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HOSOYA POLYNOMIAL, WIENER INDEX AND HYPER WIENER INDEX OF SOME FAMILIES OF GRAPHS OF DIAMETER 2

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Abstract

Let G be a simple connected graph having vertex set $V(G)$ and edge set $E(G)$. The Hosoya polynomial of G is $H(G,x) = \sum_{\{u,v\} \subset V(G)} x^{d(u,v)}$, where $d(u,v)$ denotes the distance between the vertices u and v. In this research paper, we will determine the Hosoya polynomial of some families of graphs of diameter 2. Moreover, we will determine the Wiener Index and hyper Wiener Index of the respective families.

1. Introduction

Let G be a connected graph, the vertex set and edge set of G is denoted by $V(G)$ and $E(G)$ respectively. The distance $d(u,v)$ between u and v is the length of the smallest path, where $u, v \in V(G)$. The maximum distance between the two vertices of a graph G is called the diameter of G and is denoted by $d(G)$. The degree of a vertex $u \in V(G)$ is the number of vertices joined to u or the number of edges incident with u and is denoted by d_u. The Hosoya polynomial of a graph G is a generating function that indicates about the distribution of distance in a graph. The polynomial was introduced by a Japanese chemist Haruo Hosoya in 1988. Haruo Hosoya discovered a new formula for the Wiener Index in terms of graph distance and therefore this polynomial is known by the name of its discoverer. The Hosoya polynomial of a connected graph G is defined as (Hosoya, 1988):

$$H(G,x) = \frac{1}{2} \sum_{v \in V(G)} V(G) \sum_{u \in V(G)} V(G)\ d(u,v)$$

The Hosoya polynomial of various chemical structures has been determined (Ali & Ali, 2011, Farahani, 2013 and Sadeghieh et al., 2017). Moreover, the Hosoya polynomial of some graph families have been examined (Farahani, 2015, Farahani, 2015, Narayankar et al., 2012). Also, the Hosoya polynomial of families of graphs has been studied (Stevanovic, 2001 and Wang et al., 2016).

The Wiener Index (Rezai et al., 2017) of a graph can be calculated by using the Hosoya polynomial. It is formulated as follows:

$$W(G) = \frac{\partial H(G,x)}{\partial x}|_{x=1}$$

The hyper Wiener Index (Rezai et al., 2017) of a graph can be calculated by using the Hosoya polynomial. It is formulated as follows:

$$WW(G) = H'(G,x)|_{x=1} + \frac{1}{2}H''(G,x)|_{x=1}$$

where the former and later are the first and second derivatives of the Hosoya polynomial at $x = 1$.

1.1 Definition

The Windmill graph $Wd(k,n)$ (Nagabhushana et al., 2017) is an undirected graph constructed for $k \geq 2, n \geq 2$ by joining n copies of the complete graph K_k at a shared vertex.

1.2 Definition

The Double Cones (Murugan, 2015) are graphs obtained by joining two isolated vertices to every vertex of C_n. A double Cone on $n+2$ vertices is denoted by $CO_{n+2} = C_n + 2K_1$.

1.3 Definition

The Join of two graphs (Sagan et al., 1996) is denoted by $G_1 + G_2$ and have vertex set $V(G_1 + G_2) = V_1 \cup V_2$ and edge set $E(G_1 + G_2) = E_1 \cup E_2 \cup \{uv: u \in V_1, v \in V_2\}$.

1.4 Definition

The Fan graph (Modha & Kanani, 2015) is the join of $P_n + K_1$.

1.5 Definition

The Double Fan graph (Modha & Kanani, 2015) is the join of $P_n + 2K_1$.

2. Materials and Methods

A simple calculation for finding out the Hosoya polynomial, Wiener Index and hyper Wiener Index will now be put forward.

3. Results

In this section, we determine the Hosoya polynomial, Wiener Index and hyper Wiener Index of some families of graphs of Diameter 2.

Theorem 3.1: The Hosoya polynomial of the Windmill graph $Wd(k,n)$ for all integer numbers $k \geq 4, n \geq 2$ is

$$H(Wd(k,n),x) = \frac{nk(k-1)}{2}x + \frac{(k^2-2k+1)(n^2-n)}{2}x^2$$

The Wiener Index is

$$W\big(Wd(k,n)\big) = k^2n^2 - \frac{1}{2}nk^2 - 2kn^2 - \frac{3}{2}kn + n^2 - n$$

The hyper Wiener Index is

$$WW\big(Wd(k,n)\big) = \frac{3}{2}k^2n^2 - nk^2 - 3kn^2 - \frac{3}{2}kn + \frac{3}{2}n^2 - n$$

Proof

One can see that there are $\frac{nk(k-1)}{k}$ vertices of degree $k-1$ and a center vertex of degree $n(k-1)$. Thus, we have the following partition of the vertex set of $Wd(k,n)$

$$V_{k-1} = \{v \in V(Wd(k,n)) | d_v = k-1\} \rightarrow |V_{k-1}| = \frac{nk(k-1)}{k} \quad (3.1.1)$$

$$V_{n(k-1)} = \{c \in V(Wd(k,n)) | d_c = n(k-1)\} \rightarrow |V_{n(k-1)}| = 1 \quad (3.1.2)$$

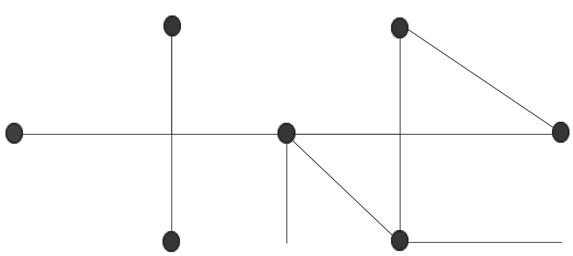

Figure 1: $Wd(4,2)$

Thus, the total number of edges are

$$|E(G)| = \frac{1}{2}[(k-1) \times |V_{k-1}| + n(k-1) \times |V_{(k-1)n}|]$$

$$|E(G)| = \frac{1}{2}[(k-1) \times \frac{nk(k-1)}{k} + n(k-1) \times 1]$$

$$|E(G)| = \frac{nk(k-1)}{2} \quad (3.1.3)$$

Now to compute the Hosoya polynomial of $Wd(k,n)$, we will use the definition of the Hosoya polynomial from (Hosoya, 1988). Thus, we have

$$H(G,x) = \sum_{k=1}^{d(G)} d(G,k)x^k \quad (3.1.4)$$

where $d(G,k)$ is the representation of the distance $d(u,v) = k$ and $1 \leq k \leq diam(G)$.

$$d(Wd(k,n),1) = |E(G)| = \frac{nk(k-1)}{2} \quad (3.1.5)$$

The total number of 1-edges paths are equal to the total number of edges. Thus, the first sentence of the Hosoya polynomial is, $\frac{nk(k-1)}{2}x$.

$$d(Wd(k,n),2) = \frac{(k^2-2k+1)(n^2-n)}{2} \quad (3.1.6)$$

There are no 2-edges paths between the center vertex and V_{k-1}. The total number of 2-edges paths between the vertices $u,v \in V_{k-1}$ are $\frac{(k^2-2k+1)(n^2-n)}{2}$. Thus, the second and last sentence of the Hosoya polynomial is $\frac{(k^2-2k+1)(n^2-n)}{2}x^2$. From equations (3.1.5) and (3.1.6), we get the desired Hosoya polynomial of the Windmill Graph $Wd(k,n)$.

$$H(Wd(k,n),x) = \frac{nk(k-1)}{2}x + \frac{(k^2-2k+1)(n^2-n)}{2}x^2 \quad (3.1.7)$$

Taking the first derivative of equation (3.1.7) at $x = 1$ will provide the Wiener index. Thus, following in the below manner

$$W\big(Wd(k,n)\big) = \frac{nk(k-1)}{2} + (k^2 - 2k + 1)(n^2 - n)x|_{x=1}$$

$$W\big(Wd(k,n)\big) = \frac{nk(k-1)}{2} + (k^2 - 2k + 1)(n^2 - n)$$

$$W\big(Wd(k,n)\big) = k^2n^2 - \frac{1}{2}nk^2 - 2kn^2 - \frac{3}{2}kn + n^2 - n \quad (3.1.8)$$

To obtain the hyper Wiener index of this family, will take first the second derivative of the Hosoya polynomial at $x = 1$.

$$H''\big(Wd(k,n)\big) = (k^2 - 2k + 1)(n^2 - n) \quad (3.1.9)$$

Now, to obtain the hyper Wiener index, add the first derivative from (3.1.8) and half of the second derivative (3.1.9) of the Hosoya polynomial. Thus, we have

$$WW\big(Wd(k,n)\big) = k^2n^2 - \frac{1}{2}nk^2 - 2kn^2 - \frac{3}{2}kn + n^2 - n + (k^2 - 2k + 1)(n^2 - n)$$

$$WW\big(Wd(k,n)\big) = \frac{3}{2}k^2n^2 - nk^2 - 3kn^2 - \frac{3}{2}kn + \frac{3}{2}n^2 - n \quad (3.1.10)$$

This completes the proof. For example, for $k = 4, n = 2$, we have the following form of Hosoya polynomial, Wiener index and hyper Wiener index,

$$H(Wd(4,2),x) = 12x + 9x^2$$

$$W\big(Wd(4,2)\big) = 6$$

$$WW(Wd(4,2)) = 8$$

Theorem 3.2: The Hosoya polynomial of the Double Cone graph $\forall n \geq 3$ is

$$H(CO_{n+2},x) = 3nx + \frac{n^2 - 3n + 2}{2}x^2$$

The Wiener Index is

$$W(CO_{n+2}) = n^2 + 2$$

The hyper Wiener Index is

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

Proof

The total number of vertices of this family are $n + 2$. First, we will partition the vertices. There are n vertices of degree 4 and 2 vertices of degree n. Thus, there are $n + 2$ vertices.

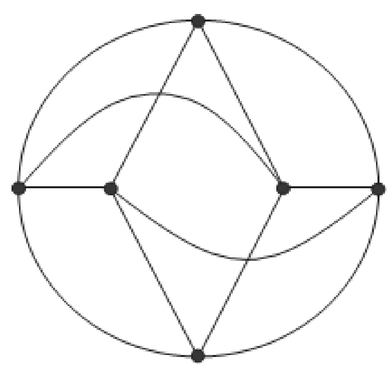

Figure 2: Double Cone graph, $C_4 + 2K_1, n = 4$

According to Theorem 3.1, the number of edges are $3n$. Now, we will compute the Hosoya polynomial of Double Cone graph.

$$d(CO_{n+2}, 1) = |E(G)| = 3n \quad (3.2.1)$$

The total number of edges contributes to the total number of 1-edges paths. Thus, the first sentence of the Hosoya polynomial is $3nx$.

$$d(CO_{n+2}, 2) = \frac{n^2 - 3n + 2}{2} \quad (3.2.2)$$

The number of 2-edges paths between the vertices $u, v \in V_n$ is 1. There are $\frac{n^2-3n}{2}$, 2-edges paths between the vertices $u, v \in V_4$. There are no 2-edges paths between the vertices of V_4 and V_n. Thus, the second sentence of the Hosoya polynomial is $\left[1 + \frac{n^2-3n}{2}\right] x^2 = \frac{1}{2}[n^2 - 3n + 2]x^2$.

Thus, we get the Hosoya polynomial of the respective family

$$H(CO_{n+2}, x) = 3nx + \frac{n^2 - 3n + 2}{2} x^2 \quad (3.2.3)$$

To obtain the Wiener index and hyper Wiener index of this family, we will follow the same steps as illustrated in Theorem 3.1. Thus, we have

$$W(CO_{n+2}) = n^2 + 2 \quad (3.2.4)$$

$$WW(CO_{n+2}) = \frac{3}{2}n^2 - \frac{3}{2}n + 3 \quad (3.2.5)$$

This completes the proof. For example, for $n = 4$, we have the following Hosoya polynomial, Wiener index and hyper Wiener index as follows:

$$H(CO_{4+2}, x) = 12x + 3x^2$$

$$W(CO_{4+2}) = 18$$

$$WW(CO_{4+2}) = 21$$

Theorem 3.3: The Hosoya polynomial of the Fan graph $\forall n \geq 2$ is

$$H(F_n, x) = (2n - 1)x + \frac{n^2 - 3n + 2}{2} x^2$$

The Wiener Index is

$$W(F_n) = n^2 - n + 1$$

The hyper Wiener Index is

$$WW(F_n) = \frac{3}{2}n^2 - \frac{5}{2}n + 2$$

Proof

The total number of vertices of this respective family are $n + 1$. From the definition and figure of the Fan graph, one can see that there are 2 vertices of degree 2, $n - 2$ vertices of degree 3 and a one vertex of degree n. Hence, we have $n + 1$ vertices.

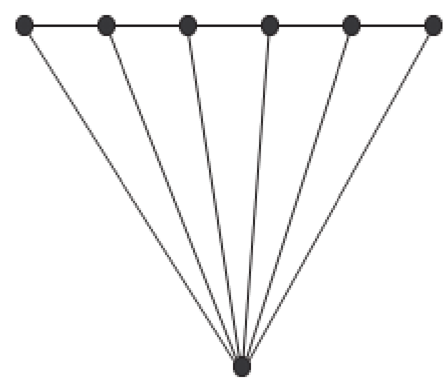

Figure 3: Fan graph, $n = 6$

According to Theorem 3.1, the number of edges are $2n - 1$. Now, we will compute the Hosoya polynomial of the Fan graph.

$$d(F_n, 1) = |E(G)| = 2n - 1 \quad (3.3.1)$$

The total number of edges contributes to the total number of 1-edges paths. Thus, the first sentence of the Hosoya polynomial is $(2n-1)x$.

$$d(F_n,2)=\frac{n^2-3n+2}{2} \quad (3.3.2)$$

There are no 2-edges paths between the vertices of s and V_2 or V_3. The only 2-edges paths are between the vertices of V_2 and V_3 which are $\frac{n^2-3n+2}{2}$ in number. Thus, the second sentence of the Hosoya polynomial is $\frac{1}{2}[n^2-3n+2]x^2$.

Thus, we get the Hosoya polynomial of the respective family

$$H(F_n,x)=(2n-1)x+\frac{n^2-3n+2}{2}x^2 \quad (3.3.3)$$

To acquire the Wiener and hyper Wiener index of this corresponding family, we will pursue the same steps as demonstrated in Theorem 3.1. Thus, we have

$$W(F_n)=n^2-n+1 \quad (3.3.4)$$

$$WW(F_n)=\frac{3}{2}n^2-\frac{5}{2}n+2 \quad (3.3.5)$$

This completes the proof. For example, for $n=6$, we have the following Hosoya polynomial, Wiener index and hyper Wiener index as follows:

$$H(F_6,x)=11x+10x^2$$

$$W(F_6)=31$$

$$WW(F_6)=41$$

Theorem 3.4: The Hosoya polynomial of the Double Fan graph df_n, $\forall n\geq 3$ is

$$H(df_n,x)=(3n-1)x+(2n-4)x^2$$

The Wiener Index is

$$W(df_n)=7n-9$$

The hyper Wiener Index is

$$WW(df_n)=9n-13$$

Proof

There are total $n+2$ vertices. From the definition and figure of the Double Fan graph, one can see that there are 2 vertices of degree n, 2 vertices of degree 3 and $n-2$ vertices of degree 4. Thus, we have $n+2$ vertices.

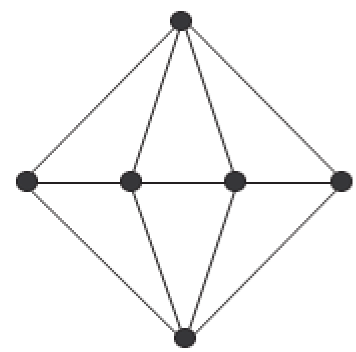

Figure 4: Double Fan graph, df_4

The total number of edges are $3n-1$. Now, we will compute the Hosoya polynomial of the Double Fan graph.

$$d(df_n,1)=|E(G)|=3n-1 \quad (3.4.1)$$

The total number of edges contributes to the total number of 1-edges paths. Thus, the first sentence of the Hosoya polynomial is $(3n-1)x$.

$$d(df_n,2)=2n-4 \quad (3.4.2)$$

There is 1, 2-edges paths between the vertices $u,v\in V_n$ and also the number of 2-edges paths between the vertices $u,v\in V_3$ is 1. The number of 2-edges paths are between the vertices of V_3 and V_4 are $2n-6$ in number. Thus, the second sentence of the Hosoya polynomial is $[2n-4]x^2$.

Thus, we get the Hosoya polynomial of the respective family

$H(df_n, x) = (3n-1)x + (2n-4)x^2$ (3.4.3)

To attain the Wiener and hyper Wiener index of this corresponding family, we will follow the same steps as exhibited in Theorem 3.1. Thus, we have

$$W(df_n) = 7n - 9 \quad (3.4.4)$$

$$WW(df_n) = 9n - 13 \quad (3.4.5)$$

This completes the proof. For example, for $n = 4$, we have the following Hosoya polynomial, Wiener index and hyper Wiener index as follows:

$$H(df_4, x) = 11x + 4x^2$$

$$W(df_4) = 19$$

$$WW(df_4) = 23$$

Theorem 3.5: The Hosoya polynomial of the family of the graph of K_n joined with P_2 at a single vertex, $\forall n \geq 3$ is

$$H(G, x) = \frac{n^2 - n + 2}{2}x + (n-1)x^2$$

The Wiener Index is

$$W(G) = \frac{n^2}{2} + \frac{3n}{2} - 1$$

The hyper Wiener Index is

$$WW(G) = \frac{1}{2}n^2 + \frac{5}{2}n - 2$$

Proof

The total number of vertices of G are $n+1$. There is 1 vertex of degree 1, $n-1$ vertices of degree $n-1$ and a one vertex of degree n. Moreover, the total number of vertices are $n+1$.

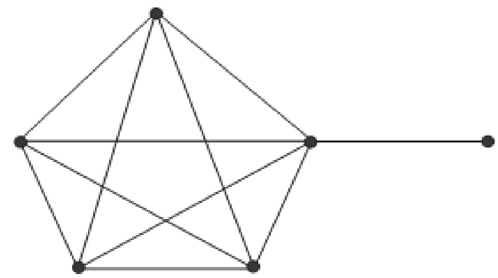

Figure 5: K_5 joined with P_2 at a single vertex

The number of edges of this family of graph are $\frac{n^2-n+2}{2}$ according to the steps performed in Theorem 3.1. The Hosoya polynomial of this family is computed as follows:

$$d(G,1) = |E(G)| = \frac{n^2 - n + 2}{2} \quad (3.5.1)$$

The total number of 1-edges paths are $\frac{n^2-n+2}{2}$. Thus, the first sentence of the Hosoya polynomial is $[\frac{n^2-n+2}{2}]x$.

$$d(G,2) = n - 1 \quad (3.5.2)$$

The total number of 2-edges paths between the vertices of V_1 and V_{n-1} are $n-1$. Also, there are no 2-dges paths between the vertices of V_1 and V_n and V_{n-1} and V_n. Thus, the second and last sentence of the Hosoya polynomial is $[n-1]x^2$.

Thus, we get the Hosoya polynomial of the respective family

$$H(G, x) = \frac{n^2 - n + 2}{2}x + (n-1)x^2 \quad (3.5.3)$$

To arrive at the final form of the Wiener and hyper Wiener index of this family, we will follow the same steps as demonstrated in Theorem 3.1. Thus, we have

$$W(G) = \frac{n^2}{2} + \frac{3n}{2} - 1 \quad (3.5.4)$$

$$WW(G) = \frac{n^2}{2} + \frac{5n}{2} - 2 \quad (3.5.5)$$

This completes the proof. For example, for $n = 5$, we have the following Hosoya polynomial, Wiener index and hyper Wiener index as follows:

$$H(G,x) = 11x + 4x^2$$

$$W(G) = 19$$

$$WW(G) = 23$$

Theorem 3.6: The Hosoya polynomial of the family of the graph of K_n joined with W_3 at a single vertex, $\forall n \geq 3$ is

$$H(G,x) = \frac{n^2 - n + 12}{2}x + (3n - 3)x^2$$

The Wiener Index is

$$W(G) = \frac{n^2}{2} + \frac{11n}{2}$$

The hyper Wiener Index is

$$WW(G) = \frac{1}{2}n^2 + \frac{17}{2}n - 3$$

Proof

The total number of vertices of G are $n + 3$. There are 3 vertices of degree 3, $n - 1$ vertices of degree $n - 1$ and a one vertex of degree $n + 2$. Thus, the total number of vertices that accompany this family are $n + 3$.

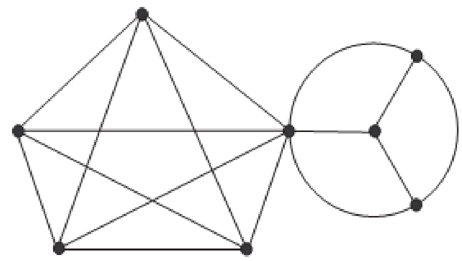

Figure 6: K_5 joined with the Wheel graph W_3 at a single vertex

The number of edges of this family of graph are $\frac{n^2-n+12}{2}$ according to the steps illustrated in Theorem 3.1. The Hosoya polynomial of this family is computed as follows:

$$d(G,1) = |E(G)| = \frac{n^2 - n + 12}{2} \quad (3.6.1)$$

The total number of 1-edges paths are $\frac{n^2-n+12}{2}$. Thus, the first sentence of the Hosoya polynomial is $[\frac{n^2-n+12}{2}]x$.

$$d(G,2) = 3n - 3 \quad (3.6.2)$$

The total number of 2-edges paths between the vertices of V_3 and V_{n-1} are $3n - 3$ and other than these pairing there are no 2-edges paths in the whole family of G. Thus, the second and last sentence of the Hosoya polynomial is $[3n - 3]x^2$.

Thus, we get the Hosoya polynomial of the respective family

$$H(G,x) = \frac{n^2 - n + 12}{2}x + (3n - 3)x^2 \quad (3.6.3)$$

To obtain the final form of the Wiener and hyper Wiener index of this family, we will follow the same steps as demonstrated in Theorem 3.1. Thus, we have

$$W(G) = \frac{n^2}{2} + \frac{11n}{2} \quad (3.6.4)$$

$$WW(G) = \frac{n^2}{2} + \frac{17n}{2} - 3 \quad (3.6.5)$$

This completes the proof. For example, for $n = 5$, we have the following Hosoya polynomial, Wiener index and hyper Wiener index as follows:

$$H(G, x) = 16x + 12x^2$$

$$W(G) = 40$$

$$WW(G) = 52$$

Theorem 3.7: The Hosoya polynomial of the family of the graph of K_n joined with one copy of K_m, $\forall n, m \geq 3$ is

$$H(G, x) = \frac{n^2 + m^2 - n - m}{2} x + (nm - n - m + 1)x^2$$

The Wiener Index is

$$W(G) = \frac{n^2 + m^2 + 4nm - 5n - 5m + 4}{2}$$

The hyper Wiener Index is

$$WW(G) = \frac{n^2 + m^2 + 6nm - 7n - 7m + 6}{2}$$

Proof

The total number of vertices of G are $n + m - 1$. There are $n - 1$ vertices of degree $n - 1$, 1 vertex of degree $m + n - 2$ and $m - 1$ vertices of degree $m - 1$. Thus, there are $n + m - 1$ vertices.

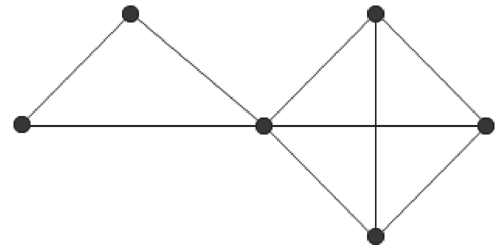

Figure 7: K_3 joined with one copy of K_4

The number of edges of this family of graph are $\frac{n^2+m^2-n-m}{2}$ according to the steps illustrated in Theorem 3.1. The Hosoya polynomial of this family is computed as follows:

$$d(G, 1) = |E(G)| = \frac{n^2 + m^2 - n - m}{2} \quad (3.7.1)$$

Thus, the first sentence of the Hosoya polynomial is $[\frac{n^2+m^2-n-m}{2}]x$.

$$d(G, 2) = nm - n - m + 1 \quad (3.7.2)$$

The total number of 2-edges paths between the vertices of V_{n-1} and V_{m-1} are $nm - n - m + 1$ and other than these pairing there are no 2-edges paths in the whole family of G. Thus, the second and last sentence of the Hosoya polynomial is $[nm - n - m + 1]x^2$.

Thus, we get the Hosoya polynomial of the respective family

$$H(G, x) = \frac{n^2 + m^2 - n - m}{2} x + (nm - n - m + 1)x^2 \quad (3.7.3)$$

To obtain the final form of the Wiener and hyper Wiener index of this family, we will follow the same steps as demonstrated in Theorem 3.1. Thus, we have

$$W(G) = \frac{n^2 + m^2 + 4nm - 5n - 5m + 4}{2} \quad (3.7.4)$$

$$WW(G) = \frac{n^2 + m^2 + 6nm - 7n - 7m + 6}{2} \quad (3.7.5)$$

This completes the proof. For example, for $n = 3, m = 4$, we have the following Hosoya polynomial, Wiener index and hyper Wiener index as follows:

$$H(G, x) = 9x + 6x^2$$
$$W(G) = 21$$
$$WW(G) = 27$$

Theorem 3.8: The Hosoya polynomial of the family of the graph of $P_2 + C_n$, $\forall n \geq 3$ is

$$H(G, x) = (3n + 1)x + \frac{n^2 - 3n}{2}x^2$$

The Wiener Index is

$$W(G) = n^2 + 1$$

The hyper Wiener Index is

$$WW(G) = \frac{3n^2}{2} - \frac{3n}{2} + 1$$

Proof

The total number of vertices of G are $n + 2$. There are n vertices of degree 4 and 2 vertices of degree $n + 1$. So, the total number of vertices that appear in this family of graphs are $n + 2$.

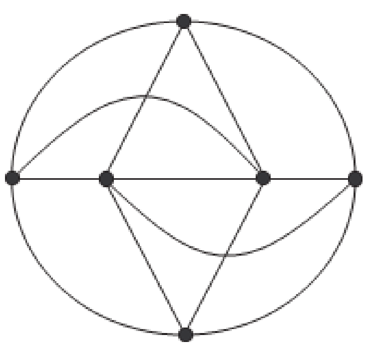

Figure 8: $P_2 + C_4$

The number of edges of this respective family of graph are $3n + 1$ according to the steps demonstrated in Theorem 3.1. The Hosoya polynomial of this family is obtained as follows:

$$d(G, 1) = |E(G)| = 3n + 1 \quad (3.8.1)$$

Thus, the first sentence of the Hosoya polynomial is $[3n + 1]x$.

$$d(G, 2) = \frac{n^2 - 3n}{2} \quad (3.8.2)$$

The total number of 2-edges paths between the vertices of $u, v \in V_4$ are $\frac{n^2-3n}{2}$ and other than these pairing there are no 2-edges paths in the entire family of G. Thus, the second and last sentence of the Hosoya polynomial is $[\frac{n^2-3n}{2}]x^2$.

Thus, we get the Hosoya polynomial of the respective family

$$H(G, x) = (3n + 1)x + (\frac{n^2 - 3n}{2})x^2 \quad (3.8.3)$$

To get the desired form of the Wiener and hyper Wiener index of this family, we will follow the same steps as demonstrated in Theorem 3.1. Thus, we have

$$W(G) = n^2 + 1 \quad (3.8.4)$$

$$WW(G) = \frac{3n^2}{2} - \frac{3n}{2} + 1 \quad (3.8.5)$$

This completes the proof. For example, for $n = 4$, we have the following Hosoya polynomial, Wiener index and hyper Wiener index as follows:

$$H(G, x) = 13x + 2x^2$$

$$W(G) = 17$$

$$WW(G) = 19$$

4. Discussion

In this paper, we have determined the Hosoya polynomial, Wiener index and hyper Wiener index of some families of graphs of Diameter 2.

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