The Schultz, Modified Schultz indices and their polynomials of the Jahangir graphs *Jn,m* for integer numbers *n=3, m≥3*

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ABSTRACT— ***Let G be a connected graph. The vertex-set and edge-set of G denoted by V(G) and E(G) respectively. The distance between the vertices u and v, d(u,v), in a graph is the number of edges in a shortest path connecting them.***

In this study, we compute the Schultz index $Sc(G)=½\sum_{u,v\in V(G)}(d_u+d_v)d(u,v)$, ***Modified Schultz index*** $Sc^*(G)=½\sum_{u,v\in V(G)}(d_u\times d_v)d(u,v)$ ***and their polynomials of the Jahangir graphs*** $J_{n,m}$ ***for integer numbers n=3, m≥3.***

Keywords— Topological Index, Schultz Index, Schultz polynomials, Jahangir graphs $J_{3,m}$.

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1. INTRODUCTION

Let G be a connected graph. The vertex-set and edge-set of G denoted by *V(G)* and *E(G)* respectively. The distance between the vertices *u* and *v, d(u,v),* in a graph is the number of edges in a shortest path connecting them. The maximum distance between two vertices of *G* is called the diameter of *G*, denoted by *d(G).*Two graph vertices are adjacent if they are joined by a graph edge. The degree of a vertex *v* is the number of vertices joining to u and denoted by d_v [1].

A topological index is a numerical quantity derived in an unambiguous manner from the structure graph of a molecule. The topological index of a molecule is a non-empirical numerical quantity that quantifies the structure and the branching pattern of the molecule. Therefore, the topological analysis of a molecule involves translating its molecular structure into a characteristic unique number (or index) that may be considered a descriptor of the molecule under examination.

One of the topological indexes is Schultz index and denoted by MTI. This index was introduced by *H. Schultz* in 1989, as the molecular topological index [2], and it is defined by:

$$Sc(G)=½\sum_{\{u,v\}\subset V(G)}(d_u+d_v)d(u,v)$$

where d_u and d_v are degrees of vertices *u* and *v*. The Schultz polynomial of *G* is defined as:

$$Sc(G,x)=½\sum_{\{u,v\}\subset V(G)}(d_u+d_v)x^{d(u,v)}$$

S. Klavžar and *I. Gutman* defined another based structure descriptors the Modified Schultz index of *G* is defined as [3]:

$$Sc^*(G)=½\sum_{\{u,v\}\subset V(G)}(d_u\times d_v)d(u,v)$$

The Modified Schultz polynomial of G is defined

$$Sc^*(G,x)=\tfrac{1}{2}\sum_{\{u,v\}\subset V(G)}(d_u\times d_v)x^{d(u,v)}$$

The Schultz, Modified Schultz indices studied and are computed in many papers series [4-19].

In this study, we compute the Schultz, Modified Schultz indices and Schultz, Modified Schultz polynomials of *Jahangir graphs* $J_{n,m}$ for integer numbers $n=3$, $m\geq 3$.

2. MAIN RESULTS

Let $J_{3,m}$ be the *Jahangir graphs* for all integer number $m\geq 3$, in this section we compute its Schultz, Modified Schultz indices and polynomials. The Jahangir graphs $J_{n,m}$ is a graph on $nm+1$ vertices i.e., a graph consisting of a cycle C_{nm} with one additional vertex which is adjacent to m vertices of C_{nm} at distance n to each other on C_{nm}.

For more details about the Jahangir graphs $J_{n,m}$ reader can see the paper series [20-30].

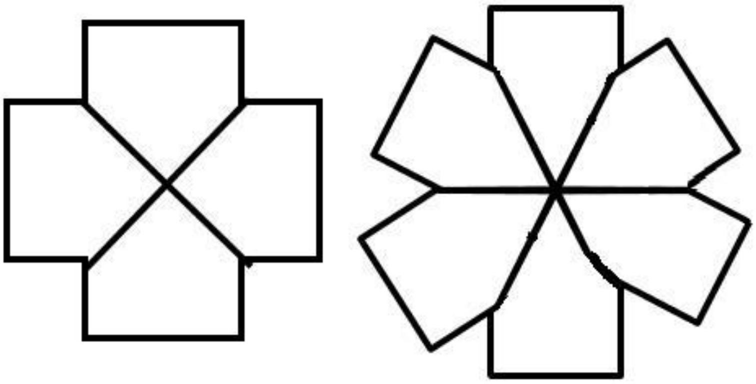

Figure 1. Two first Jahangir graphs $J_{3,4}$ and $J_{3,6}$.

Theorem 1. Let $J_{n,m}$ be the Jahangir graphs for integer numbers $n=3$, $m\geq 3$. Then, compute its Schultz, Modified Schultz polynomials and indices are equal to:

- The Schultz polynomial

$$Sc(J_{3,m},x)=m(m+17)x^1+5m(m+3)x^2+2m(5m-6)x^3+4m(2m-5)x^4$$

- The Modified Schultz polynomial

$$Sc^*(J_{3,m},x)=m(3m+16)x^1+\tfrac{1}{2}m(17m+23)x^2+4m(3m-4)x^3+4m(2m-5)x^4$$

- The Schultz index $Sc(J_{3,m})= m(78m-69)$.
- The Modified Schultz index $Sc^*(J_{3,m})= m(88m-89)$.

Proof. Consider the Jahangir graph $J_{3,m}$ (see Figure 1). By using [20-30], we know that this graph has $|V(J_{3,m})|=2m+m+1$ vertices and the number of edges is equal to $|E(J_{3,m})|=\frac{2\times 2m+3\times m+m\times 1}{2}=4m$.

Since $2m$ vertices of C_{3m} have degree two and m vertices of C_{3m} have degree three and one additional vertex (Center vertex) of $J_{3,m}$ has degree m.

We define three sub-sets of vertex set $V(J_{3,m})$ as:

$$A=V_2(J_{3,m})=\{v\in V(J_{3,m})|\ d_v=2\}$$
$$B=V_3(J_{3,m})=\{v\in V(J_{3,m})|\ d_v=3\}$$
$$C=V_m(J_{3,m})=\{v\in V(J_{3,m})|\ d_v=m=d_c\}$$

And obviously $A\cup B\cup C=V(J_{3,m})$ and $A\cap B\cap C=\emptyset$.

From Figure 1 and definition of Jahangir graph $J_{3,m}$, one can see that for all vertices u,v in $V(J_{3,m})$, $\exists d(u,v)\in\{1,2,3,4\}$ and the diameter of the Jahangir graph $J_{3,m}$ is equal to $d(J_{3,m})=4$. Obviously we have the $\binom{3m+1}{2}=\frac{(3m+1)(3m+2)}{2}$ distinct shortest path between vertices u and v of $J_{3,m}$.

Now, we should compute all cases of distinct paths between vertices of the Jahangir graph $J_{3,m}$ to achieve our aims. From the structure of the Jahangir graph $J_{3,m}$, we can see that there are m 1-edges paths (edges) between the vertex c and vertices of B or V_3, such that $d_c+d_v=m+3$, $d_c\times d_v=3m$. There are two 1-edges paths starts a vertex v of $B=V_3$ and ends vertices of $A=V_2$ (such that $d_u+d_v=5$, $d_u\times d_v=6$). And there are m 1-edges paths (edges) between two adjacent vertices v and u in A that $d_u+d_v=d_u\times d_v=4$. Thus, the first sentences of the Schultz and Modified Schultz polynomials of the Jahangir graph $J_{3,m}$ are equal to $(4m+5\times 2m+(m+3)m)x^1=(m^2+17m)x^1$ and $(4m+6\times 2m+3m\times m)x^1=(3m^2+16m)x^1$, respectively.

Now, we present all other cases of 2-edges paths, 3-edges paths and 4-edges paths of the Jahangir graph $J_{3,m}$, in following table and alternatively we can compute all coefficients of the Schultz and Modified Schultz polynomials of $J_{3,m}$ easily.

Table 1. All exist edges paths and alternative coefficients of the Schultz and Modified Schultz polynomials of the Jahangir graph $J_{3,m}$.

The distance $d(u,v)=i$	Cases of degree d_u & d_v	Repetitions of i-edges paths	A term of i^{th} sentence of Schultz polynomial	A term of i^{th} sentence of Modified Schultz polynomial
1	2 & 2	$m=\|B\|$	$4m$	$4m$
1	2 & 3	$2m=\|A\|$	$10m$	$12m$
1	3 & m	$m=\|B\|$	$(m+3)m$	$3m^2$
2	2 & 2	m	$4m$	$4m$
2	2 & 3	$2\|B\|$	$10m$	$12m$
2	2 & m	$2m=\|A\|$	$2m(m+2)$	$4m^2$
2	3 & 3	$½\|B\| (\|B\|-1)$	$3m(m-1)$	$\frac{9}{2}m(m-1)$
3	2 & 2	$\|A\|$	$8m$	$8m$
3	3 & 2	$\|B\|(\|A\|-4)$	$10m(m-2)$	$12m(m-2)$
4	2 & 2	$½\|A\|(\|A\|-5)$	$4m(2m-5)$	$4m(2m-5)$

Thus, by using the results from Table 1 and the definition of the Schultz, Modified Schultz polynomials and indices of the graph G, we have following computations for $Sc(J_{3,m},x)$, $Sc^*(J_{3,m},x)$, $Sc(J_{3,m})$ and $Sc^*(J_{3,m})$, $\forall m\geq 3$.

$$Sc(J_{3,m},x)=½\sum_{\{u,v\}\subset V(J_{2,m})}(d_u+d_v)x^{d(u,v)}$$

$$=(4m+10m+m(m+3))x^1+(4m+10m+2m(m+2)+3m(m-1))x^2+(8m+10m(m-2))x^3+4m(2m-5)x^4$$

$$=m(m+17)x^1+5m(m+3)x^2+2m(5m-6)x^3+4m(2m-5)x^4$$

and

$$Sc^*(J_{3,m},x)=½\sum_{\{u,v\}\subset V(G)}(d_u\times d_v)x^{d(u,v)}$$

$$=(4m+12m+3m^2)x^1+(4m+12m+4m^2+\tfrac{9}{2}m(m-1))x^2+(8m+12m(m-2))x^3+4m(2m-5)x^4$$

$$=m(3m+16)x^1+½m(17m+23)x^2+4m(3m-4)x^3+4m(2m-5)x^4.$$

Now, by using the first derivative of the Schultz, Modified Schultz polynomials of the Jahangir graph $J_{3,m}$, (evaluated at $x=1$), we can compute the Schultz, Modified Schultz indices as:

$$Sc(J_{3,m})=\left.\frac{\partial Sc(J_{3,m},x)}{\partial x}\right|_{x=1}$$

$$=[m(m+17)x^1+5m(m+3)x^2+2m(5m-6)x^3+4m(2m-5)x^4]'|_{x=1}$$

$$=[m(m+17)\times 1+5m(m+3)\times 2+2m(5m-6)\times 3+4m(2m-5)\times 4]$$

$$=78m^2-69m=m(78m-69).$$

And

$$Sc^*(J_{3,m})=Sc^*(J_{3,m},x)'|_{x=1}$$

$$=[m(3m+16)x^1+½m(17m+23)x^2+4m(3m-4)x^3+4m(2m-5)x^4]'|_{x=1}$$

$$=m(3m+16)\times 1+½m(17m+23)\times 2+4m(3m-4)\times 3+4m(2m-5)\times 4$$

$$=m(88m-89).$$

Here these completed the proof of Theorem 1. ■

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