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ON THE HOSOYA POLYNOMIAL AND WIENER INDEX OF JUMP GRAPH

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Abstract. In this paper, we obtain the expressions for Wiener index and Hosoya polynomial of a graph with diameter ≤ 3. Further, we obtain Wiener index and Hosoya polynomial of jump graph of certain graph families. In addition, we give bounds for Wiener index of *jump graph*.

1. Introduction

All graphs considered in this paper are connected, finite, undirected with no loops and multiple edges. Let G be a graph with vertex set $V = V(G) = \{v_1, v_2, ..., v_n\}$ and an edge set $E = E(G) = \{e_1, e_2, ..., e_m\}$. Thus, $|V| = n$ and $|E| = m$. As usual n is said to be the order and m the size of G. The *distance* $d_G(v_i, v_j)$ (or simply $d(v_i, v_j)$) between two vertices v_i and v_j is the length of the shortest path between the vertices v_i and v_j in G. The shortest $v_i - v_j$ path is often called *geodesic*. The *diameter* of a connected graph G, denoted by $diam(G)$, is the length of any longest geodesic. The *degree* $d_G(v_i)$ *of a vertex* v_i in G is the number of edges incident to v_i. The *degree* $d_G(e)$ *of an edge* $e = uv$ of G in $L(G)$ is given by $d_G(e) = d_G(u) + d_G(v) - 2$. The *eccentricity* $e(v)$ of a vertex v in G is defined to be $e(v) = max\{d(u, v)|u \in V\}$. A *unicyclic graph* [15] is a connected graph and have just one cycle.

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In practice, G corresponds to what is known as the *molecular graph* of an organic compound. The molecular graph is a graph where vertices corresponds to atoms and edges corresponds to bonds. The *Wiener index* is a graph invariant that belongs to the molecular structure-descriptors called topological indices, which are used for the design of molecules with desired properties. In 1947, Harold Wiener [21] used the following formula to calculate the boiling point t_B of alkanes:

$$t_B = aW(G) + bW_p(G) + c.$$

In this formula a, b, c are constants for a given isomeric group and $W_p(G)$, the *Wiener polarity index* of G [5, 10] which is defined as follows:

$$W_p(G) = |\{(u, v) : d_G(u, v) = 3; u, v \in V\}|.$$

The *Wiener index* (or *Wiener number*) [21] $W(G)$ of a graph G is the sum of distances between all (unordered) pairs of vertices of G, i.e.,

$$W(G) = \sum_{i<j} d_G(v_i, v_j).$$

The *Wiener index* $W(G)$ of the graph G is also defined by

$$W(G) = \frac{1}{2} \sum_{v_i, v_j \epsilon V(G)} d_G(v_i, v_j),$$

where the summation is over all possible pairs $v_i, v_j \in V(G)$. For complete review on Wiener index, refer [6, 14]. The distance number of a vertex u of a graph G denoted by $d(u \mid G)$ and is defined as [13]

$$d(u \mid G) = \sum_{v \in V(G)} d_G(u, v).$$

Then

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} d(u \mid G).$$

The Wiener polynomial was initially defined by Haruo Hosoya [16] and termed in honour of Harold Wiener who coined the Wiener index. The Hosoya polynomial [18] of a connected graph G is denoted by $W(G;q)$ and is defined by

$$W(G;q) = \sum_{i<j} q^{d_G(v_i,v_j)},$$

where q is a parameter.The relation between Hosoya polynomial and Wiener index is

$$W(G) = \frac{d}{dq}(W(G;q))\Big|_{q=1.} \tag{1.1}$$

Hence, we can derive the expression for the Wiener index of G from that of the Hosoya polynomial of G.

Let $G = (V(G), E(G))$ be a graph. The complement $\overline{G}$ of G is the graph with the same vertex set as G, in which two vertices are adjacent if and only if they are not adjacent in G. The *line graph* [15] $L(G)$ of G is the graph whose vertex set $V(L(G)) = E(G)$ in which two vertices are adjacent if and only if they correspond to adjacent edges in G. If G is a (n, m) graph whose vertices have degrees $d_G(v_i)$, then the line graph $L(G)$ has $n_L = m$ vertices and $m_L = -m + \frac{1}{2}\sum_{i=1}^{n} d_G^2(v_i)$ edges.

Chartrand [2] introduced the concept of *jump graph* $J(G)$ of a graph and determined all the graphs G for which sequence $\{J^k(G)\}$ of iterated jump graphs converges, diverges or terminates. *Jump graph* $J(G)$ of a graph G is a graph whose vertices are the edges of G and two vertices of $J(G)$ are adjacent if and only if they are nonadjacent edges of G. Evidently, the jump graph $J(G)$ of G is complement of the line graph $L(G)$ of G. If G is a (n, m) graph whose vertices have degrees $d_G(v_i)$, then the jump graph $J(G)$ has $n_J = m$ vertices and $m_J = \frac{m(m+1)}{2} - \frac{1}{2}\sum_{i=1}^{n} d_G^2(v_i)$ edges.

In [22], B. Wu and X. Guo characterized the connected jump graphs with diameter r for which $1 \leq r \leq 4$. Moreover, they determined all the self-complementary jump graphs. In [23], B. Wu and J. Meng characterized the hamiltonian jump graphs. Let G be a graph of size $m \geq 1$. Then, $J(G)$ is connected [2] if and only if G contains no edge that is adjacent to every other edge of G, unless $G = K_4$ or C_4.

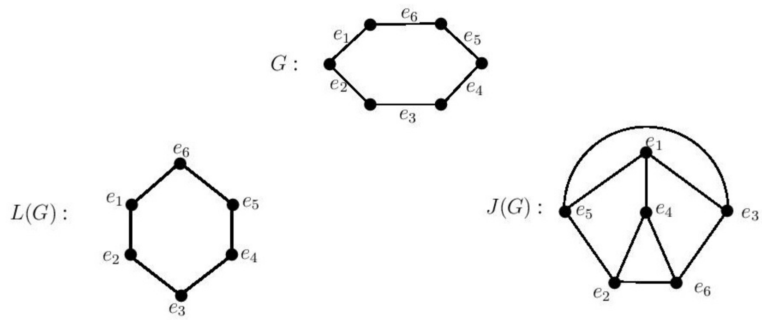

FIGURE 1. self-explanatory examples of a graph G, its line graph $L(G)$ and jump graph $J(G)$.

In chemical literature, there have been a few earlier attempts to shift from ordinary molecular graph to their transformations. The line graph is used in [7, 8, 9]. Attempts to use graph complements were recently reported in [19]. In the present work, we obtain the expressions for Wiener index and Hosoya polynomial of graphs with diameter ≤ 3. Further, we obtain Wiener index and Hosoya polynomial of jump graph of certain graph families. In addition, we give bounds for Wiener index of *jump graph*. The star S_n is a complete bipartite graph $K_{1,n-1}$ and the vertex of degree $n-1$ in S_n is called the *central vertex* of S_n. The graph G obtained from S_p and S_q by joining their central vertices by an edge is called a *double star*[1] and is denoted by $S_{p,q}$.

The first Zagreb index [12] is defined as

$$M_1(G) = \sum_{v_i \in V} d_G^2(v_i) = \sum_{i=1}^{n} d_G^2(v_i),$$

is one among the widely studied degree-based indices, which was introduced by Gutman et al. in 1972. For graph-theoretical terminology and notation we follow [13, 15]. The following Theorems are useful for proving our main results.

Theorem 1.1. [18] *The Wiener polynomial satisfies the following conditions:*

(i): *$deg(W(G;q))$ equals the diameter of G.*

(ii): $[q^o]W(G;q) = 0$.

(iii): $[q^1]W(G;q) = |E(G)|$, *where E(G) is an edge set of G.*

(iv): $W(G;1) = \binom{|V(G)|}{2}$, *where $V(G)$ is the vertex set of G.*

(v): $W'(G;1) = W(G)$.

In Wiener polynomial $W(G;q)$, the coefficients of q^0 is always zero and the coefficients of q^1 is equal to the number of edges of graph G. Wiener polynomial at $q = 1$ gives $\binom{|V(G)|}{2}$ and differentiating the Wiener polynomial at $q = 1$ gives the Wiener index of graph G.

Theorem 1.2. [20] *If G is a (n, m) graph with $diam(G) \leqslant 2$, then*

$$W(G) = n(n-1) - m.$$

Theorem 1.3. [4] *If G is a simple graph with n vertices and m edges, then*

$$2m(2p+1) - pn(1+p) \leq \sum_{i=1}^{n} d_G^2(v_i), \text{ where } p = \lfloor \tfrac{2m}{n} \rfloor,$$

and equality holds if and only if the difference of the degrees of any two vertices of graph G is at most one. Here $\lfloor x \rfloor$ denotes the greatest positive integer less than or equal to x.

Theorem 1.4. [3] *If G is a simple graph with n vertices and m edges, then*

$$\sum_{i=1}^{n} d_G^2(v_i) \leq m[\tfrac{2m}{n-1} + n - 2].$$

Theorem 1.5. [4] *Let G be a connected graph with n vertices and m edges. Then*

$$\sum_{i=1}^{n} d_G^2(v_i) = m[\tfrac{2m}{n-1} + n - 2]$$

if and only if G is a star graph or a complete graph.

Theorem 1.6. [17] *If G is a connected graph with vertex set $V = \{v_1, v_2, ..., v_n\}$ and edge set $E = \{e_1, e_2, ..., e_m\}$, then*

$$W(L(G)) \geq \sum_{i=1}^{n} \tfrac{d_G(v_i)(d_G(v_i)-1)}{2} + m(m-1) - \sum_{i=1}^{m} d_G(e_i).$$

Theorem 1.7. [11] *For any nontrivial tree T_n of order n, $M_1(P_n) \leq M_1(T_n)$.*

2. Results on the Wiener index of jump graph of a graph

In literature, till today we have direct expression to calculate Wiener index of the graphs whose *diameter* ≤ 2. But there is no analogous expression for graphs with *diameter* ≥ 3. We now establish an expression to find Wiener index of graphs with *diameter* ≤ 3. We use this theorem to find the Wiener index of jump graphs.

Theorem 2.1. *For any graph G of order n, size m with $diam(G) \leq 3$,*

$$W(G) = n(n-1) - m + W_p(G).$$

Proof. Suppose G is a graph of order n and size m with $diam(G) \leq 3$. Define the sets $A = \{v_i \in V : e(v_i) = 2\}$ and $B = \{v_i \in V : e(v_i) = 3\}$, where $|A| + |B| = n$. If $v_i \in A$, then define two sets A_1 and A_2 as $A_1 = \{v \in V : d_G(v_i, v) = 1\}$ and $A_2 = \{v \in V : d_G(v_i, v) = 2\}$. Obviously $|A_1| + |A_2| = n - 1$. Then

$$\begin{aligned} d(v_i \mid G) &= |A_1| + 2|A_2| \\ &= (n-1) + |A_2| \\ &= (n-1) + (n-1-|A_1|) \\ &= 2n - 2 - d_G(v_i) \qquad (2.1) \end{aligned}$$

If $v_i \in B$, then define three sets B_1, B_2 and B_3 as $B_1 = \{v \in V : d_G(v_i, v) = 1\}$, $B_2 = \{v \in V : d_G(v_i, v) = 2\}$ and $B_3 = \{v \in V : d_G(v_i, v) = 3\}$. Clearly $|B_1| + |B_2| + |B_3| = n - 1$. Then

$$\begin{aligned} d(v_i \mid G) &= |B_1| + 2|B_2| + 3|B_3| \\ &= (n-1) + |B_2| + 2|B_3| \\ &= (n-1) + (n-1-|B_1|) + |B_3| \\ &= 2n - 2 - d_G(v_i) + P_{v_i} \qquad (2.2) \end{aligned}$$

where P_{v_i} is the number of vertices which are at a distance 3 from vertex v_i.
Now,

$$\begin{aligned} W(G) &= \frac{1}{2}\sum_{i=1}^{n} d(v_i \mid G) \\ &= \frac{1}{2}\left(\sum_{v_i\in A} d(v_i \mid G) + \sum_{v_i\in B} d(v_i \mid G)\right). \end{aligned}$$

From Eqs. (2.1) and (2.2), we have

$$\begin{aligned} W(G) &= \frac{1}{2}\left\{\sum_{v_i\in A}(2n-2-d_G(v_i)) + \sum_{v_i\in B}(2n-2-d_G(v_i)+P_{v_i})\right\} \\ &= \frac{1}{2}\left\{(2n-2)(|A|+|B|) - \sum_{v_i\in A} d_G(v_i) - \sum_{v_i\in B} d_G(v_i) + \sum_{v\in B} P_{v_i}\right\} \\ &= n(n-1) - \frac{1}{2}\sum_{i=1}^{n} d_G(v_i) + \frac{1}{2}(2W_p(G)) \\ &= n(n-1) - m + W_p(G). \end{aligned}$$

□

Lemma 2.1. *For any nontrivial tree* $T_n \notin \{S_n, S_{p,q}\}$, *diam*$(J(T_n)) \leq 3$.

Proof. If $T_n \in \{S_n, S_{p,q}\}$, then $J(T_n)$ is disconnected and one cannot determine its Wiener index. Thus, consider the nontrivial tree $T_n \notin \{S_n, S_{p,q}\}$. If e_i and e_j are vertices in $J(T_n)$ corresponding to nonadjacent edges of G, then e_i and e_j are adjacent in $J(T_n)$ and obviously $d_{J(T_n)}(e_i, e_j) = 1$. If e_i and e_j are vertices in $J(T_n)$ corresponding to adjacent edges of G, then we have following two cases:

Case 1. If there exist a common edge e_k which is not adjacent to both e_i and e_j in G, then

$$d_{J(T_n)}(e_i, e_j) = d_{J(T_n)}(e_i, e_k) + d_{J(T_n)}(e_k, e_j) = 2.$$

Case 2. If the above case does not hold, then there exist two nonadjacent edges e_s and e_t in G such that e_s is not adjacent to e_i and e_t is not adjacent to e_j in G. Therefore,

$$d_{J(T_n)}(e_i, e_j) = d_{J(T_n)}(e_i, e_s) + d_{J(T_n)}(e_s, e_t) + d_{J(T_n)}(e_t, e_j) = 3.$$

□

Theorem 2.2. *For any nontrivial tree* $T_n \notin \{S_n, S_{p,q}\}$ *of order* n,

$$W(J(T_n)) = \tfrac{1}{2}\left[(n-1)(n-4) + \sum_{i=1}^{n} d_G^2(v_i)\right] + K,$$

where K *is the number of pairs of adjacent edges* $(a \sim b)$ *such that all other edges are adjacent either to an edge* a *or to an edge* b *in* G.

Proof. Let $T_n \notin \{S_n, S_{p,q}\}$ be nontrivial tree of order n. Then by Lemma 2.1, $diam(J(T_n)) \leq 3$. Therefore, from Theorem 2.1,
we have

$$W(J(T_n)) = n_J(n_J - 1) - m_J + W_p(J(T_n)).$$

By definition of Wiener polarity index, $W_p(J(T_n))$ is number of pair of vertices which are at distance $3 = K$, i.e., obviously the number of pairs of adjacent edges $(a \sim b)$ which are adjacent either to an edge a or to an edge b in G.
Hence

$$\begin{aligned} W(J(T_n)) &= m(m-1) - \frac{1}{2}\left[m(m+1) - \sum_{i=1}^{n} d_G^2(v_i)\right] + K \\ &= \frac{1}{2}\left[m(m-3) + \sum_{i=1}^{n} d_G^2(v_i)\right] + K. \end{aligned}$$

For a tree, we have $m = n-1$ and $W(J(T_n)) = \frac{1}{2}\left[(n-1)(n-4) + \sum_{i=1}^{n} d_G^2(v_i)\right] + K$.

□

Theorem 2.2 can also be written as, $W(J(T_n)) = \frac{1}{2}\left[(n-1)(n-4) + M_1(T_n)\right] + K$.

Corollary 2.1. *For any nontrivial tree T_n of order n,*

$$W(J(P_n)) \leq W(J(T_n)).$$

Proof. From Theorem 1.7,

$$\begin{aligned} M_1(P_n) \leq M_1(T_n) \quad &\Longrightarrow \quad 2(2n-3) \leq M_1(T_n) \\ &\Longrightarrow \quad \frac{1}{2}[(n-1)(n-4) + 2(2n-3)] + K \leq \frac{1}{2}[(n-1)(n-4) + M_1(T_n)] + K. \end{aligned}$$

Therefore, by Theorem 2.2, $W(J(P_n)) \leq W(J(T_n))$. □

Corollary 2.2. *For any path P_n of order $n \geq 6$,*

$$W(J(P_n)) = \tfrac{n^2-n-2}{2}.$$

Proof. For any path P_n of order $n \geq 6$, the distance between the adjacent vertices of $J(P_n)$ which corresponds to edges of P_n is one where the edges in P_n are nonadjacent and the distance between nonadjacent vertices in $J(P_n)$ is two which corresponds to adjacent edges in P_n. Therefore, $K = 0$. From Theorem 2.2,

$$\begin{aligned} W(J(P_n)) &= \frac{1}{2}\left[(n-1)(n-4) + \sum_{i=1}^{n} d_G^2(v_i)\right] + K \\ &= \frac{1}{2}[(n-1)(n-4) + 2(2n-3)] \\ &= \frac{n^2-n-2}{2}. \end{aligned}$$

□

Theorem 2.3. *If $K_{a,b}$ is the complete bipartite graph, then*

$$W(J(K_{a,b})) = \begin{cases} \frac{ab}{2}[ab+a+b-3] & if \;\; a,b > 2, \\ \frac{ab}{2}[ab+a+b-3] + b & if \;\; a = 2,\; b > 2. \end{cases}$$

Proof. If $a = 1$, then $K_{a,b}$ is star and $J(K_{a,b})$ is totally disconnected. If $a = b = 2$, then $J(K_{a,b})$ is disconnected.

For $a, b > 2$: In $J(K_{a,b})$, the distance between adjacent vertices is one which corresponds to nonadjacent edges of $K_{a,b}$ and the distance between nonadjacent vertices in $J(K_{a,b})$ is two when the edges of $K(a,b)$ are adjacent.

Thus, $diam(J(K_{a,b})) = 2$.

From Theorem 1.2,

$$W(J(K_{a,b})) = n_J(n_J - 1) - m_J.$$

For $K_{a,b}$, $n_J = ab$, $m_J = \frac{ab(ab+1)}{2}$ and $\sum_{i=1}^{n} d_G^2(v_i) = ab(a+b)$.

Therefore,

$$\begin{aligned} W(J(K_{a,b})) &= ab(ab-1) - \left[\frac{ab(ab+1)}{2} - \frac{1}{2}ab(a+b)\right] \\ &= \frac{ab}{2}(ab + a + b - 3). \end{aligned}$$

For $a = 2,\ b > 2$:

$$diam(J(K_{a,b})) = 3.$$

From Theorem 2.1, we have $W(J(K_{a,b})) = n_J(n_J - 1) - m_J + W_p(J(K_{a,b}))$

Note that, $W_p(J(K_{a,b})) = b$.

Hence

$$W(J(K_{a,b})) = \frac{ab}{2}(ab + a + b - 3) + b.$$

□

Theorem 2.4. *Let G be a graph of order n and size m with no edge adjacent to all other edges. Then*

$$W(J(G)) \geq \tfrac{1}{2}\left[m(m-3) + \sum_{i=1}^{n} d_G^2(v_i)\right].$$

Equality holds for $diam(J(G)) \leq 2$.

Proof. For each vertex v_i, there are $d_G(v_i)$ edges incident to v_i. These $d_G(v_i)$ edges form a complete graph $K_{d_G(v_i)}$ in $L(G)$, and they form a totally disconnected graph $\overline{K_{d_G(v_i)}}$ in $J(G)$. Hence contributes the value $\binom{d_G(v_i)}{2}$ to the $W(L(G))$ and atleast the value $2\binom{d_G(v_i)}{2}$ to the $W(J(G))$.

Consider an edge $e = uv$ which is adjacent to $d_G(e) = d_G(u)+d_G(v)-2$ edges at u and v taken together. Hence the edge e is not adjacent to the remaining $(m-1-d_G(e))$ edges of G. Therefore, the vertex e is adjacent to these $(m-1-d_G(e))$ vertices in $J(G)$. Hence each such edge e contributes the value $(m-1-d_G(e))$ to $W(J(G))$. Thus,

$$\begin{aligned} W(J(G)) &\geq \sum_{i=1}^{n}[d_G(v_i)(d_G(v_i)-1)] + \frac{1}{2}\sum_{i=1}^{m}[m-1-d_G(e_i)] \\ &= \sum_{i=1}^{n}(d_G^2(v_i) - d_G(v_i)) + \frac{1}{2}\left[m(m-1) - \sum_{i=1}^{m} d_G(e_i)\right] \\ &= \sum_{i=1}^{n} d_G^2(v_i) - 2m + \frac{1}{2}\left[m(m-1) - 2\left(-m + \frac{1}{2}\sum_{i=1}^{n} d_G^2(v_i)\right)\right] \\ &= \frac{1}{2}\left[m(m-3) + \sum_{i=1}^{n} d_G^2(v_i)\right]. \end{aligned}$$

Hence, $W(J(G)) \geq \frac{1}{2}\left[m(m-3) + \sum_{i=1}^{n} d_G^2(v_i)\right]$.

For the equality:

If $diam(J(G)) \leq 2$, then distance between nonadjacent vertices in $J(G)$ contributes exactly the value $2\binom{d_G(v_i)}{2}$ to $W(J(G))$.

Therefore,

$$\begin{aligned} W(J(G)) &= \sum_{i=1}^{n}[d_G(v_i)(d_G(v_i)-1)] + \frac{1}{2}\sum_{i=1}^{m}[m-1-d_G(e_i)] \\ &= \frac{1}{2}\left[m(m-3) + \sum_{i=1}^{n} d_G^2(v_i)\right]. \end{aligned}$$

□

Corollary 2.3. *If G is a $r-$regular graph with n vertices, then*

$$W(J(G)) \geq \frac{nr}{2}\left(\frac{nr+4r-6}{4}\right).$$

Proof. If G is a $r-$regular graph, then $d_G(v_i) = r$ for all $v_i \in V(G)$, and $m = \frac{nr}{2}$.
Therefore, from Theorem 2.4,
we have

$$\begin{aligned} W(J(G)) &\geq \frac{(\frac{nr}{2})(\frac{nr}{2}-3)}{2} + \frac{1}{2}\sum_{i=1}^{n} r^2 \\ &= \frac{nr}{2}\left[\frac{nr-6}{4} + r\right] \\ &= \frac{nr}{2}\left(\frac{nr+4r-6}{4}\right). \end{aligned}$$

Hence, $W(J(G)) \geq \frac{nr}{2}\left(\frac{nr+4r-6}{4}\right)$. □

Corollary 2.4. *For any cycle C_n of order $n \geq 5$,*

$$W(J(C_n)) = \frac{n(n+1)}{2}.$$

Proof. For any cycle C_n of order $n \geq 5$, the distance between the adjacent vertices of $J(C_n)$ which corresponds to the nonadjacent edges of C_n is one and the distance between the nonadjacent vertices in $J(C_n)$ is two which corresponds to the adjacent edges in C_n.
Therefore, $diam(J(C_n)) \leq 2$.
Thus from Theorem 2.4, we have

$$W(J(G)) = \frac{1}{2}\left[m(m-3) + \sum_{i=1}^{n} d_G^2(v_i)\right].$$

Since cycle C_n of order n has $m = n$ edges and degree of each vertex is two.
Therefore, $\sum\limits_{i=1}^{n} d_G^2(v_i) = 4n$.
Thus,

$$W(J(C_n)) = \frac{n(n+1)}{2}.$$

□

Next, we determine the Wiener index of jump graph of a wheel. For $n \geq 4$, a wheel W_n is defined to be the graph $K_1 + C_{n-1}$ having $m = 2(n-1)$ edges.

Corollary 2.5. *If W_n is a wheel of order $n \geq 6$, then*

$$W(J(W_n)) = \frac{5n^2-7n+2}{2}.$$

Proof. For any wheel graph W_n of order $n \geq 6$, the distance between adjacent vertices of $J(W_n)$ is one which corresponds to nonadjacent edges of W_n and the distance between nonadjacent vertices in $J(W_n)$ is two when the edges in W_n are adjacent. Therefore, $diam(J(W_n)) \leq 2$.
Thus from Theorem 2.4, we have

$$W(J(G)) = \frac{1}{2}\left[m(m-3) + \sum_{i=1}^{n} d_G^2(v_i)\right].$$

Since W_n has one vertex of degree $(n-1)$ and remaining $(n-1)$ vertices are of degree three. Then $\sum_{i=1}^{n} d_G^2(v_i) = (n-1)(n+8)$.
Thus,

$$W(J(W_n)) = \frac{5n^2-7n+2}{2}.$$

□

Corollary 2.6. *For any complete graph K_n of order $n \geq 5$,*

$$W(J(K_n)) = \frac{n(n-1)(n-2)(n+5)}{8}.$$

Proof. For any complete graph K_n of order $n \geq 5$, the distance between the adjacent vertices of $J(K_n)$ is one which corresponds to nonadjacent edges of K_n and the distance between the nonadjacent vertices in $J(K_n)$ is two which corresponds to adjacent edges in K_n.
Therefore, $diam(J(K_n)) \leq 2$.

Thus from Theorem 2.4, we have

$$W(J(K_n)) = \frac{1}{2}[m(m-3) + \sum_{i=1}^{n} d_G^2(v_i)].$$

For a complete graph, $m = \frac{n(n-1)}{2}$ and degree of each vertex is $(n-1)$.
Therefore, $\sum_{i=1}^{n} d_G^2(v_i) = n(n-1)^2$.
Thus,

$$W(J(K_n)) = \frac{n(n-1)(n-2)(n+5)}{8}.$$

□

Corollary 2.7. *Let G be any graph with n vertices such that $diam(J(G)) \leq 2$. Then*

$$\tfrac{n^2-n-2}{2} \leq W(J(G)) \leq \tfrac{n(n-1)(n-2)(n+5)}{8}.$$

Lower bound holds if G is a path and upper bound holds if G is a complete graph.

Proof. From Theorem 1.3, $2m(2p+1) - pn(1+p) \leq \sum_{i=1}^{n} d_G^2(v_i)$ and equality holds for a path. For a path of order n, $p = \lfloor \frac{2m}{n} \rfloor = 1$.
Therefore,

$$\begin{aligned} 2(2n-3) &\leq \sum_{i=1}^{n} d_G^2(v_i) \\ (2n-3) + \frac{m(m-3)}{2} &\leq \frac{m(m-3)}{2} + \frac{1}{2}\sum_{i=1}^{n} d_G^2(v_i) \end{aligned}$$

From Theorem 2.4, we have

$$\frac{n^2-n-2}{2} \leq W(J(G)).$$

Again from Theorems 1.4 and 1.5, we have

$$\sum_{i=1}^{n} d_G^2(v_i) \leq m\left[\frac{2m}{n-1} + (n-2)\right]$$

and equality holds if and only if G is a star graph or a complete graph. If G is a star graph, then $J(G)$ is disconnected. Therefore, we consider only complete graph. For

a complete graph, $m = \binom{n}{2}$ and $\sum\limits_{i=1}^{n} d_G^2(v_i) = n(n-1)^2$.
Thus,

$$\frac{m(m-3)}{2} + \frac{1}{2}\sum_{i=1}^{n} d_G^2(v_i) \leq \frac{m(m-3)}{2} + \frac{1}{2}n(n-1)^2.$$

Now from Theorem 2.4, we have

$$\begin{aligned} W(J(G)) &\leq \frac{n(n-1)}{2}\left[\left(\frac{n^2-n-6}{4}\right) + (n-1)\right] \\ &= \frac{n(n-1)}{8}(n^2+3n-10) \\ &= \frac{n(n-1)(n-2)(n+5)}{8}. \\ \text{Hence}, W(J(G)) &\leq \frac{n(n-1)(n-2)(n+5)}{8}. \end{aligned}$$

□

Now, the simple reduced form of Theorem 1.6 is as follows:

Lemma 2.2. *Let G be a connected graph with vertex set $V = \{v_1, v_2, ..., v_n\}$. Then*

$$W(L(G)) \geq m^2 - \tfrac{1}{2}\sum_{i=1}^{n} d_G^2(v_i).$$

Proof. Let G be a connected graph with vertex set $V = \{v_1, v_2, ..., v_n\}$ and edge set $E = \{e_1, e_2, ..., e_m\}$.

Then

$$\begin{aligned}
W(L(G)) &\geq \sum_{i=1}^{n} \frac{d_G(v_i)(d_G(v_i)-1)}{2} + m(m-1) - \sum_{i=1}^{m} d_G(e_i) \\
&= \frac{1}{2}\sum_{i=1}^{n} d_G^2(v_i) - \frac{1}{2}\sum_{i=1}^{n} d_G(v_i) + m^2 - m - \sum_{i=1}^{m} d_G(e_i) \\
&= \frac{1}{2}\sum_{i=1}^{n} d_G^2(v_i) - \frac{1}{2}(2m) + m^2 - m - 2\left(-m + \frac{1}{2}\sum_{i=1}^{n} d_G^2(v_i)\right) \\
&= \frac{1}{2}\sum_{i=1}^{n} d_G^2(v_i) + m^2 - \sum_{i=1}^{n} d_G^2(v_i) \\
&= m^2 - \frac{1}{2}\sum_{i=1}^{n} d_G^2(v_i).
\end{aligned}$$

Hence, $W(L(G)) \geq m^2 - \frac{1}{2}\sum_{i=1}^{n} d_G^2(v_i)$. □

Theorem 2.5. *Let G be a connected graph of order n and size m with no edge adjacent to all other edges of G. Then*

$$W(L(G)) + W(J(G)) \geq \tfrac{3}{2}\, m(m-1).$$

Proof. Let G be a connected graph with vertex set $V = \{v_1, v_2, ..., v_n\}$.
Then from Lemma 2.2, we have

$$W(L(G)) \geq m^2 - \frac{1}{2}\sum_{i=1}^{n} d_G^2(v_i). \tag{2.3}$$

Now from Theorem 2.4, we have

$$W(J(G)) \geq \frac{1}{2}\left[m(m-3) + \sum_{i=1}^{n} d_G^2(v_i)\right]. \tag{2.4}$$

By adding Eqs. (2.3) and (2.4), we obtain

$$W(L(G)) + W(J(G)) \geq \frac{3}{2}m(m-1).$$

□

Theorem 2.6. *Let $G \neq K_2 \cdot K_3$ be a unicyclic graph. Then $W(J(G)) \geq W(\overline{G})$ with equality only if G is the cycle graph C_n.*

Proof. It is evident from the fact that, $L(C_n)$ and C_n are isomorphic. Hence $\overline{L(C_n)}$ and $\overline{C_n}$ are isomorphic. Obviously $J(C_n)$ and $\overline{C_n}$ are isomorphic. Therefore, $W(J(C_n)) = W(\overline{C_n})$.

Assume that, G is different from C_n. Suppose $G = K_2 \cdot K_3$. Then $J(G)$ is diconnected.

As unicyclic graph have an equal number of vertices and edges, one can construct bijective mapping between edge and vertex sets of G. We choose following mapping g of the edges onto vertices.

Let the vertices belonging to the (unique) cycle of G be $\{v_1, v_2, ..., v_p\}$ such that v_i is adjacent to v_{i+1}, $i = 1, 2, ..., p$, assuming that $v_{p+1} = v_1$. If $e_i = v_i v_{i+1}$ is an edge of G, belonging to its cycle, then for $i = 1, 2, ..., p$, $g(e_i) = v_i$. Let $e'' = uv$ be an edge of G not belonging to the cycle. Let v_i be any vertex of G, belonging to the cycle. If the distance between u and v_i is smaller than the distance between v and v_i, then $g(e'') = v$.

The bijection g has the following property:

If the edges e_i and e_j are not adjacent in G, then the vertices $g(e_i) = v_i$ and $g(e_j) = v_j$ are not adjacent in G. i.e., if vertices e_i and e_j are adjacent in $J(G)$, then the vertices v_i and v_j are adjacent in $\overline{G}$. This implies $J(G)$ is isomorphic to a spanning subgraph of $\overline{G}$.

This result follows from the fact that Wiener index of a graph cannot exceed the Wiener index of its connected spanning subgraph. If G is different from C_n, then $\overline{G}$ possess more edges than $J(G)$ and the inequality in this result must be strict. □

3. Results on the Hosoya Polynomial of jump graph of a graph

In literature, till today we have direct expression to calculate Hosoya polynomial of the graphs whose *diameter* ≤ 2. But there is no analogous expression for graphs with *diameter* ≥ 3. We now establish an expression to find Hosoya polynomial of graphs with *diameter* ≤ 3. We use this theorem to find the Hosoya polynomial of jump graphs.

Theorem 3.1. *Let G be a graph of order n and size m with $diam(G) \leq 3$. Then*

$$W(G;q) = W_p(G)q^3 + \left(\binom{n}{2} - W_p(G) - m\right)q^2 + mq$$

and

$$W(G) = W_p(G) + n(n-1) - m.$$

Proof. Let G be a graph of order n and size m with $diam(G) \leq 3$. Then by definition of Hosoya polynomial,
we have

$$W(G;q) = \sum_{u,v \in V(G)} q^{d_G(u,v)}$$

and by Theorem 1.1, the highest power of polynomial is equal to the diameter of G. Let $A_i(G) = |\{(u,v) : d_G(u,v) = i\}|$ for $i = 1, 2, 3$. Therefore, the expected Hosoya polynomial for G is

$$W(G;q) = \sum_{i=1}^{3} A_i(G)q^i.$$

By definition of $A_i(G)$,
we have
$A_1(G) = m$, $A_3(G) = W_p(G)$ and $A_2(G) = \binom{n}{2} - m - W_p(G)$.
Therefore,

$$W(G;q) = W_p(G)q^3 + \left(\binom{n}{2} - W_p(G) - m\right)q^2 + mq. \tag{3.1}$$

From Eq. (1.1), the Wiener index of G is

$$\begin{aligned} W(G) &= \frac{d}{dq}(W(G;q))\Big|_{q=1} \\ &= 3W_p(G) + 2\left(\binom{n}{2} - W_p(G) - m\right) + m \\ &= W_p(G) + n(n-1) - m. \qquad (3.2) \end{aligned}$$

□

Corollary 3.1. *For a nontrivial tree $T_n \notin \{S_n, S_{a,b}\}$ of order n, the Hosoya polynomial is given by*

$$\begin{aligned} W(J(T_n);q) &= Kq^3 + \left(\binom{n-1}{2} - K - \frac{m(m+1)}{2} + \frac{1}{2}\sum_{i=1}^{n} d_G^2(v_i)\right)q^2 \\ &\quad + \left(\frac{m(m+1)}{2} - \frac{1}{2}\sum_{i=1}^{n} d_G^2(v_i)\right)q. \end{aligned}$$

and $W(J(T_n)) = \frac{1}{2}\left[(n-1)(n-4) + \sum_{i=1}^{n} d_G^2(v_i)\right] + K$ *, where K is the number of pairs of adjacent edges $(a \sim b)$ such that all other edges are either adjacent to an edge a or adjacent to an edge b in G.*

Proof. From Lemma 2.1, the $diam(J(T_n)) \leq 3$. Therefore, by definition of Wiener polarity index, $W_p(J(T_n))$ is number of pair of vertices which are at distance $3 = K$. Therefore, K is obviously the number of pairs of adjacent edges $(a \sim b)$ which are either adjacent to an edge a or adjacent to an edge b in G.

Thus, the proof follows by substituting the Wiener polarity index $W_p(J(T_n))$ and order of the tree T_n in Eqs. (3.1) and (3.2). □

Corollary 3.2. *For a complete bipartite graph $K_{a,b}$ the Hosoya polynomial is given by*

$$W(J(K_{a,b});q) = \begin{cases} \frac{1}{2}ab(a+b-2)q^2 + \frac{ab(ab+1)}{2}q & if\ a,b > 2, \\ bq^3 - 3bq^2 + \frac{2b(2b+1)}{2}q & if\ a = 2, b > 2, \end{cases}$$

and

$$W(J(T_n)) = \begin{cases} \frac{ab}{2}[ab+a+b-3] & if \quad a,b>2, \\ b[3b-1]+b & if \quad a=2, b>2. \end{cases}$$

Proof. <u>$For\ a,b>2$</u> : In $J(K_{a,b})$, the distance between the adjacent vertices of $J(K_{a,b})$ is one which corresponds to nonadjacent edges of $K_{a,b}$ and the distance between the nonadjacent vertices in $J(K_{a,b})$ is two which corresponds to adjacent edges in $K_{a,b}$, therefore $diam(J(K_{a,b}))=2$.

<u>$For\ a=2\ ,b>2$</u> : $diam(J(K_{a,b})=3$ and $W_p(J(K_{a,b}))=b$.

Thus, the proof follows by substituting the above values and the order of $K_{a,b}$ in Eqs. (3.1) and (3.2). □

Corollary 3.3. *For a cycle C_n of order $n \geq 5$, the Hosoya polynomial is given by*

$$W(J(C_n);q) = nq^2 + \frac{n(n-3)}{2}q$$

and

$$W(J(C_n)) = \frac{n(n+1)}{2}.$$

Proof. For any cycle C_n of order $n \geq 5$, the distance between the adjacent vertices of $J(C_n)$ is one which corresponds to nonadjacent edges of C_n and the distance between the nonadjacent vertices in $J(C_n)$ is two which corresponds to adjacent edges in C_n, i.e., $diam(J(C_n)) \leq 2$. Therefore, $W_p(J(C_n))=0$.

Thus, the proof follows by substituting the Wiener polarity index $W_p(J(C_n))$ and order of the cycle C_n in Eqs. (3.1) and (3.2). □

Corollary 3.4. *For a wheel W_n of order $n \geq 6$, the Hosoya polynomial is given by*

$$W(J(W_n);q) = \frac{1}{2}(n^2+3n-4)q^2 + \frac{1}{2}(3n^2-13n+10)q \quad and$$

$$W(J(W_n)) = \frac{5n^2-7n+2}{2}.$$

Proof. For any wheel W_n of order $n \geq 6$, the distance between the adjacent vertices of $J(W_n)$ is one which corresponds to nonadjacent edges of W_n and the distance between the nonadjacent vertices in $J(W_n)$ is two which corresponds to adjacent edges in W_n. Therefore, $diam(J(W_n)) \leq 2$. Thus, $W_p(J(W_n)) = 0$.

Hence, the proof follows by substituting the Wiener polarity index $W_p(J(W_n))$ and order of W_n in Eqs. (3.1) and (3.2). □

Corollary 3.5. *For a complete graph K_n of order $n \geq 5$, the Hosoya polynomial is given by*

$$\begin{aligned} W(J(K_n);q) &= \frac{1}{2}(n^3 - 3n^2 + 2n)q^2 + \frac{1}{4}n(n-1)(n^2 - 3n + 4)q \quad \textit{and} \\ W(J(K_n)) &= \frac{n(n-1)(n-2)(n+5)}{8}. \end{aligned}$$

Proof. For any complete graph K_n of order $n \geq 5$, the distance between the adjacent vertices of $J(K_n)$ is one which corresponds to nonadjacent edges of K_n and the distance between the nonadjacent vertices in $J(K_n)$ is two which corresponds to adjacent edges in K_n. Therefore, $diam(J(K_n)) \leq 2$. Thus, $W_p(J(K_n)) = 0$.

Hence, the proof follows by substituting the Wiener polarity index $W_p(J(K_n))$ and order of K_n in Eqs. (3.1) and (3.2). □

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