pair of vertices are of distance two

$(n-9)+(n-10)+(n-11)+(n-12)$ pair of vertices are of distance three

and so on.

$$W(G_2^2(P_n);q) = \{4n-10\}q + \{4n-26\}q^2 + \{4n-42\}q^3 + \{4n-58\}q^4 + \ldots + 6q^{\left[\frac{n}{4}\right]}, \qquad \text{if} \quad n \equiv 0; 1 \bmod 4$$

$$W(G_2^2(P_n);q) = \{4n-10\}q + \{4n-26\}q^2 + \{4n-42\}q^3 + \{4n-58\}q^4 + \ldots + q^{\left[\frac{n}{4}\right]+1}, \qquad \text{if} \quad n \equiv 2 \bmod 4$$

$$W(G_2^2(P_n);q) = \{4n-10\}q + \{4n-26\}q^2 + \{4n-42\}q^3 + \{4n-58\}q^4 + \ldots + 3q^{\left[\frac{n}{4}\right]+1}, \qquad \text{if} \quad n \equiv 3 \bmod 4$$

$$W(G_2^2(P_n);q) = \begin{cases} \sum_{i=1}^{\left[\frac{n}{4}\right]} \{2(2n+1) - 4(4i-1)\}\, q^i & \text{if} \quad n \equiv 0, 1 \bmod 4 \\ \sum_{i=1}^{\left[\frac{n}{4}\right]} \{2(2n+1) - 4(4i-1)\}\, q^i + q^{\left[\frac{n}{4}\right]+1} & \text{if} \quad n \equiv 2 \bmod 4 \\ \sum_{i=1}^{\left[\frac{n}{4}\right]} \{2(2n+1) - 4(4i-1)\}\, q^i + 3q^{\left[\frac{n}{4}\right]+1} & \text{if} \quad n \equiv 3 \bmod 4 \end{cases}$$

Hence,

$$W(G_2^2(P_n);q) = \sum_{i=1}^{\left[\frac{n}{4}\right]} \{(4n+2) - 4(4i-1)\}q^i, \qquad \text{if} \quad n \equiv 0; 1 \bmod 4$$

$$= \sum_{i=1}^{\left[\frac{n}{4}\right]} \{(4n+2) - 4(4i-1)\}q^i + \left(\sum_{j=1}^{\ell-1}\right) q^{\left[\frac{n}{4}\right]+1}, \qquad n \equiv \ell \bmod 4 \;\&\; \ell = 2, 3.$$

Theorem 2.3: The Wiener polynomial of $G_2^3(P_n)$ is

$$W(G_2^3(P_n); q) = \sum_{i=1}^{\left[\frac{n}{6}\right]} \{(6n+3) - 6(6i-2)\}q^i, \qquad \text{if } n \equiv 0, 1 \bmod 6$$

$$= \sum_{i=1}^{\left[\frac{n}{6}\right]} \{(6n+2) - 6(6i-2)\}q^i$$

$$+ \left(\sum_{j=1}^{\ell-1}\right) q^{\left[\frac{n}{6}\right]+1}, \; n \equiv \ell \bmod 6 \;\&\; \ell = 2, 3, 4, 5.$$

Proof: Wiener polynomials of $G_2^3(P_n)$ for different values of n are as follows:

n	Wiener polynomial
4	$15q$
5	$21q$
6	$27q + q^2$
7	$33q + (1+2)q^2$
8	$39q + (1+2+3)q^2$
9	$45q + (1+2+3+4)q^2$
10	$51q + (1+2+3+4+5)q^2$
11	$57q + 21q^2$
12	$63q + 27q^2 + q^3$
13	$69q + 33q^2 + (1+2)q^3$
14	$75q + 39q^2 + (1+2+3)q^3$
15	$81q + 45q^2 + (1+2+3+4)q^3$
16	$87q + 51q^2 + (1+2+3+4+5)q^3$
17	$93q + 57q^2 + 21q^3$

From the above table the highest degree of the polynomial is

$$\left[\frac{n}{6}\right] \text{ if } n \equiv 0, 1 \bmod 6 \quad \text{and} \quad \left[\frac{n}{6}\right] \text{ if } n \equiv 2, 3, 4, 5 \bmod 6.$$

The minimum degree in $G_2^3(P_n)$ is 6 and

$$(n-1) + (n-2) + (n-3) + (n-4) + (n-5) + (n-6)$$

pair of vertices are of distance one

$$(n-7)+(n-8)+(n-9)+(n-10)+(n-11)+(n-12)$$

pair of vertices are of distance two

$$(n-13)+(n-14)+(n-15)+(n-16)+(n-17)+(n-18)+(n-19)$$

pair of vertices are of distance three and so on.

$$W(G_2^3(P_n);q)=\{6n-21\}q+\{6n-57\}q^2+\{6n-112\}q^3+\{6n-135\}q^4+\ldots$$

Hence,

$$W(G_2^3(P_n);q)=\begin{cases}\sum_{i=1}^{\left[\frac{n}{6}\right]}\{(6n+2)-6(6i-2)\}q^i & n\equiv 0,1 \bmod 6\\ \sum_{i=1}^{\left[\frac{n}{6}\right]}\{(6n+2)-6(6i-2)\}q^i & \\ \qquad +\left(\sum_{j=1}^{\ell-1} j\right)q^{\left[\frac{n}{6}\right]+1}, & n\equiv \ell \bmod 6 \ \& \ \ell=2,3,4,5.\end{cases}$$

Hence in general,

The Wiener polynomial of $G_2^k(P_n)$ is

$$W(G_2^k(P_n);q)=\begin{cases}\sum_{i=1}^{\left[\frac{n}{2k}\right]}\{k(2n+1)-2k(2ki-(k-1))\}q^i, & n\equiv 0,1 \bmod 6\\ \sum_{i=1}^{\left[\frac{n}{2k}\right]}\{k(2n+1)-2k(2ki-(k-1))\}q^i & \\ \qquad +\left(\sum_{j=1}^{\ell-1} j\right)q^{\left[\frac{n}{2k}\right]+1}, & n\equiv \ell \bmod 2k \ \& \\ & \ell=2,3,\ldots,(2k-1).\end{cases}$$

Result 2.1:

$$W(K_n) < W(G_2^k(P_n)) < W(C_n),\ K = 1, 2, \ldots$$

Example 2.1: Using theorems 2.1, 2.2 and 2.3 we have

$W(G_2^1(P_{10});q)=17q+13q^2+9q^3+5q^4+q^5,$ $\quad W(G_2^1(P_{10})=95$

$W(G_2^2(P_{10});q)=30q+14q^2+q^3,$ $\quad W(G_2^2(P_{10})=61$

$W(G_2^3(P_{10});q)=39q+6q^2,$ $\quad W(G_2^3(P_{10})=51$

$W(G_2^4(P_{10});q)=44\text{q}+\text{q}2,$ $\quad W(G_2^2(P_{10})=46$

$W(G_2^5(P_{10});q)=45q$ $\quad W(G_2^2(P_{10})=45=W(K_{10})$

Corollary 2.1: The Wiener Index for $G_2^1(P_n)$ is

$$W(G_2^1(P_n)) = \begin{cases} \dfrac{n(n+2)(2n-1)}{24}, & n \text{ is even} \\ \dfrac{(n^2-1)(2n+3)}{24}, & n \text{ is odd} \end{cases}$$

Proof:

$$W(G_2^1(P_n)) = \sum_{i=1}^{\frac{n}{2}} i((2n+1)-4i), \qquad n \text{ is even}$$

$$= (2n+1) \sum_{i=1}^{\frac{n}{2}} i - 4 \sum_{i=1}^{\frac{n}{2}} i^2$$

$$= \frac{(2n+1)n(n+2)}{8} - \frac{n(n+1)(n+2)}{6}$$

$$= \frac{n(n+2)(2n-1)}{24}, \qquad n \text{ is even}$$

$$W(G_2^1(P_n)) = \sum_{i=1}^{\frac{n-1}{2}} i((2n+1)-4i), \qquad n \text{ is odd}$$

$$= (2n+1) \sum_{i=1}^{\frac{n-1}{2}} i - 4 \sum_{i=1}^{\frac{n-1}{2}} i^2$$

$$= \frac{(2n+1)(n-1)(n+1)}{8} - \frac{n(n+1)(n-1)}{6}$$

$$= \frac{(2n+3)(n^2-1)}{24}, \qquad n \text{ is odd}$$

In corollary 2.1 Wiener Index for $W(C_n)$ is involved, this shows the relationship between $W(C_n)$ and $W(G_2^1(P_n))$.

Corollary 2.2:

$$W(C_n) - \sum_{i=1}^{\frac{n-2}{2}} i^2 = W[G_2^1(P_n)], \qquad n \text{ is even}$$

$$W(C_n) - \sum_{i=1}^{\frac{n-3}{2}} (i^2 + i) = W[G_2^1(P_n)], \qquad n \text{ is odd}$$

Proof:

$$W(C_n) - \sum_{i=1}^{\frac{n-2}{2}} i^2 = \frac{n^3}{8} - \frac{n(n-1)(n-2)}{24}, \qquad n \text{ is even}$$

$$= \frac{2n^3 + 3n^2 - 2n}{24}$$

$$= \frac{n(2n^2+3n-2)}{24}$$

$$= \frac{n(n+2)(2n-1)}{24} = W(G_2^1(P_n)), \quad n \text{ is even}$$

$$W(C_n) - \sum_{i=1}^{\frac{n-3}{2}} (i^2+i) = \frac{n(n^2-1)}{8} - \frac{(n-3)(n-2)(n-1)}{24} - \frac{(n-3)(n-1)}{8}$$

$$= \frac{(n-1)}{24}[2n^2+5n+3]$$

$$= \frac{(2n+3)(n^2-1)}{24} = W(G_2^1(P_n)), \quad n \text{ is odd}$$

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