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Computing the Hosoya Polynomial, Wiener Index and Hyper-Wiener Index of the Harary Graph

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Abstract The distance $d(u,v)$ between two vertices u and v of a connected graph G is equal to the length of a shortest path that connects u and v. The Hosoya polynomial was introduced by *H. Hosoya* in 1988 and defined as $H(G,x)= \frac{1}{2}\sum_{v\in(V)}\sum_{u\in(V)} x^{d(u,v)}$. Also, the Wiener index $W(G)$ is the sum of all distances between vertices of G as $W(G)=\frac{1}{2}\sum_{v\in(V)}\sum_{u\in(V)} d(u,v)$ whereas the hyper-Wiener index $WW(G)$ is defined as $WW(G)=\frac{1}{2}\sum_{v\in V(G)}\sum_{u\in V(G)} (d(u,v)+d(u,v)^2)$. In this paper, we compute the Hosoya polynomial of the Harary graph. Also we compute the Wiener index and hyper Wiener index of this family of *Regular graph*s.

Keywords Harary graph, Topological Indices, Hosoya polynomial, Wiener Index, Hyper-Wiener index

1. Introduction

Let $G=(V,E)$ be a simple connected graph. The vertex-set and edge-set of G denoted by $V=V(G)$ and $E=E(G)$, respectively. An edge $e=uv$ of a graph G is joined between two vertices u and v. The distance between vertices u and v, $d(u,v)$, in a graph is the number of edges in a shortest path connecting them and the diameter of a graph G, $D(G)$ is the longest topological distance in G.

A topological index of a graph is a single unique number characteristic of the graph and is mathematically invariant under graph automorphism. The topological index of a molecular graph G is a non-empirical numerical quantity that quantifies the structure and the branching pattern of G.

Usage of topological indices in biology and chemistry began in 1947 when *H. Wiener* [1, 2] introduced *Wiener index* to demonstrate correlations between physicochemical properties of organic compounds and the index of their molecular graphs.

The *hyper-Wiener index* is one of distance-based graph invariants, (based structure descriptors), used for predicting physico–chemical properties of organic compounds. The hyper-Wiener index was introduced by *M. Randić* in 1993 [3, 4]. The Wiener index and the hyper Wiener index of G are defined as follows:

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

$$WW(G)=\frac{1}{2}\sum_{v\in V(G)}\sum_{u\in V(G)} (d(u,v)+d(u,v)^2) \tag{2}$$

respectively.

The *Hosoya polynomial* was first introduced by *H. Hosoya*, in 1988 [5] and define as follows:

$$H(G,x)= \frac{1}{2}\sum_{v\in(V)}\sum_{u\in(V)} x^{d(u,v)}. \tag{3}$$

In references [6-20], some properties and more historical details of the Wiener and Hyper Wiener indices and the Hosoya polynomial of molecular graphs are studded.

2. Main Result

The aim of this section is to obtain a closed formula of Hosoya polynomial, Wiener index and hyper-Wiener index of the Harary graph $H_{2r+1,2n}$. At first we need the following definition.

Definition 1 [21-24]. Let r and n be two positive integer numbers and $n\geq r+1$, then in the Harary graph $H_{2r+1,2n}$, two vertices i and j are joined if and only if $|i-j|\leq r$ or $j=i+n$ $(\forall i,j\in\mathbb{Z}_{2n})$.

Example 1. In case $r=2$ and $n=6$ $(6\geq 2+1)$, the Harary graph $H_{5,12}$ is shown in Figure 1. By Definition 1, one can see that the vertex v_1 is joined with the vertices v_2,v_3, v_{12},v_{11} and

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v_7, since 7-1=6 and for all numbers 2,3,11 and 12 $(\in\mathbb{Z}_{12})$, $|1-2|=|1-12|<|1-3|=|1-11|\leq 2$.

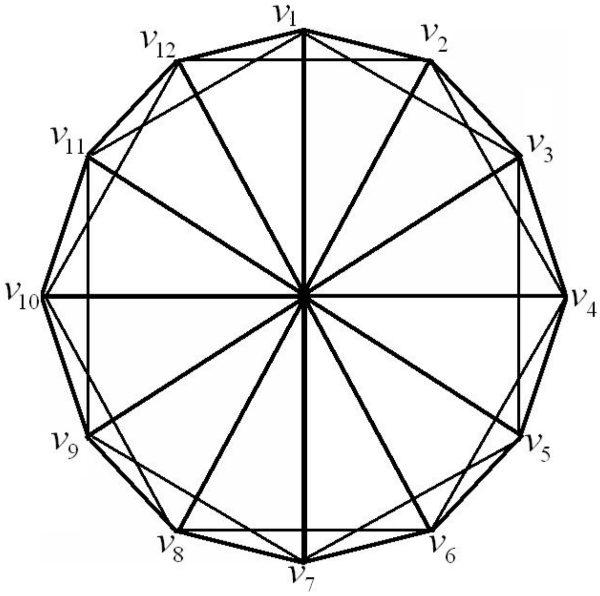

Figure 1. The Harary graph $H_{5,12}$

It is easy to see that this $2r+1$-regular graph has $2n$ vertices and $2n(2r+1)/2= n(2r+1)$ edges. And obviously for $n=r+1$, $H_{2r+1,2r+2}$ is automorphic with the complete graph K_{2r+2}. Also for $r=1$, $H_{3,2n}$ is automorphic with the Moebius graph M_{2n}. More information can be found in [1, 12, 18, 25] and Figure 1. Here, we have the following theorems, which are main results in this work.

Theorem 1. Let G be the Harary graph $H_{2r+1,2n}$ for given positive integer number r and n. Then, the Hosoya polynomial of $H_{2r+1,2n}$ is

$$\begin{aligned} H\left(H_{2r+1,2n}\right) &= n\left(2r+1\right)x^1+\sum_{d=2}^{\left[n/2r\right]} 4nx^d \\ &+2n\left(n-r-2\left[n/2r\right]+1\right)x^{\left[n/2r\right]+1} \end{aligned} \tag{4}$$

Proof. Consider the Harary graph $G=H_{2r+1,2n}$ as order $2n$ $(=|V(H_{2r+1,2n})|)$. From definition of the Harary graph, this implies that for all two vertices $v_i,v_j\in V(H_{2r+1,2n})$ $d(v_i,v_j)=1$ if and only if $i-r\leq j\leq i+r$ or $|j-i|=n$ $(\forall i,j=1,2,\ldots,n)$, thus the coefficient of the first term in the Hosoya polynomial of G (x^1) is equal to $|E(H_{2r+1,2n})|=2rn+n$.

On the other hand from the structure of $H_{2r+1,2n}$, $\forall i,j\in\mathbb{Z}_{2n}$ & $|i-j|\leq r$ or $|i-j|=n$ $d(v_i,v_{i\pm(r+j)})= d(v_i,v_{i+n\pm j})=2$, since for a vertex $v_i\in V(H_{2r+1,2n})$, v_i,v_j, $v_i,v_{i\pm r}$, v_i,v_{i+n}, $v_{i\pm r}v_{i\pm r+j}$ and $v_{i+n},v_{i+n\pm j}$ belong to $E(H_{2r+1,2n})$. Hence the coefficient of the second term in $H(H_{2r+1,2n},x)$ is $4n$.

Also by similar argument, one can see that for all vertices of G, $d(v_i,v_{i\pm(dr+j)})$ and $d(v_i,v_{i+n\pm((d-1)r+j)})$ are equal to $d+1$, where $2\leq d\leq \left[2n-4r/2\times 2r\right]=\left[n-2r/2r\right]=\left[\frac{n}{2r}\right]-1$. This implies that the diameter of Harary graph $H_{2r+1,2n}$ will be $\left[n/2r\right]+1$. It is easy to see that the latest coefficient in $H(H_{2r+1,2n},x)$ is equal to $\binom{2n}{2}-\frac{1}{2}\left[2n(2r+1)+8n\left(\left[n/2r\right]-1\right)\right]$.

Therefore by using the definition of Hosoya polynomial, we have

$$\begin{aligned} H(H_{2r+1,2n},x) &= \frac{1}{2}\sum_{v\in V\left(H_{2r+1,2n}\right)}\ \sum_{u\in V\left(H_{2r+1,2n}\right)} x^{d(v,u)} \\ &= \sum_{i,j=1}^{n} x^{d\left(v_i,v_j\right)} \\ &= \frac{1}{2}\left[2n\left(2r+1\right)x^1+4\left(2n\right)x^2+4\left(2n\right)x^3+\ldots+4\left(2n\right)x^{\left[n/2r\right]}+4n\left(n-r-2\left[n/2r\right]+1\right)x^{\left[n/2r\right]+1}\right]. \end{aligned}$$

And this complete the proof of Theorem 1.

According to Equation 3, we can obtain the Wiener index and the hyper-Wiener index of the Harary graph $H_{2r+1,2n}$ by the Hosoya polynomial.

Theorem 2. Let $H_{2r+1,2n}$ be the Harary graph ($\forall r,n\in\mathbb{Z}$ & $n\geq r+1$). Then, the Wiener index of $H_{2r+1,2n}$ is equal to

$$W(H_{2r+1,2n})=2n\left(n-1/2+\left(n-r\right)\left[n/2r\right]-\left[n/2r\right]^2\right)$$

Proof. Consider the Harary graph $G= H_{2r+1,2n}$. From definitions of the Wiener index and Hosoya Polynomial of G (Equations 1 and 3), we see that the Wiener index $W(G)$ is the first derivative of the Hosoya polynomial $H(G,x)$ evaluated at $x=1$. Thus

$$W(H_{2r+1,2n}) = \left.\frac{\partial H(H_{2r+1,2n},x)}{\partial x}\right|_{x=1}$$

$$= \frac{\partial n(2r+1)x^1}{\partial x}|_{x=1} + \frac{\partial \sum_{d=2}^{[n/2r]} 4nx^d}{\partial x}|_{x=1} + \frac{\partial 2n\left(n-r-2\left[n/2r\right]+1\right)x^{[n/2r]+1}}{\partial x}|_{x=1}$$

$$= n(2r+1) + 4n\sum_{d=2}^{[n/2r]} d + 2n\left(n-r-2\left[n/2r\right]+1\right)\left(\left[n/2r\right]+1\right)$$

$$= 2nr + n + \frac{4n}{2}\left(\left[n/2r\right]+2\right)\left(\left[n/2r\right]-1\right) + 2n\left(n-r+1+(n-r-1)\left[n/2r\right]-2\left[n/2r\right]^2\right)$$

$$= 2nr + n + 2n\left(\left[n/2r\right]^2 + \left[n/2r\right]-2\right) + 2n\left(n-r+1+(n-r-1)\left[n/2r\right]-2\left[n/2r\right]^2\right)$$

$$= 2n\left(n-1/2+(n-r)\left[n/2r\right]-\left[n/2r\right]^2\right)$$

Here the proof of Theorem 2 is completed.

As an immediately result from Theorem 2, we have.

Theorem 3. For given positive integer numbers r and n ($n\geq r+1$), the hyper-Wiener index of the Harary graph $H_{2r+1,2n}$ is equal to

$$WW(H_{2r+1,2n}) = 2n\left(2n-1+\left(3n-3r+1/3\right)\left[n/2r\right]+(n-r-3)\left[n/2r\right]^2-4/3\left[n/2r\right]^3\right).$$

Proof. Let $H_{2r+1,2n}$ be the Harary graph ($\forall r,n\in\mathbb{Z}$ & $n\geq r+1$). According to Equation 2, we can compute the hyper-Wiener index of $H_{2r+1,2n}$ as follows:

$$WW\left(H_{2r+1,2n}\right) = \frac{1}{2}\sum_{v\in V\left(H_{2r+1,2n}\right)}\sum_{u\in V\left(H_{2r+1,2n}\right)}\left(d(v,u)+d(v,u)^2\right)$$

$$= W\left(H_{2r+1,2n}\right) + \frac{1}{2}\sum_{v\in V\left(H_{2r+1,2n}\right)}\sum_{u\in V\left(H_{2r+1,2n}\right)} d(v,u)^2$$

$$= W\left(H_{2r+1,2n}\right) + n(2r+1) + 4n\sum_{d=2}^{[n/2r]} d^2 + 2n\left(n-r-2\left[n/2r\right]+1\right)\left(\left[n/2r\right]+1\right)^2$$

$$= W\left(H_{2r+1,2n}\right) + 2nr + n + \frac{4n}{6}\left[n/2r\right]\left(\left[n/2r\right]+1\right)\left(2\left[n/2r\right]+1\right) - 4n$$

$$+2n\left(n-r+1+(2n-2r)\left[n/2r\right]+(n-r-3)\left[n/2r\right]^2-2\left[n/2r\right]^3\right)$$

$$= W\left(H_{2r+1,2n}\right) + 2nr + n + \frac{4n}{6}\left[n/2r\right]\left(\left[n/2r\right]+1\right)\left(2\left[n/2r\right]+1\right) - 4n$$

$$+2n\left(n-r+1+(2n-2r)\left[n/2r\right]+(n-r-3)\left[n/2r\right]^2-2\left[n/2r\right]^3\right)$$

$$= W\left(H_{2r+1,2n}\right) + 2n\left(n-1/2+\left(2n-2r+1/3\right)\left[n/2r\right]+(n-r-2)\left[n/2r\right]^2-4/3\left[n/2r\right]^3\right)$$

Finally, $WW(H_{2r+1,2n}) = 2n\left(2n-1+\left(3n-3r+1/3\right)\left[n/2r\right]+(n-r-3)\left[n/2r\right]^2-4/3\left[n/2r\right]^3\right)$.

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