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Extremal Graphs under Wiener–type Invariants

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Abstract. Let $d(G,k)$ be the number of pairs of vertices of a graph G that are at distance k, λ a real number, and $W_\lambda(G) = \sum_{k\geq 1} d(G,k)k^\lambda$. $W_\lambda(G)$ is called the Wiener-type invariant of G associated to real number λ. In this paper, the Wiener-type invariant of the Cartesian product of graphs is computed. As an application the Tratch−Stankevich−Zefirov of C_4 nanotubes and nanotori are computed. We also find some new bound for this graph invariant.

1 Introduction

Throughout this paper graph means simple connected graph. The distance between two vertices u and v of a graph G is denoted by $d_G(u,v)$ ($d(u,v)$ for short). It is defined as the number of edges in a minimum path connecting them. Let $d(G,k)$ be the number of pairs of vertices of G that are at distance k, λ a real number, and $W_\lambda(G) = \sum_{k=1}^{d} d(G,k)k^\lambda$, where $d = \mathrm{diam}(G)$ denotes the diameter of the graph G. $W_\lambda(G)$ is called the Wiener-type invariant of G associated to real number λ, see [2, 14] for details. Note that $d(G,0)$ and $d(G,1)$ represent the number of vertices and edges, respectively. The case of $\lambda = 1$ is called the classical Wiener index [17]. The quantities $WW = \frac{1}{2}[W_1 + W_2]$ and $TSZ = \frac{1}{6}W_3 + \frac{1}{2}W_2 + \frac{1}{3}W_1$ are the so-called hyper-Wiener index and Tratch−Stankevich−Zefirov index [3].

The Cartesian product $G \times H$ of graphs G and H is a graph such that $V(G\times H) = V(G)\times V(H)$, and any two vertices (a,b) and (u,v) are adjacent in $G\times H$ if and only

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if either $a = u$ and b is adjacent with v, or $b = v$ and a is adjacent with u, see [7] for details.

Throughout this paper, C_n, P_n and K_n denote the cycle, path and complete graphs on n vertices. The complement of a graph G is a graph H on the same vertices such that two vertices of H are adjacent if and only if they are not adjacent in G. The graph H is usually denoted by $\bar{G}$. Our other notations are standard and taken mainly from [1, 5, 16].

2 Main Results

In this section, an exact formula for the Wiener-type invariants of the Cartesian product of graphs is presented. We begin with the following lemma which crucial throughout the paper.

Lemma 2.1. Let G and H be graphs. Then we have:

(a) $|V(G \times H)| = |V(G)| \times |V(H)|$,

(b) $|E(G \times H)| = |E(G)| \times |V(H)| + |V(G)| \times |E(H)|$,

(c) $G \times H$ is connected if and only if G and H are connected.

(d) If $(a, c), (b, d) \in V(G \times H)$ then $d_{G\times H}((a, c), (b, d)) = d_G(a, b) + d_H(c, d)$,

(e) The Cartesian product of graphs is associative and commutative.

Proof. The parts (a−e) are consequences of definitions and some well-known results of the book of Imrich and Klavžar, [7]. ■

The Wiener index of the Cartesian product graphs was studied in [4]. In [13], Klavžar, Rajapakse and Gutman computed the Szeged index of the Cartesian product of graphs. The present authors, [6, 8, 9, 10, 11, 12, 18], computed exact formulas for the hyper-Wiener, vertex PI, edge PI, the first Zagreb, the second Zagreb, the edge Wiener and the edge Szeged indices of some graph operations.

Lemma 2.2. Suppose G and H are connected graphs, $|V(G)| = m$, $|V(H)| = n$ and λ is a positive integer. Then

$$\begin{aligned} W_\lambda(G \times H) &= m^2 W_\lambda(H) + 2\binom{\lambda}{1} W(G) W_{\lambda-1}(H) + 2\binom{\lambda}{2} W_2(G) W_{\lambda-2}(H) \\ &+ \cdots + 2\binom{\lambda}{\lambda-1} W_{\lambda-1}(G) W(H) + n^2 W_\lambda(G) \ . \end{aligned}$$

Proof. Suppose $\{u_1, \ldots, u_m\}$ and $\{v_1, \ldots, v_n\}$ are vertices of G and H, respectively. Then by Lemma 2.1 and definition of W_λ,

$$\begin{aligned}
W_\lambda(G \times H) &= \sum_{\{u,v\}} d^\lambda_{G\times H}(u,v) = \frac{1}{2}\sum_{(u_i,v_k)}\sum_{(u_j,v_l)} d^\lambda_{G\times H}((u_i,v_k),(u_j,v_l)) \\
&= \frac{1}{2}\sum_{k,l=1}^{n}\sum_{i,j=1}^{m}(d_G(u_i,u_j)+d_H(v_k,v_l))^\lambda \\
&= \frac{1}{2}\sum_{k,l=1}^{n}\sum_{i,j=1}^{m}\left(\sum_{r=0}^{\lambda}\binom{\lambda}{r} d^r_G(u_i,u_j)d^{\lambda-r}_H(v_k,v_l)\right) \\
&= \frac{1}{2}\sum_{k,l=1}^{n}\sum_{i,j=1}^{m}(d^\lambda_H(v_k,v_l)+\binom{\lambda}{1}d_G(u_i,u_j)d^{\lambda-1}_H(v_k,v_l) \\
&+ \cdots + \binom{\lambda}{\lambda-1}d^{\lambda-1}_G(u_i,u_j)d_H(v_k,v_l)+d^\lambda_G(u_i,u_j)) \\
&= m^2W_\lambda(H) + 2\binom{\lambda}{1}W(G)W_{\lambda-1}(H) + 2\binom{\lambda}{2}W_2(G)W_{\lambda-2}(H) \\
&+ \cdots + 2\binom{\lambda}{\lambda-1}W_{\lambda-1}(G)W(H) + n^2W_\lambda(G)\,,
\end{aligned}$$

proving the lemma. ■

Corollary 2.3. With notation of Lemma 2.2, $TSZ(G \times H) = |V(H)|^2TSZ(G) + |V(G)|^2TSZ(H) + W(G)W_2(H) + W(H)W_2(G) + 2W(G)W(H)$.

Proof. By Lemma 2.2, we have:

$$\begin{aligned}
TSZ(G \times H) &= \frac{1}{6}W_3(G\times H) + \frac{1}{2}W_2(G\times H) + \frac{1}{3}W(G\times H) \\
&= \frac{1}{6}|V(H)|^2W_3(G) + W(G)W_2(H) + W_2(G)W(H) \\
&+ \frac{1}{6}|V(G)|^2W_3(H) + \frac{1}{2}|V(H)|^2W_2(G) + 2W(G)W(H) \\
&+ \frac{1}{2}|V(G)|^2W_2(H) + \frac{1}{3}W(G)|V(H)|^2 + \frac{1}{3}W(H)|V(G)|^2 \\
&= |V(H)|^2TSZ(G) + |V(G)|^2TSZ(H) + W(G)W_2(H) \\
&+ W(H)W_2(G) + 2W(G)W(H)\,,
\end{aligned}$$

as desired. ■

Consider a net $G[n,m] = P_n \times P_m$. By Corollary 2.3, one can compute the Tratch–Stankevich–Zefirov index of $G[n,m]$ as follows:

$$\begin{aligned} TSZ(P_n \times P_m) &= \frac{1}{120}m^2n^5 + \frac{1}{24}m^2n^4 + \frac{1}{36}m^2n^3 - \frac{1}{12}m^2n^2 - \frac{13}{360}m^2n \\ &+ \frac{1}{120}m^5n^2 + \frac{1}{24}m^4n^2 + \frac{1}{36}m^3n^2 - \frac{13}{360}mn^2 + \frac{1}{72}m^4n^3 \\ &- \frac{1}{72}m^4n + \frac{1}{72}m^2n^4 - \frac{1}{72}mn^4 + \frac{1}{18}m^3n^3 \\ &- \frac{1}{18}mn^3 - \frac{1}{18}m^3n + \frac{1}{18}mn\ . \end{aligned}$$

In the next corollary, we compute the Tratch–Stankevich–Zefirov index of nanotubes and nanotori covered by C_4.

Corollary 2.4. The Tratch–Stankevich–Zefirov index of C_4 nanotubes and nanotori are computed as follows:

i) If m is even then,

$$\begin{aligned} TSZ(P_n \times C_m) &= \frac{1}{120}m^2n^5 + \frac{1}{24}m^2n^4 + \frac{1}{18}m^2n^3 - \frac{23}{360}m^2n + \frac{1}{384}m^5n^2 \\ &+ \frac{1}{24}m^3n^2 + \frac{1}{48}m^4n^2 + \frac{1}{144}m^4n^3 - \frac{1}{144}m^4n + \frac{1}{96}m^3n^4 \\ &+ \frac{1}{24}m^3n^3 - \frac{1}{24}m^3n\ . \end{aligned}$$

ii) If m is odd then,

$$\begin{aligned} TSZ(P_n \times C_m) &= \frac{1}{120}m^2n^5 + \frac{1}{24}m^2n^4 + \frac{5}{144}m^2n^3 - \frac{13}{192}m^2n^2 - \frac{31}{720}m^2n \\ &+ \frac{1}{384}m^5n^2 - \frac{11}{384}mn^2 + \frac{1}{48}m^4n^2 - \frac{7}{2976}m^3n^2 + \frac{1}{144}m^4n^3 \\ &- \frac{1}{144}m^4n + \frac{1}{96}m^3n^4 - \frac{1}{96}mn^4 + \frac{1}{24}m^3n^3 - \frac{1}{24}mn^3 \\ &- \frac{1}{24}m^3n + \frac{1}{24}mn\ . \end{aligned}$$

iii) If m and n are even then,

$$\begin{aligned} TSZ(C_n \times C_m) &= \frac{1}{384}m^2n^5 + \frac{1}{16}m^2n^3 + \frac{1}{48}m^2n^4 + \frac{1}{12}m^2n^2 + \frac{1}{384}n^2m^5 \\ &+ \frac{1}{16}n^2m^3 + \frac{1}{48}n^2m^4 + \frac{1}{192}n^3m^4 + \frac{1}{192}n^4m^3 + \frac{1}{32}m^3n^3\ . \end{aligned}$$

iv) If m and n are odd then,

$$\begin{aligned} TSZ(C_n \times C_m) &= \frac{1}{384}m^2n^5 - \frac{5}{96}m^2n^2 + \frac{1}{48}m^2n^4 + \frac{7}{192}m^2n^3 + \frac{13}{384}nm^2 \\ &+ \frac{1}{384}n^2m^5 + \frac{1}{48}n^2m^4 + \frac{7}{192}n^2m^3 - \frac{13}{384}n^2m + \frac{1}{192}m^4n^3 \\ &- \frac{1}{192}nm^4 + \frac{1}{192}m^3n^4 - \frac{1}{192}mn^4 + \frac{1}{32}m^3n^3 - \frac{1}{32}m^3n \\ &- \frac{1}{32}mn^3 + \frac{1}{32}mn \ . \end{aligned}$$

v) If m is odd and n is even then,

$$\begin{aligned} TSZ(C_n \times C_m) &= \frac{1}{384}m^2n^5 + \frac{3}{64}m^2n^3 + \frac{1}{48}m^2n^4 + \frac{1}{64}m^2n^2 + \frac{1}{384}n^2m^5 \\ &+ \frac{1}{48}n^2m^4 + \frac{5}{96}n^2m^3 - \frac{19}{384}n^2m + \frac{1}{192}n^3m^4 + \frac{1}{192}m^3n^4 \\ &- \frac{1}{192}mn^4 + \frac{1}{32}m^3n^3 - \frac{1}{32}mn^3 \ . \end{aligned}$$

From now on λ denotes a positive real number. In what follows, the extremal graphs with respect to the Wiener-type invariant are determined.

Lemma 2.5. Suppose G is an incomplete connected graph with n vertices, $n \geq 3$. Then $W_\lambda(G) \geq (1-2^\lambda)|E(G)| + 2^\lambda\binom{n}{2}$ with equality if and only if $diam(G) = 2$.

Proof. Since λ is positive,

$$\begin{aligned} W_\lambda(G) &= \sum_{k=1}^{d} d(G,k)k^\lambda = d(G,1) + \sum_{k=2}^{d} d(G,k)k^\lambda \\ &\geq d(G,1) + 2^\lambda \sum_{k=2}^{d} d(G,k) = |E(G)| + 2^\lambda\left(\binom{n}{2} - |E(G)|\right) \\ &= (1-2^\lambda)|E(G)| + 2^\lambda\binom{n}{2} , \end{aligned}$$

proving the lemma. Clearly the equality holds if and only if $diam(G) = 2$. ■

Corollary 2.6. Suppose G is satisfied the conditions of Lemma 2.5. If $diam(G) = 2$ then $W_\lambda(G) \geq n - 1 + 2^\lambda$ with quality if and only if G is isomorphic to P_3.

Proof. By Lemma 2.5 and this fact that in the $n-$vertex graphs of diameter 2, $n-1 \leq |E(G)| \leq \binom{n}{2} - 1$, we have:

$$W_\lambda(G) \geq |E(G)| - 2^\lambda |E(G)| + 2^\lambda \binom{n}{2} \geq n - 1 - 2^\lambda \binom{n}{2} + 2^\lambda + 2^\lambda \binom{n}{2} = n - 1 + 2^\lambda \ .$$

On the other hand, $n-1 = \binom{n}{2} - 1$ if and only if $n = 3$ and since $diam(G) = 2$, $G \cong P_3$. ■

In 1956, Nordhaus and Gaddum [15] proved that for the chromatic number $\chi(G)$ of a graph G is satisfied the inequality $2\sqrt{n} \leq \chi(G) + \chi(\bar{G}) \leq n+1$. In recent years, too many authors named such an inequality for a given topological index, a Nordhaus-Gaddum type inequality [19]. In what follows a Nordhaus-Gaddum type inequality for the Wiener-type invariant of graphs is proved.

Corollary 2.7. Suppose G and $\bar{G}$ are connected incomplete $n-$vertex graphs with $n \geq 3$. Then $W_\lambda(G) + W_\lambda(\bar{G}) \geq \binom{n}{2}(1+2^\lambda)$ with equality if and only if $diam(G) = diam(\bar{G}) = 2$.

Proof. By Lemma 2.5,

$$\begin{aligned} W_\lambda(G) + W_\lambda(\bar{G}) &\geq (1-2^\lambda)|E(G)| + 2^\lambda \binom{n}{2} + (1-2^\lambda)|E(\bar{G})| + 2^\lambda \binom{n}{2} \\ &= (1-2^\lambda)(|E(G)| + |E(\bar{G})|) + 2^{\lambda+1}\binom{n}{2} \\ &= (1-2^\lambda)\binom{n}{2} + 2^{\lambda+1}\binom{n}{2} = \binom{n}{2}(1+2^\lambda)\,, \end{aligned}$$

as desired. ■

Lemma 2.8. Suppose G is a $n-$vertex connected graph with $n \geq 5$ and $diam(G) = diam(\bar{G}) = 3$. Then $W_\lambda(G) + W_\lambda(\bar{G}) < \binom{n}{2}(1+3^\lambda)$.

Proof. Suppose $t_k = d(G,k)$ and $\bar{t}_k = d(\bar{G},k)$. It is clear that $t_2 + t_3 = \bar{t}_1$, $\bar{t}_2 + \bar{t}_3 = t_1$ and $t_1 + \bar{t}_1 = \binom{n}{2}$. Then,

$$\begin{aligned} W_\lambda(G) + W_\lambda(\bar{G}) &= \sum_{k=1}^{3}(t_k + \bar{t}_k)k^\lambda = (t_1 + \bar{t}_1) + 2^\lambda(t_2 + \bar{t}_2) + 3^\lambda(t_3 + \bar{t}_3) \\ &< \binom{n}{2} + 3^\lambda(t_2 + \bar{t}_2 + t_3 + \bar{t}_3) = \binom{n}{2}(1+3^\lambda)\,, \end{aligned}$$

proving the lemma. ■

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References

[1] M. V. Diudea, I. Gutman, L. Jäntschi, *Molecular Topology*, Nova, Huntington, 2001.

[2] I. Gutman, A property of the Wiener number and its modifications, *Indian J. Chem.* **36A** (1997) 128–132.

[3] I. Gutman, A. A. Dobrynin, S. Klavžar, L. Pavlović, Wiener–type invariants of trees and their relation, *Bull. Inst. Combin. Appl.* **40** (2004) 23–30.

[4] A. Graovac, T. Pisanski, On the Wiener index of a graph, *J. Math. Chem.* **8** (1991) 53–62.

[5] F. Harary, *Graph Theory*, AddisonWesley, Reading, 1969.

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

[7] W. Imrich, S. Klavžar, *Product Graphs — Structure and Recognition*, Wiley, New York, 2000.

[8] M. H. Khalifeh, H. Yousefi–Azari, A. R. Ashrafi, The first and second Zagreb indices of some graph operations, *Discr. Appl. Math.* **157** (2009) 804–811.

[9] M. H. Khalifeh, H. Yousefi–Azari, A. R. Ashrafi, S. G. Wagner, Some new results on distance–based graph invariants, *Eur. J. Combin.* **30** (2009) 1149–1163.

[10] M. H. Khalifeh, H. Yousefi–Azari, A. R. Ashrafi, The hyper–Wiener index of graph operations, *Comput. Math. Appl.* **56** (2008) 1402–1407.

[11] M. H. Khalifeh, H. Yousefi–Azari, A. R. Ashrafi, Vertex and edge PI indices of Cartesian product graphs, *Discr. Appl. Math.* **156** (2008) 1780–1789.

[12] M. H. Khalifeh, H. Yousefi–Azari, A. R. Ashrafi, I. Gutman, The edge Szeged index of product graphs, *Croat. Chem. Acta* **81** (2008) 277–281.

[13] S. Klavžar, A. Rajapakse, I. Gutman, The Szeged and the Wiener index of graphs, *Appl. Math. Lett.* **9** (1996) 45–49.

[14] S. Klavžar, I. Gutman, A theorem on Wiener–type invariants for isometric subgraphs of hypercubes, *Appl. Math. Lett.* **19** (2006) 1129–1133.

[15] E. A. Nordhaus, J. W. Gaddum, On complementary graphs, *Amer. Math. Month.* **63** (1956) 175–177.

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

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

[18] H. Yousefi–Azari, B. Manoochehrian, A. R. Ashrafi, The PI index of product graphs, *Appl. Math. Lett.* **21** (2008) 624–627.

[19] L. Zhang, B. Wu, The Nordhaus–Gaddum–type inequalities for some chemical indices, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 189–194.