MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **71** (2014) 373-382

ISSN 0340 - 6253

Harary Index of Some Nano–Structures

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(Received September 15, 2012)

Abstract

The Harary index of a simple connected graph G, H(G), is defined as the summation of $d(u,v|G)^{-1}$ over non-ordered pairs of vertices, where d(u,v|G) denotes the distance between vertices u and v of G. In this paper, we suggest a method for computing the Harary index of the Cartesian product of graphs. Then as our main purpose of this paper, we apply this result to compute the Harary index of some molecular graphs related to polyomino structures and nanostructures.

1 Introduction

Throughout the paper, all of graphs are considered to be simple and connected. A simple graph is an undirected graph without any loops or multiple edges. Let G be a graph with the vertex set $V(G)$ and the edge set $E(G)$. The distance between the vertices u and v of G is denoted by $d(u,v|G)$ and defined as the number of edges in a shortest path connecting them. The diameter of G is the maximum of distance among all pairs of vertices of G and denoted by $diam(G)$. Also, we use $|S|$ to denote the cardinality of a set S and we denote by $[q^i]f(q)$, the coefficient of q^i in a polynomial $f(q)$.

A chemical graph or a molecular graph is a graph related to the structure of a chemical compound. Each vertex of this graph represented an atom of the molecule and covalent bonds between atoms are represented by edges between the corresponding vertices. In theoretical chemistry, the physico-chemical properties of chemical compounds are often modeled by the molecular graph based molecular structure descriptors, which are also referred to as topological indices [1]. Among the variety of those indices, which are designed to capture the

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different aspects of molecular structure, Wiener index is the best known one. Wiener index is the first reported distance-based topological index which was introduced by the Chemist, Harold Wiener, in 1947 [2,3]. Wiener used his index, for the calculation of the boiling points of alkanes. From graph-theoretical point of view, Wiener index of G is defined as $W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v|G)$. In [4], the Wiener polynomial of G, was introduced. If q is a parameter, the Wiener polynomial of G is denoted by $W(G;q)$ and defined as $W(G;q) = \sum_{\{u,v\}\subseteq V(G)} q^{d(u,v|G)}$. In fact, $W(G;q) = \sum_{i=1}^{diam(G)} d(G,i)q^i$, where $d(G,i)$ is the number of all pairs of vertices of G, which are at distance i. It is clear that, the first derivative of the Wiener polynomial of G in $q=1$, is equal to the Wiener index of G, i.e., $W'(G;1) = W(G)$.

Harary index was introduced in 1993, by Plavšić et al. in honor of Professor Frank Harary, due to his influence in development of graph theory and especially to its application in Chemistry. Harary index of G is denoted by $H(G)$ and defined as follows [5]:

$$H(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d(u,v|G)}.$$

For more details on the Harary index and its applications in Chemistry see [6-8]. Now, let us recall the definition of the Cartesian product of graphs. Let G_1 and G_2 be two graphs with the set of vertices $V(G_1)$ and $V(G_2)$ and the set of edges $E(G_1)$ and $E(G_2)$, respectively . The Cartesian product of G_1 and G_2 denoted by $G_1 \times G_2$, is a graph with the vertex set $V(G_1)\times V(G_2)$ and two vertices (u_1,u_2) and (v_1,v_2) of $G_1 \times G_2$, are adjacent if and only if $[u_1 = v_1 \ and \ u_2v_2 \in E(G_2)]$ or $[u_2 = v_2 \ and \ u_1v_1 \in E(G_1)]$.

According to the proof of Theorem 1 in [9], the distance between the vertices (u_1,u_2) and (v_1,v_2) of $G_1 \times G_2$, is equal to $d((u_1,u_2),(v_1,v_2)|G_1 \times G_2) = d(u_1,v_1|G_1) + d(u_2,v_2|G_2)$.

Therefore, $diam(G_1 \times G_2) = diam(G_1) + diam(G_2)$.

The Harary index of some graph operations containing join, composition, disjunction and symmetric difference have been computed previously [10]. But the Harary index of the Cartesian product of graphs has not been considered yet. In this paper, we suggest a method for computing the Harary index of the Cartesian product of graphs. Then as our main purpose of this paper, we apply our results to compute the Harary index of some molecular graphs related to polyomino chains and some nanotubes and nanotori. .The interested readers for more information on computing topological indices of graph operations can be referred to [11-13].

2 Discussion and results

In this section, we present a method to find the Harary index of the Cartesian product of graphs.

Theorem 2.1. Let G_1 and G_2 be two graphs with the set of vertices $V(G_1)$ and $V(G_2)$, respectively. Then $W(G_1 \times G_2;q) = 2W(G_1;q)W(G_2;q) + |V(G_2)|W(G_1;q) + |V(G_1)|W(G_2;q)$.

Proof. See Proposition 1.4 in [4]. □

Lemma 2.2. Let P_n and C_n be the n-vertex path and cycle, respectively. We have:

(i) $W(P_n;q) = (n-1)q + (n-2)q^2 + ... + q^{n-1}$;

(ii) $W(C_{2n};q) = 2n(q + q^2 + ... + q^{n-1}) + nq^n$;

(iii) $W(C_{2n+1};q) = (2n+1)(q + q^2 + ... + q^n)$.

Proof. See Theorem 1.2 in [4].□

By definition of the Wiener polynomial, it is clear that $d(G,i)$ is the coefficient of q^i in $W(G;q)$. So the Harary index of G can also be defined in terms of $d(G,i)$, as follows:

Definition 2.3. The Harary index of G is defined as follows:

$$H(G) = \sum_{i=1}^{diam(G)} \frac{d(G,i)}{i} = \sum_{i=1}^{diam(G)} \frac{[q^i]W(G,q)}{i}.$$

From now on, for any positive integer n, let $\varphi_n = \sum_{i=1}^{n} \frac{1}{i}$.

Lemma 2.4. We have the following specific Harary indices.

(i) $H(P_n) = n\varphi_n - n$;

(ii) $H(C_{2n}) = 2n\varphi_n - 1$;

(iii) $H(C_{2n+1}) = (2n+1)\varphi_n$.

Proof. By Lemma 2.2 and definition 2.3, the proof is obvious.□

Lemma 2.5. Let G_1 and G_2 be two graphs with the set of vertices $V(G_1)$ and $V(G_2)$, respectively. Then $d(G_1 \times G_2, i) = [q^i](2W(G_1;q)W(G_2;q)) + |V(G_2)|d(G_1,i) + |V(G_1)|d(G_2,i)$.

Proof. By Theorem 2.1, we have:

$d(G_1 \times G_2, i) = [q^i]W(G_1 \times G_2; q) = [q^i](2W(G_1;q)W(G_2;q) + |V(G_2)|W(G_1;q) + |V(G_1)|W(G_2;q)) =$
$[q^i](2W(G_1;q)W(G_2;q)) + |V(G_2)| \; ([q^i] \; W(G_1;q)) + |V(G_1)| \; ([q^i] \; W(G_2;q)) =$
$[q^i](2W(G_1;q)W(G_2;q)) + |V(G_2)|d(G_1,i) + |V(G_1)|d(G_2,i)$. □

Theorem 2.6. Let G_1 and G_2 be two graphs. Then

$$H(G_1 \times G_2) = 2\sum_{i=1}^{diam(G_1)+diam(G_2)} \frac{[q^i](W(G_1;q)W(G_2;q))}{i} + |V(G_2)|H(G_1) + |V(G_1)|H(G_2).$$

Proof. By definition 2.3 and the previous Lemma, we have:

$$H(G_1 \times G_2) = \sum_{i=1}^{diam(G_1 \times G_2)} \frac{d(G_1 \times G_2, i)}{i} =$$

$$\sum_{i=1}^{diam(G_1 \times G_2)} \frac{[q^i](2W(G_1;q)W(G_2;q)) + |V(G_2)|d(G_1,i) + |V(G_1)|d(G_2,i)}{i} =$$

$$\sum_{i=1}^{diam(G_1 \times G_2)} \frac{[q^i](2W(G_1;q)W(G_2;q))}{i} + |V(G_2)| \sum_{i=1}^{diam(G_1 \times G_2)} \frac{d(G_1,i)}{i} + |V(G_1)| \sum_{i=1}^{diam(G_1 \times G_2)} \frac{d(G_2,i)}{i}.$$

Since for every $i > diam(G_1)$, $d(G_1,i) = 0$ and similarly for every $i > diam(G_2)$, $d(G_2,i) = 0$, we have:

$$H(G_1 \times G_2) = 2\sum_{i=1}^{diam(G_1)+diam(G_2)} \frac{[q^i](W(G_1;q)W(G_2;q))}{i} + |V(G_2)| \sum_{i=1}^{diam(G_1)} \frac{d(G_1,i)}{i} + |V(G_1)| \sum_{i=1}^{diam(G_2)} \frac{d(G_2,i)}{i}$$

$$= 2\sum_{i=1}^{diam(G_1)+diam(G_2)} \frac{[q^i](W(G_1;q)W(G_2;q))}{i} + |V(G_2)|H(G_1) + |V(G_1)|H(G_2). \square$$

3 Main results

In this section, we use Theorem 2.6 to find the Harary index of linear polyomino chain, C_4- nanotubes and C_4-nanotori.

Harary index of linear polyomino chain

In Figure 1, you can see the graph $P_m \times P_n$.

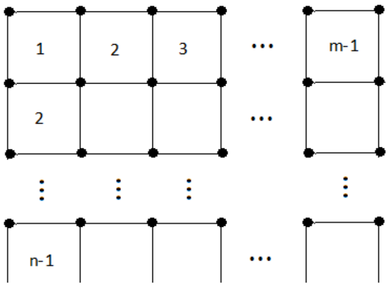

Figure 1. The graph $P_m \times P_n$.

In the following Theorem, we find the Harary index of $P_m \times P_n$.

Theorem 3.1. Let $G = P_m \times P_n$. Then

$$H(G) = \frac{1}{3}(2(n+m)^2 - m(n^2-1) - n(m^2-1) - nm - 1) - \frac{n}{3}(n^2+3nm-1)\varphi_n - \frac{m}{3}(m^2+3nm-1)\varphi_m + \frac{n+m}{3}((n+m)^2-1)\varphi_{m+n-2}.$$

Proof. Without lost of generality, let $n \le m$ and $\alpha_i = [q^i](W(P_m;q)W(P_n;q))$. By Theorem 2.6, we should find α_i for $1 \le i \le diam(P_m) + diam(P_n) = m+n-2$. So we have:

(i) If $1 \le i \le n$, then $\alpha_i = \sum_{j=1}^{i-1}(m-j)(n+j-i) = \frac{i^3}{6} - \frac{m+n}{2}i^2 + \frac{6nm+3n+3m-1}{6}i - nm$;

(ii) If $n+1 \le i \le m$, then $\alpha_i = \sum_{j=1}^{n-1}(n-j)(m+j-i) = -\frac{n(n-1)}{2}i + \frac{n(n-1)(n+3m+1)}{6}$;

(iii) If $m+1 \le i \le m+n-2$, then

$$\alpha_i = \sum_{j=1}^{m+n-(i+1)} j(m+n-i-j) = -\frac{i^3}{6} + \frac{m+n}{2}i^2 - \frac{3n^2+3m^2+6nm-1}{6}i + \frac{(n+m)^3-(n+m)}{6}.$$

Now, by Lemma 2.4 and Theorem 2.6, the proof is straightforward.□

Note that, the graph $P_2 \times P_{n+1}$ made by n squares is called ladder graph with $2n+2$ vertices and denoted by L_n (see figure 2). Also, this graph is the molecular graph related to the polyomino structures and called the linear polyomino chain.

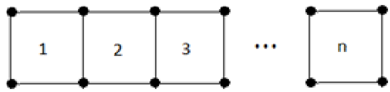

Figure 2. *Linear polyomino chain* L_n .

Corollary 3.2. Harary index of the linear polyomino chain L_n is as follows:

$$H(L_n) = (4n+6)\varphi_{n+1} - 5(n+1).$$

Proof. Using the previous Theorem, the proof is obvious.□

Harary index of C_4-nanotubes

Let $G = P_m \times C_n$, then $G = TUC_4(n,m)$ is a C_4-nanotube (see figure 3) [14].

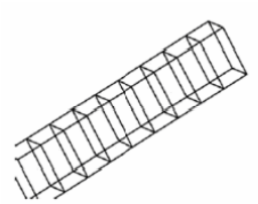

Figure 3. *A* C_4*-nanotube*.

In the following Theorem, we find the Harary index of C_4-nanotubes.

Theorem 3.3. Let $G = P_m \times C_{2n+1} = TUC_4(2n+1,m)$, then

$$H(G) = (2n+1)(n - nm + 1 - (n^2 + 2nm + n + m)\varphi_n - m^2\varphi_m + (n+m)(n+m+1)\varphi_{m+n-1}) .$$

Proof. Let $\alpha_i = [q^i](W(P_m;q)W(C_{2n+1};q))$. According to the Theorem 2.6, we should find α_i for $1 \le i \le diam(P_m) + diam(C_{2n+1}) = m + n - 1$. So we consider two following cases:

Case I: Let $n \le m$.

(i) If $1 \le i \le n$, then $\alpha_i = (2n+1)\sum_{j=1}^{i-1}(m-j) = -\frac{2n+1}{2}i^2 + \frac{(2n+1)(2m+1)}{2}i - m(2n+1)$;

(ii) If $n+1 \le i \le m$, then $\alpha_i = (2n+1)\sum_{j=1}^{n}(m+j-i) = -n(2n+1)i + \frac{n(2n+1)(n+2m+1)}{2}$;

(iii) If $m+1 \le i \le m+n-1$, then

$$\alpha_i = (2n+1)\sum_{j=1}^{m+n-i} j = \frac{2n+1}{2}i^2 - \frac{(2n+1)(2n+2m+1)}{2}i + \frac{(2n+1)(n+m)(n+m+1)}{2}.$$

Case II: Let $m \le n$.

(i) If $1 \le i \le m$, then $\alpha_i = (2n+1)\sum_{j=1}^{i-1}(m-j) = -\frac{2n+1}{2}i^2 + \frac{(2n+1)(2m+1)}{2}i - m(2n+1)$;

(ii) If $m+1 \le i \le n$, then $\alpha_i = (2n+1)\sum_{j=1}^{m-1} j = \frac{m(m-1)(2n+1)}{2}$;

(iii) If $n+1 \le i \le n+m-1$, then

$$\alpha_i = (2n+1)\sum_{j=1}^{m+n-i} j = \frac{2n+1}{2}i^2 - \frac{(2n+1)(2n+2m+1)}{2}i + \frac{(2n+1)(n+m)(n+m+1)}{2}.$$

Now, by Lemma 2.4 and Theorem 2.6, we can obtain the desire result.□

Theorem 3.4. Let $G = P_m \times C_{2n} = TUC_4(2n,m)$, then

$$H(G) = 2n^2(1-m) + m(2n-1) - 2n^2(n+2m)\varphi_n - 2m^2 n\varphi_m + 2n(n+m)^2\varphi_{n+m-1}.$$

Proof. Let $\alpha_i = [q^i](W(P_m;q)W(C_{2n};q))$. To find α_i $(1 \le i \le m+n-1)$, we consider two following cases:

Case I: Let $n \le m$.

(i) If $1 \le i \le n$, then $\alpha_i = 2n\sum_{j=1}^{i-1}(m-j) = -ni^2 + n(2m+1)i - 2nm$;

(ii) If $n+1 \le i \le m$, then $\alpha_i = 2n\sum_{j=1+i-n}^{i-1}(m-j) + n(n+m-i) = n(1-2n)i + n(n^2+2nm-m)$;

(iii) If $m+1 \le i \le m+n-1$, then

$$\alpha_i = 2n\sum_{j=1+i-n}^{m-1}(m-j) + n(n+m-i) = ni^2 - 2n(n+m)i + n(n+m)^2.$$

Case II: Let $m \le n$.

(i) If $1 \le i \le m$, then $\alpha_i = 2n\sum_{j=1}^{i-1}(m-j) = -ni^2 + n(2m+1)i - 2nm$;

(ii) If $m+1 \le i \le n$, then $\alpha_i = 2n\sum_{j=1}^{m-1}(m-j) = nm(m-1)$;

(iii) If $n+1 \le i \le n+m-1$, then $\alpha_i = 2n\sum_{j=1}^{m+n-(i+1)} j + n(n+m-i) = ni^2 - 2n(n+m)i + n(n+m)^2$.

Now, by Lemma 2.4 and Theorem 2.6, the proof is straightforward.□

Harary index of C_4-nanotori

Let $G = C_m \times C_n$, then $G = TC_4(n,m)$ is a C_4-nanotorus (see figure 4) [15]. In the following

Theorem, we find the Harary index of C_4-nanotori.

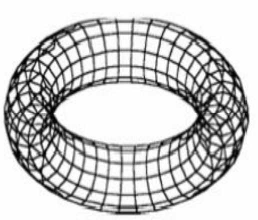

Figure 4. *A* C_4*-nanotorus*.

Theorem 3.5. Let $G = C_{2m} \times C_{2n+1} = TC_4(2n+1,2m)$, then

$$H(G) = -(2n+1)(1+2m(2n+1)\varphi_n + 4m^2\varphi_m - 2m(2n+2m+1)\varphi_{n+m}).$$

Proof. Let $\alpha_i = [q^i](W(C_{2m};q)W(C_{2n+1};q))$. By Theorem 2.6, we should find α_i for $1 \le i \le diam(C_{2m}) + diam(C_{2n+1}) = m+n$. So we consider two following cases:

Case I: Let $n \le m$.

(i) If $1 \le i \le n$, then $\alpha_i = 2m(2n+1)(i-1)$;

(ii) If $n+1 \le i \le m$, then $\alpha_i = 2mn(2n+1)$;

(iii) If $m+1 \le i \le n+m$, then $\alpha_i = m(2n+1)(2n+2m-2i+1)$.

Case II: Let $m \le n$.

(i) If $1 \le i \le m$, then $\alpha_i = 2m(2n+1)(i-1)$;

(ii) If $m+1 \le i \le n$, then $\alpha_i = m(2n+1)(2m-1)$;

(iii) If $n+1 \le i \le n+m$, then $\alpha_i = m(2n+1)(2n+2m-2i+1)$.

Now, the result can be obtained by easy calculation.□

Theorem 3.6. Let $G = C_{2m} \times C_{2n} = TC_4(2n,2m)$, then

$$H(G) = \frac{-2(n^2+m^2+nm)}{n+m} - 8mn^2\varphi_n - 8m^2n\varphi_m + 8nm(n+m)\varphi_{n+m}.$$

Proof. Without lost of generality, let $n \le m$ and set $\alpha_i = [q^i](W(C_{2m};q)W(C_{2n};q))$. We have:

(i) If $1 \le i \le n$, then $\alpha_i = 4mn(i-1)$;

(ii) If $n+1 \le i \le m$, then $\alpha_i = 2mn(2n-1)$;

(iii) If $m+1 \le i \le m+n-1$, then $\alpha_i = 4nm(n+m-i)$;

(iv) $\alpha_{m+n} = nm$.

Now, by Lemma 2.4 and Theorem 2.6, the proof is straightforward.□

Theorem 3.7. Let $G = C_{2m+1} \times C_{2n+1} = TC_4(2n+1, 2m+1)$, then

$$H(G) = -(2n+1)(2m+1)((2n+1)\varphi_n + (2m+1)\varphi_m - 2(n+m+1)\varphi_{n+m}).$$

Proof. Without lost of generality, let $n \le m$ and set $\alpha_i = [q^i](W(C_{2m+1};q)W(C_{2n+1};q))$. We have the following cases:

(i) If $1 \le i \le n$, then $\alpha_i = (2n+1)(2m+1)(i-1)$;

(ii) If $n+1 \le i \le m$, then $\alpha_i = n(2n+1)(2m+1)$;

(iii) If $m+1 \le i \le n+m$, then $\alpha_i = (2n+1)(2m+1)(n+m+1-i)$.

Now, using Lemma 2.4 and Theorem 2.6, the proof is completed.□

Acknowledgement: This work was partially supported by Center of Excellence of Algebraic Hyperstructures and its Applications of Tarbiat Modares University (CEAHA). We would like to thank the referee for a number of helpful comments and suggestions.

References

[1] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1992.

[2] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.

[3] H. Wiener, Correlation of heats of isomerization and differences in heats of vaporization of isomers among the paraffin hydrocarbons, *J. Amer. Chem. Soc.* **69** (1947) 2636–2638.

[4] B. E. Sagan, Y. Yeh, P. Zhang, The Wiener polynomial of a graph, *Inter. J. Quantum Chem.* **60** (1996) 959–969.

[5] D. Plavšić, S. Nikolić, N. Trinajstić, Z. Mihalić, On the Harary index for the characterization of chemical graphs, *J. Math. Chem.* **12** (1993) 335–350.

[6] M. V. Diudea, T. Ivanciuc, S. Nikolić, N. Trinajstić, Matrices of reciprocal distance polynomials and derived numbers, *MATCH Commun. Math. Comput. Chem.* **35** (1997) 41–64.

[7] B. Lučić, A. Miličević, S. Nikolić, N. Trinajstić, Harary index twelve years later, *Croat. Chem. Acta.* **75** (2002) 847–868.

[8] B. Zhou, X. Cail, N. Trinajstić, On Harary index, *J. Math. Chem.* **44** (2008) 611–618.

[9] D. Stevanović, Hosoya polynomial of composite graphs, *Discr. Math.* **235** (2001) 237–244.

[10] S. Hossein–Zadeh, A. Hamzeh, A. R. Ashrafi, Wiener–type invariants of some graph operations, *Filomat* **23** (2009) 103–113.

[11] M. Azari, A. Iranmanesh, Computation of the edge Wiener indices of the sum of graphs, *Ars Combin.* **100** (2011) 113–128.

[12] M. Azari, A. Iranmanesh, A. Tehranian, Computation of the first edge Wiener index of a composition of graphs, *Studia Univ. Babes Bolyai Chem*. **4** (2010) 183–196.

[13] M. Azari, A. Iranmanesh, A. Tehranian, A method for calculating an edge version of the Wiener number of a graph operation, *Util. Math.* **87** (2012) 151–164.

[14] P. E. John, M. V. Diudea, Wiener index of zig–zag polyhex nanotubes, *Croat. Chem. Acta*. **77** (2004) 127–132.

[15] M. V. Diudea, P. E. John, Covering polyhedral tori, *MATCH Commun. Math. Comput. Chem*. **44** (2001) 103–116.