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Research article

On the Schultz and Modified Schultz Polynomials of Some Harary Graphs

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Abstract

Let *G=(V,E)* be a simple connected graph of finite order $n=|V|$, with the vertex set *V* and the edge set *E*. The distance $d(u,v)$ between two vertices *u* and *v* of *G* is equal to the length of a shortest path that connects *u* and *v*. The Wiener index $W(G)=\frac{1}{2}\sum_{\{v,u\}\subset V(G)} d(v,u)$, the Schultz molecular topological index $Sc(G,x)=\frac{1}{2}\sum_{\{u,v\}\subseteq V(G)}(d_u+d_v)x^{d(u,v)}$ and the Modified Schultz molecular topological index $Sc^*(G,x)=\frac{1}{2}\sum_{\{u,v\}\subseteq V(G)}(d_u\times d_v)x^{d(u,v)}$ are based on the distances between the vertices of molecular graphs.

In this paper, we focus on the structure of an important regular graph and compute Schultz polynomial, Modified Schultz polynomial and their topological indices of the Harary graph $H_{2m,n}$

Keywords: Wiener index; Schultz polynomial; Modified Schultz polynomial; Regular graph, Harary graph.

Introduction

Let *G=(V,E)* be a simple connected graph of finite order $n=|V|$, such that it has vertex set *V=V(G)* and edge set *E=E(G)*. The distance between vertices u and *v* of *G*, denoted by *d(u,v)*, is the number of edges in a shortest path connecting them. An edge $e=uv$ of graph G is joined between two vertices u and v ($d(u,v)=1$). Also, the degree of a vertex $v \in V(G)$ is the number of adjacent vertices with v and denoted by d_v. A general reference for the notation in graph theory is [1].

In graph theory, we have many invariant polynomials for any graphs, that they have usually integer coefficients. Also, topological indices are real numbers related to a structural graph of a molecule. Such indices based on the distances in graph are widely used for establishing relationships between the structure of a molecular graph and their physicochemical properties. Usage of topological indices in biology and chemistry began in 1947 when chemist *Harold Wiener* [2] introduced Wiener index to demonstrate correlation between physicochemical properties of organic compounds and the index of their molecular graphs and defined as:

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

Also, for this topological index, there is Hosoya Polynomial. The Hosoya polynomial was introduced by *H. Hosoya*, in 1988 [3] and define as follow:

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

Another based structure descriptors is the "*molecular topological index*" (Schultz index) was introduced by *Harry P. Schultz* in 1989 [4]. The Schultz index is defined as:

$$Sc(G) = \frac{1}{2}\sum_{\{u,v\} \subset V(G)} (d_u + d_v) d(u,v)$$

where d_u and d_v are degrees of vertices u and v.

S. Klavžar and *I. Gutman* in 1997 [5] defined the Modified Schultz polynomial of G is defined as:

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

Now, let G be a connected graph. The Schultz polynomial of G is:

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

Also the modified Schultz polynomial of G is defined as:

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

Obviously, $Sc(G) = \frac{\partial Sc(G,x)}{\partial x}|_{x=1}$ and $Sc^*(G) = \frac{\partial Sc^*(G,x)}{\partial x}|_{x=1}$. These molecular topological polynomials and indices studied in many papers [6-9] and computed for some nanotubes in a series of papers [10-13].

In this paper, we obtained a closed formula of the Schultz polynomial, Modified Schultz polynomial and their topological indices for an interesting regular graph that called *Harary graph*. The general form of the Harary graph $H_{2m,n}$ is defined as follows:

Definition 1 [1, 14-17]. Let m and n be two positive integer numbers, then the Harary graph $H_{2m,n}$ is constructed as follows:

It has vertices $1,2.n-1,n$ and two vertices i and j are joined if $i-m \le j \le i+m$ (where addition is taken modulo n).

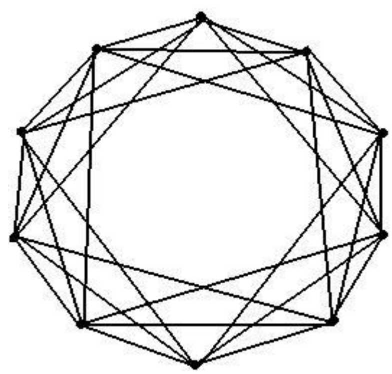

Figure1: The Harary graph $H_{6,10}$.

Results and Discussion

In this section we compute the Schultz polynomial, the Modified Schultz polynomial, the Schultz index and the Modified Schultz index of the Harary graph $H_{2m,n}$ in the following theorem.

Theorem 1. Let $G=H_{2m,n}$ be the Harary graph $\forall\, m,n \in \mathbb{N}$. Then,

- The Schultz polynomial of G is equal to

$$Sc(H_{2m,n};x)=\sum_{d=1}^{\left[\frac{n}{2m}\right]} 4nm^2x^d + 4md\left(H_{2m,n},\left[\frac{n}{2m}\right]+1\right)x^{\left[\frac{n}{2m}\right]+1}$$

- The Modified Schultz polynomial of G is equal to:

$$Sc^*(H_{2m,n};x)=\sum_{d=1}^{\left[\frac{n}{2m}\right]} 4nm^3x^d + 4m^2d\left(H_{2m,n},\left[\frac{n}{2m}\right]+1\right)x^{\left[\frac{n}{2m}\right]+1}$$

where
$$d\left(H_{2m,n},\left[\frac{n}{2m}\right]+1\right)=\begin{cases} n\times\left|m\times\left[\frac{n}{2m}\right]-\left[\frac{n}{2}\right]\right| & n \quad odd \\ n\times\left|m\times\left[\frac{n}{2m}\right]-\left[\frac{n}{2}\right]\right|-\frac{n}{2} & n \quad even \end{cases}$$

So, the Schultz index of $H_{2m,n}$ is

- If n be odd ($=2q+1$): $Sc(H_{2m,2q+1}) = 2m(2q+1)\left(2q+(2q-m)\left[{}^{q}\!/\!_{m}\right]-m\left[{}^{q}\!/\!_{m}\right]^2\right)$
- If n be even ($=2q$): $Sc(H_{2m,2q}) = 4qm\left(2q-1+(2q-m-1)\left[{}^{q}\!/\!_{m}\right]-m\left[{}^{q}\!/\!_{m}\right]^2\right)$

And the Modified Schultz index of G is

- If $n=2q+1$, $Sc^*(G) = 2nm^2\left(2q+(2q-m)\left[{}^{q}\!/\!_{m}\right]-m\left[{}^{q}\!/\!_{m}\right]^2\right)$
- If $n=2q$, $Sc^*(H_{2m,2q}) = 2nm^2\left(2q-1+(2q-m-1)\left[{}^{q}\!/\!_{m}\right]-m\left[{}^{q}\!/\!_{m}\right]^2\right)$

Before prove the main theorem, we need the following denotations.

Denotation 1. Let $d(u,v)=i$ is distance between vertices u and v of G. Then, $D_i=\{(u,v)\,|\,u,v\in V(G), d(u,v)=i\}$ and we denoted the size of D_i by $d(G,i)$. Suppose the topological diameter $d(G)$ is the longest topological distance in G. Therefore, the Hosoya polynomial of G is defined as:

$$H(\mathrm{G,x}) = \sum_{\{u,v\}\subset V(G)} x^{d(u,v)} = \sum_{i=0}^{d(G)} d(G,i)x^{d(u,v)}$$

and we obtain the Wiener index of G from the Hosoya polynomial of G, that is equal to:

$$W(\mathrm{G}) = \frac{1}{2}\sum_{v\in V(G)}\sum_{u\in V(G)} d(u,v) = \sum_{i=0}^{d(G)} d(G,i)d(u,v)$$

Denotation 2. Let G be an r-regular graph and for all vertex v of G, $d_v=r$. Thus, the Schultz and Modified Schultz polynomials of G will be

$$Sc(\mathrm{G,x}) = 2r\sum_{i=0}^{d(G)} d(G,i)x^{d(u,v)}$$

and

$$Sc^*(\mathrm{G,x}) = r^2\sum_{i=0}^{d(G)} d(G,i)x^{d(u,v)}$$

respectively.

Proof of Theorem 1. Consider the Harary graph $G=H_{2m,n}$ (Figure 1). This $2m$-regular graph has n vertices. In other words, $|V(H_{2m,n})|=n$ $(\forall m,n\in\mathbb{N})$ and has mn edges, since two vertices $v_i,v_j\in V(H_{2m,n})$ are adjacent if and only if $|i-j|\leq m$,

thus, $$|E(H_{2m,n})| = \frac{n(2m)}{2} = mn.$$

From the structure of $H_{2m,n}$ (Figure 1), one can see that all vertices of $H_{2m,n}$ have similar geometrical and topological conditions then the number of path as distance i in $H_{2m,n}$ ($d(H_{2m,n},i)$) is a multiple of the number of vertices (n). For example $\forall\, v\in V(H_{2m,n})$, there are $2m=d_v(H_{2m,n},1)$ paths as distance 1 (or all edges incident to v) in $H_{2m,n}$, therefore,

$$d_v(H_{2m,n},1)=2m\times n=2|E(H_{2m,n})|.$$

So, the first sentence of the Schultz polynomial and Modified Schultz polynomial of G is equal to $\frac{1}{2}(4m\times 2mnx^1)$ and $\frac{1}{2}(4m^2\times 2mnx^1)$, respectively.

From Figure 1, one can see that $\forall\, i=1,2,\dots,n\ \&\ v_i,v_{i+m}\in V(H_{2m,n})$, $d(v_i,v_{i\pm m+j})=2$ for all $j\in\square_m$ $(=\{0,2,\dots,m-1\})$ and $d_{vi}(H_{2m,n},2)=2m=2|\square_m|$. Since $v_iv_{i\pm m}$ and $v_{i\pm m}v_{i\pm m+j}$ are from $E(H_{2m,n})$ and $d(v_i,v_{i\pm m})=d(v_{i\pm m},v_{i\pm m+j})=1$. This implies that the second sentence of the Schultz polynomial and Modified Schultz polynomial of G is equal to $\frac{1}{2}n(4m\times 2mx^2)$ and $\frac{1}{2}n(4m^2\times 2mx^2)$, respectively.

Now, for vertices v_i and v_{i+m} of $V(H_{2m,n})$, $d(v_i,v_{i\pm m})=d(v_{i\pm m},v_{i\pm 2m})=d(v_{i\pm 2m},v_{i\pm 3m})=\ \dots=d(v_{i\pm(k-1)m},v_{i\pm km})=1$ such that $i\in\square_n$ $(=\{1,2,\dots,n\})$ and $k\leq\left[\frac{n/2}{m}\right]$. Thus

$\forall\, d=1,\dots,k;$ $\qquad d(v_i,v_{i\pm dm})=d$

and obviously $\qquad d(v_i,v_{i\pm dm+j})=d+1$ $(j=1,2,\dots,m-1)$.

These mentions imply that $\forall\, d=1,\dots,[n/2m],$ two sentences $\frac{1}{2}n(4m\times 2mx^d)$ and $\frac{1}{2}n(4m^2\times 2mx^d)$ are in the two polynomials "*Schultz*" and "*Modified Schultz*" of the Harary graph $G=H_{2m,n}$, respectively.

It is easy to see that the diameter $d(H_{2m,n})$ of the Harary graph $H_{2m,n}$ is equal to $d(H_{2m,n})=d(v_i,v_{i+[n/2m]})=[n/2m]+1$ $(\forall\, i\in\{1,2,\dots,n\})$.

Because for a vertex v_i of G $(\forall\, i\in\{1,2,\dots,n\})$, the distance between vertices v_i and $v_{i\pm([n/2m]m+j)}$ or $v_{i\pm[n/2]}$ is equal to $d(H_{2m,n})$ for all $j=1,2,\dots,[n/2]$. So $\forall\, v_i\in V(H_{2m,n})$ for an odd integer number n, $d_{vi}(H,[n/2m]+1)=|[n/2]-m\times[n/2m]|$ and also for an even integer number n $(=2q)$, $d(H,d(H))=q(|[q]-m\times[q/m]|-1)$.

Now, we enumerate all distinct shortest path between any $u,v\in V(H_{2m,n})$. Thus the Schultz polynomial of $H_{2m,n}$ is equal to:

$$\begin{aligned}
Sc\left(H_{2m,n},\mathrm{x}\right)&=\frac{1}{2}\sum_{\mathrm{v}\in \mathrm{V}\left(H_{2m,n}\right)}\sum_{u\in \mathrm{V}\left(H_{2m,n}\right)}(d_u+d_v)x^{d(u,v)}\\
&=\sum_{\substack{i,j=1\\ \{v_i,v_j\}\subset V(H_{2m,n})}}^{n}\left(d_{v_i}+d_{v_j}\right)x^{d\left(v_i,v_j\right)}\\
&=4m\sum_{i=1}^{n}\sum_{j=0}^{m-1}\sum_{k=0}^{\left[\frac{n}{2m}\right]}x^{d\left(v_i,v_{i\pm k+j}\right)}\\
&=4m\sum_{i=0}^{d(H_{2m,n})}d(H_{2m,n},i)x^{d(H_{2m,n},i)}
\end{aligned}$$

$$=4nm^2x^1+4nm^2x^2+\ldots+4nm^2x^{[n/2m]}+4m\times d(H_{2m,n},\left[{}^{n}\!/\!{}_{2m}\right]+1)x^{\left[{}^{n}\!/\!{}_{2m}\right]+1}$$

where $d(H_{2m,n},\left[{}^{n}\!/\!{}_{2m}\right]+1)=\begin{cases} n\times\left|m\times\left[\frac{n}{2m}\right]-\left[\frac{n}{2}\right]\right| & n \quad odd \\ n\times\left|m\times\left[\frac{n}{2m}\right]-\left[\frac{n}{2}\right]\right|-\frac{n}{2} & n \quad even \end{cases}$

And the Schultz index of $H_{2m,n}$ is

If n be odd: $Sc(H_{2m,n})=\frac{\partial Sc\left(H_{2m,n},\mathrm{x}\right)}{\partial x}|_{x=1}$.

$$=\frac{\partial\sum_{d=1}^{\left[{}^{n}\!/\!{}_{2m}\right]}4nm^2x^d+4mn\left(\left[{}^{n}\!/\!{}_{2}\right]-m\times\left[{}^{n}\!/\!{}_{2m}\right]\right)x^{\left[{}^{n}\!/\!{}_{2m}\right]+1}}{\partial x}|_{x=1}$$

$$=4nm^2\sum_{d=1}^{\left[{}^{n}\!/\!{}_{2m}\right]}d+4mn\left(\left[{}^{n}\!/\!{}_{2m}\right]+1\right)\left(\left[{}^{n}\!/\!{}_{2}\right]-m\times\left[{}^{n}\!/\!{}_{2m}\right]\right)$$

Now, for $n=2q+1$:

$$Sc(H_{2m,2q+1})=4m\left(2q+1\right)\left({}^{1}\!/\!{}_{2}\left[{}^{q}\!/\!{}_{m}\right]\left(\left[{}^{q}\!/\!{}_{m}\right]+1\right)m+\left(q-m\left[{}^{q}\!/\!{}_{m}\right]\right)\left(\left[{}^{q}\!/\!{}_{m}\right]+1\right)\right)$$

$$=4m\left(2q^2+q\right)+2m\left[{}^{q}\!/\!{}_{m}\right]\left(4q^2+2q\left(1-m\right)-m\right)-2m^2\left(2q+1\right)\left[{}^{q}\!/\!{}_{m}\right]^2.$$

Also, if n be an arbitrary even positive integer number ($n=2q$), then

$$Sc(H_{2m,2q})=\frac{\partial\sum_{d=1}^{\left[{}^{q}\!/\!{}_{m}\right]}8qm^2x^d+8mq^2-8qm^2\left[{}^{q}\!/\!{}_{m}\right]-4qmx^{\left[{}^{q}\!/\!{}_{m}\right]+1}}{\partial x}|_{x=1}$$

$$=8qm^2\sum_{d=1}^{\left[{}^{q}\!/\!{}_{m}\right]}d+4qm\left(2q-1\right)+4qm\left(2q-2m-1\right)\left[{}^{q}\!/\!{}_{m}\right]-8qm^2\left[{}^{q}\!/\!{}_{m}\right]^2$$

$$=4qm\left(2q-1+\left(2q-m-1\right)\left[{}^{q}\!/\!{}_{m}\right]-m\left[{}^{q}\!/\!{}_{m}\right]^2\right)$$

Now, the Modified Schultz polynomial of $H_{2m,n}$ is equal to:

$$Sc^*\left(H_{2m,n},\mathrm{x}\right)=\frac{1}{2}\sum_{\{\mathrm{v,u}\}\subset\mathrm{V}\left(H_{2m,n}\right)}d_u\times d_v x^{d(u,v)}$$

$$= \sum_{\substack{i,j=1 \\ \{v_i,v_j\}\subset V(H_{2m,n})}}^{n} \left(d_{v_i} \times d_{v_j}\right) x^{d(v_i,v_j)}$$

$$= 4m^2 \sum_{i=0}^{d(H_{2m,n})} d(H_{2m,n}, i) x^{d(H_{2m,n},i)}$$

$$=4nm^3x^1 + 4nm^3x^2 + \ldots + 4nm^3x^{[n/2m]} + 4m^2 \times d(H_{2m,n}, \left[\tfrac{n}{2m}\right]+1) x^{\left[\frac{n}{2m}\right]+1}$$

where $d(H_{2m,n}, \left[\tfrac{n}{2m}\right]+1) = \begin{cases} n\times\left|m\times\left[\frac{n}{2m}\right]-\left[\frac{n}{2}\right]\right| & n \quad odd \\ n\times\left|m\times\left[\frac{n}{2m}\right]-\left[\frac{n}{2}\right]\right| - \frac{n}{2} & n \quad even \end{cases}$

By according to the Schultz polynomial of $H_{2m,n}$, one can to see that $Sc^*(H_{2m,n})=m\times Sc(H_{2m,n})$. Since $Sc^*(H_{2m,n}) = \frac{\partial Sc^*(H_{2m,n};x)}{\partial x}\big|_{x=1} = m\frac{\partial Sc(H_{2m,n};x)}{\partial x}\big|_{x=1}$ and alternatively, for the Modified Schultz index of $H_{2m,n}$ we have easily:

- If $n=2q+1$, $Sc^*(H_{2m,2q+1}) = 2m^2(2q+1)\left(2q+(2q-m)\left[\tfrac{q}{m}\right]-m\left[\tfrac{q}{m}\right]^2\right)$
- If $n=2q$, $Sc^*(H_{2m,2q}) = 4qm^2\left(2q-1+(2q-m-1)\left[\tfrac{q}{m}\right]-m\left[\tfrac{q}{m}\right]^2\right)$

Here, the proof of theorem is completed.□

Conclusion

In this paper, topological polynomials called *"Schultz, Modified Schultz"* and their indices of an important regular graph were determined.

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