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COMPUTATION OF THE WIENER INDEX OF HARARY GRAPH $H_{2r+1, 2m+1}$

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Abstract

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. The *Wiener index* was introduced by *Harold Wiener* in 1947. This index is defined as the sum of distance between all vertices of a graph and is equal to $W(G) = \sum_{\{u, v\} \subset V(G)} d(u, v)$. The *Hosoya polynomial* was introduced by H. Hosoya in 1988 and defined as $H(G, x) = \sum_{\{u, v\} \subset V(G)} x^{d(u, v)}$. In this paper, the Hosoya polynomial and the Wiener index of *Harary graph* $H_{2r+1, 2m+1}$ are computed.

Keywords and phrases: regular graph, Harary graph, distance, Hosoya polynomial, Wiener index.

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1. Introduction

Let $G = (V, E)$ be a simple connected graph. We denote the set of vertices of connected graph G with $V(G)$ and set of edges with $E(G)$. An edge $e = uv$ of a graph G is joined between two vertices u and v. In a molecular graph, each vertex denotes an atom and edges denote the bond between atoms. A topological index is a real number which describes the molecular 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.

The oldest topological index which is the Wiener index was introduced by chemist *Harold Wiener* in 1947 [20]. He introduced this index for comparing and describing the relation between Physical-Chemical properties. The definition of this index is as follows:

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

where $u, v \in V(G)$ and $d(u, v)$ is the shortest distance between them.

The Wiener index of many molecular graphs has been computed. For more details and chemical applications and mathematical properties of these topological indices see paper series [5, 7, 8, 12-16, 18, 20-22, 24, 25].

The Hosoya polynomial was first introduced by H. Hosoya, in 1988 [10] and is defined as follows:

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

If we denote by $d(G, k)$ the number of vertex pairs of G, the distance of which is equal to k. Then we can rewrite the Hosoya polynomial and the Wiener index as

$$H(G, x) = \sum_{i=1}^{d(G)} d(G, i) x^i,$$

$$W(G) = \sum_{i=1}^{d(G)} d(G, i) \times i,$$

where $d(G)$ be the diameter of G and is the longest topological distance in G.

We encourage the readers to consult [2-4, 6, 9, 10, 17, 23] and references therein for background material as well as basic computational techniques.

The Hosoya polynomial $H(G, x)$ and the Wiener index $W(G)$ of regular *Harary graph* $H_{2r+1, 2m+1}$ are computed in this paper.

2. Main Results

The general form of the Harary graph $H_{2r+1, 2m+1}$ is defined as follows:

Definition [19]**.** Let r and m be two positive integer numbers, then the Harary graph $H_{2r+1, 2m+1}$ with $2m+1$ vertices is constructed as follows:

It has vertices $1, 2, \ldots, 2m, 2m+1$ and two vertices i and j are joined if and only if $i - r \leq j \leq i + r$ or $j = i + m$ or $j = i + m + 1$ $\forall i = 1, \ldots, m$.

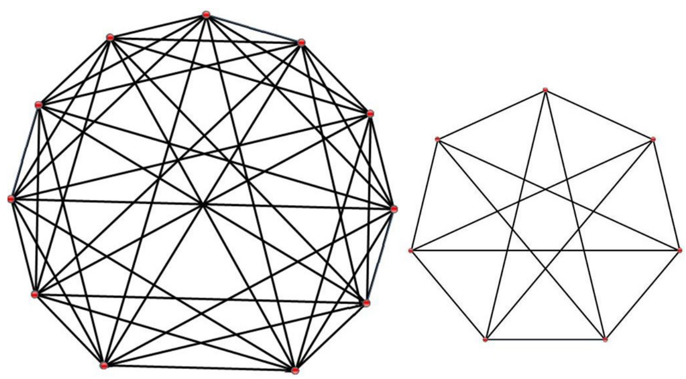

Figure1. The Harary graphs $H_{7,11}$ and $H_{3,7}$.

Obviously, from the definition of $2r+2$-regular graph $H_{2r+1, 2m+1}$, one can see that $\forall r, m \in \mathbb{N}$, and $m = r+1$, $H_{2r+1, 2r+3}$ is automorphic with the complete graph K_{2r+3} (see Figures 1, 2 and [1, 6, 11]).

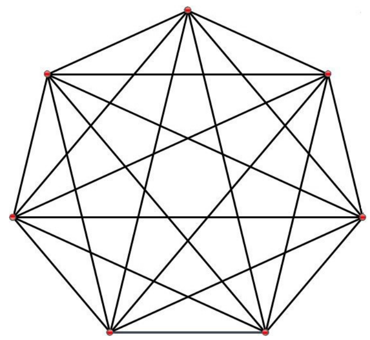

Figure 2. The Harary graph $H_{5,7}$ that is automorphic with the complete graph K_7.

Theorem 1. *Consider the Harary graph* $H = H_{2r+1,2m+1} (\forall r, m \in \mathbb{N})$. *Then the Hosoya polynomial* $H(H, x)$ *of Harary graph* $H_{2r+1,2m+1}$ *is equal to*

$$H(H_{2r+1,2m+1}, x) = (2m+1)\Big[(r+1)x^1 + 2r\sum_{k=2}^{\lfloor m+r-1/2 \rfloor} x^k$$
$$+ (m + r - \lfloor m + r - 1/2 \rfloor - 1)x^{\lceil m+r-1/2 \rceil}\Big].$$

Proof of Theorem 1. Let $H = H_{2r+1,2m+1}$ be the Harary graph with $2m+1$ vertices for all positive integer number r and m. From definition of regular graph $H_{2r+1,2m+1}$, it is obvious that for $i = 1, 2, \ldots, 2m, 2m+1$:

$$|V_i| = |\{v_j \in V(H) | i - r \leq j \leq i + r \text{ or } j = i + m \text{ or } j = i + m + 1\}| = 2r + 2 = d(v_i).$$

Thus

$$|E(H_{2r+1,2m+1})| = 1/2\,(2r+2) \times (2m+1) = (r+1)(2m+1).$$

(Obviously $m = \left\lceil |V(H)|/2 \right\rceil$). So the coefficient of the first sentence in the Hosoya polynomial of H is $d(H, 1) = (r+1)(2m+1)$.

Also from the structure of $H_{2r+1,2m+1}$ (see Figure 1), one can see that $\forall i, j \in \mathbb{N}_m$ and a vertex $v_i \in V(H_{2r+1,2m+1})$, v_iv_j, $v_iv_{i\pm r}$, $v_{i\pm r}v_{i\pm r+j}v_iv_{i+m}$ and $v_iv_{i+m+1} (= v_iv_{i-m})$ are edges of $E(H_{2r+1,2m+1})$ if $|i - j| \in \{1, \ldots, r, m, m+1\}$, thus $d(v_i, v_{i\pm(r+j)}) = d(v_i, v_{i\pm j\pm m}) = 2$, so for the coefficient of second sentence of $H(H, x)$, we have $2d(H, 2) = 4r(2m+1)$.

On the other hand, from the definition of $2r+2$-regular graph *H*, it is easy to see that by above mentioned results $d(H_{2r+1, 2m+1}, k) = 2r(2m+1)$ (the coefficient of kth sentence of $H(H, x)$). Such that

$$m + 1 - (r+1) - 1 - 2(k-1)r \geq 0 \rightarrow k \leq \lfloor m + r - 1/2 \rfloor.$$

And also, this implies that the diameter $d(H)$ of $H_{2r+1, 2m+1}$ is equal to $\lceil m + r - 1/2 \rceil$.

Therefore the coefficient in last sentence of $H(H_{2r+1, 2m+1}, x)$ is equal to

$$d(H, d(H)) = \binom{2m+1}{2} - [(r+1)(2m+1) + 2r(2m+1)(\lfloor m + r - 1/2 \rfloor - 1)]$$

$$= (2m+1)(m + r - \lfloor m + r - 1/2 \rfloor - 1),$$

since $\sum_{i=1}^{d(H)} d(H, i) = \binom{|W(H)|}{2}$.

Now, we refer to the definition of Hosoya polynomial and its index, thus we have following computation for $H_{2r+1, 2m+1}$:

$$H(H_{2r+1, 2m+1}, x)$$

$$= \frac{1}{2} \sum_{\substack{\{v_i, v_j\} \subset V(H) \\ i,\, j = 1, \ldots, 2m+1}} x^{d(v_i, v_j)}$$

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

$$= r+1)(2m+1)x^1 + 2r(2m+1)x^2 + 2r(2m+1)x^3 + \ldots + 2r(2m+1)x^{\lfloor m+r-1/2 \rfloor}$$

$$+ (2m+1)(m + r - \lfloor m + r - 1/2 \rfloor - 1)x^{\lfloor m+r-1/2 \rfloor}$$

$$= (r+1)(2m+1)x^1 + 2r(2m+1)\sum_{k=2}^{\lfloor m+r-1/2 \rfloor} x^k$$

$$+ (2m+1)(m + r - \lfloor m + r - 1/2 \rfloor - 1)x^{\lfloor m+r-1/2 \rfloor}$$

$$= (2m+1)[(r+1)x^1 + 2r\sum_{k=2}^{\lfloor m+r-1/2 \rfloor} x^k + (m + r - \lfloor m + r - 1/2 \rfloor - 1)x^{\lfloor m+r-1/2 \rfloor}].$$

Here, the proof of Theorem 1 is completed.

Theorem 2. *The Wiener index* $W(H)$ *of Harary graph* $H_{2r+1,\,2m+1}$ $(\forall r,\, m \in \mathbb{N})$ *are equal to*

- *For* $m = 2q$ *and* $r = 2p$,

$$W(H_{4p+1,\,4q+1}) = (4q+1)[p^3 + 4p^2q + 2pq^2 - 5p^2 + q^2 - 4pq + 6p + 1].$$

- **For** $m = 2q$ *and* $r = 2p + 1$,

$$W(H_{4p+3,\,4q+1}) = (4q+1)[4p^3 + 8p^2q + 4pq^2 + 3q^2 - p^2 + 2pq - 2q + 2].$$

- **For** $m = 2q + 1$ *and* $r = 2p$,

$$W(H_{4p+1,\,4q+3}) = (4q+3)[4p^3 + 4pq^2 + 8p^2q - 2pq - 3p^2 + q^2 + 2p + 1].$$

- *For* $m = 2q + 1$ *and* $r = 2p + 1$,

$$W(H_{4p+3,\,4q+3}) = (4q+3)[4p^3 + 8p^2q + 4pq^2 + 2pq - p^2 + 3q^2 - q + p + 2].$$

Proof of Theorem 2. Consider the Harary graph $H = H_{2r+1,\,2m+1}$ for two positive integer numbers *r and m.* Then, to compute the Wiener index of the Harary graph *H,* we consider four cases as above

Case 1. $\forall r,\, m \in \mathbb{N}$, m and r be even. Let $m = 2q$ and $r = 2p$, then

$$W(H_{4p+1,\,4q+1}) = \sum_{k=1}^{d(H)} d(H,\, k) \times k$$

$$= (4p+1)[(2p+1) + 2 \times 4p + \ldots + 4p(p + q - 1)$$

$$+ (2q + 2p - (p + q - 1) - 1)(p + q)]$$

$$= (4q+1)[(2p+1) + 4p\sum_{k=2}^{p+q-1} k + (p+q)(p+q)]$$

$$= (4q+1)[(2p+1) + 4p\sum_{k=2}^{p+q-1} k + (p+q)(p+q)]$$

$$= (4q+1)[2p+1+2p(p^2+q^2+2pq-3q-3p+2)$$

$$+ p^2+q^2+2pq]$$

$$= (4q+1)[2p+1+p^3+2pq^2+4p^2q-6pq-6p^2$$

$$+4p+p^2+q^2+2pq]$$

$$= (4q+1)[p^3+4p^2q+2pq^2-5p^2+q^2-4pq+6p+1].$$

Case 2. $\forall r,\ m \in \mathbb{N},\ m$ even and r odd. Let $m = 2q$ and $r = 2p+1,$ then

$$W(H_{4p+3,4q+1}) = \sum_{k=1}^{d(H)} d(H,\ k) \times k$$

$$= (4q+1)[(2p+1+1) + 2(2p+1)\sum_{k=2}^{p+q} k + (2q+2p+1$$

$$-(p+q)-1)(p+q)]$$

$$= (4q+1)[2(p+1) + 2(2p+1)\sum_{k=1}^{p+q-1} k + (p+q)(p+q)]$$

$$= (4q+1)[2(p+1) + 2(2p+1)(p^2+q^2+2pq-q-p)$$

$$+(p+q)(p+q)]$$

$$= (4q+1)[2p+2+2(2p+1)(p^2+q^2+2pq-q-p)$$

$$+p^2+q^2+2pq]$$

$$= (4q+1)[2p+2+4p^3+8p^2q+4pq^2-2p^2+2q^2-2q$$

$$-2p+p^2+q^2+2pq]$$

$$= (4q+1)[4p^3+8p^2q+4pq^2+3q^2-p^2+2pq-2q+2].$$

Case 3. $\forall r,\ m \in \mathbb{N},\ m$ odd and r even. Let $m = 2q+1$ and $r = 2p,$ then

$$W(H_{4p+1,4q+3}) = (4q+3)[(2p+1) + 4p\sum_{k=2}^{p+q} k + (2q+1+2p-(p+q)-1)(p+q)]$$

$$= (4q+3)[2p+1+4p(p^2+q^2+2pq-q-p)+(p+q)(p+q)]$$

$$= (4q+3)[2p+1+4p^3+4pq^2+8p^2q-4pq-4p^2$$

$$+ p^2 + q^2 + 2pq]$$

$$= (4q+3)[4p^3+4pq^2+8p^2q-2pq-3p^2+q^2+2p+1].$$

Finally,

Case 4. $\forall r, m \in \mathbb{N}$, m and r be odd. Let $m = 2q+1$ and $r = 2p+1$, then

$$W(H_{4p+3,4q+3}) = (4q+3)[(2p+1+1) + 2(2p+1)\sum_{k=2}^{p+q} k$$

$$+ (2q+1+2p+1-(p+q)-1)(p+q+1)]$$

$$= (4q+3)[(2p+2) + 2(2p+1)(p^2+q^2+2pq-q-p)$$

$$+ (p+q+1)(p+q+1)]$$

$$= (4q+3)[(2p+2) + (4p^3+8p^2q+4pq^2-2p^2+2q^2$$

$$-2q-2p) + (p^2+q^2+2pq+q+p)]$$

$$= (4q+3)[4p^3+8p^2q+4pq^2+2pq-p^2+3q^2-q+p+2].$$

And these complete the proof of Theorem 2.

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