Journal of Mathematical Nanoscienese 7 (2) (2017) 79–83

Journal of Mathematical Nanoscience

Available Online at: http://jmathnano.srttu.edu

On the modified Wiener number

Maryam Jalali-Rad *

Department of Pure Mathematics, Faculty of Mathematical Sciences, University of Kashan, Kashan, I. R. Iran

Academic Editor: Alireza Ashrafi

Abstract. The Graovac-Pisanski number is defined in 1991 e.g. more than 50 years after the definition of Wiener number by Graovac and Pisanski. They called this new index as modified Wiener number based on the sum of distances between all the pairs $(u,\alpha(u))$ where α stands in the automorphism group of given graph. In this paper, we investigate some results on the Graovac-Pisanski number.

Keywords. automorphism of graph, Wiener number, orbit.

1 Introduction

By a graph we mean a collection of points and lines connecting them and we call them as vertices and edges, denoted by $V(\Gamma)$ and $E(\Gamma)$, respectively. Two vertices x and y are adjacent if $xy \in E(\Gamma)$. The distance between two arbitrary vertices $x,y \in V(\Gamma)$ denoted by $d(x,y)$ is the length of the shortest path between them. The Wiener number is defined as half sum of the distances between all the pairs of vertices in Γ , see [15]. In other words,

$$W(\Gamma) = \frac{1}{2} \sum_{x,y \in V(\Gamma)} d(x,y). \tag{1}$$

Let Γ be a graph and $uv \in E$ is an edge. An automorphism of Γ is a permutation β on $V(\Gamma)$ with this property that $\beta(uv) \in E(\Gamma)$ if and only if $\beta(u)\beta(v) \in E(\Gamma)$, where $\beta(u)$ denotes to image of vertex u. The automorphism group of graph Γ is denoted by $Aut(\Gamma)$.

*Corresponding author (Email address: jalali6834@gmail.com).
DOI: 10.22061/jmns.2017.512

The orbit of the vertex $u \in V(\Gamma)$ is the set $u^\Gamma = \{\alpha(u) : \alpha \in Aut(\Gamma)\}$. The graph Γ is said to be transitive if it has only one orbit. This means that for every pair of vertices such as $u, v \in V(\Gamma)$, there is an automorphism $\sigma \in Aut(\Gamma)$ such that $\sigma(u) = v$.

The modified wiener number of graph Γ is defined by Graovac and Pisanski in 1991 as follows [10]:

$$\hat{W}(\Gamma) = \frac{|V(\Gamma)|}{2|G|} \sum_{x \in V(\Gamma)} \sum_{\alpha \in G} d(x, \alpha(x)), \tag{2}$$

where $G = Aut(\Gamma)$. Ghorbani and Klavžar in [9] proposed the name "Graovac-Pisanski index". It is thus an unfortunate fact that the term modified Wiener index is nowadays used also for an invariant different from the one of Graovac and Pisanski.

Theorem 1.1. [10]. Let Γ is a graph with automorphism group $G = Aut(\Gamma)$ and vertex set $V(\Gamma)$. Let $V_1, V_2, \ldots, V_k$ be all orbits of action G on $V(\Gamma)$. Then

$$\hat{W}(\Gamma) = |V(\Gamma)| \sum_{i=1}^{k} \frac{W(V_i)}{|V_i|}. \tag{3}$$

From Theorem 1.1, one can see easily that a graph is vertex-transitive if and only if $\hat{W}(\Gamma) = W(\Gamma)$. Similarly, $\hat{W}(\Gamma) = 0$ if and only if $Aut(\Gamma) \cong id$. This means that for all graph Γ, if $w_\Gamma = W(\Gamma)$ then we have $\hat{W}(\Gamma) \in [0, w_\Gamma]$. In addition, if Γ is a non-vertex-transitive graph then $\hat{W}(\Gamma) \in [1, w_\Gamma]$.

2 Results

In this section, first we define a new topological index base on the distance between a vertex and all images of it under the action of automorphism group. In continuing, we investigate some new results on the partial modified Wiener number. In [3] the authors proved that

$$\Delta(g) = \sum_{\alpha \in G} d(g, \alpha(g)) \tag{4}$$

is a classical function and Ghorbani et. al in [8] showed that this function can be interpreted in terms of irreducible characters of G. Hence, the distance between all pair of vertices in a same orbit are important.

Definition 1. Let Γ is a graph with automorphism group $G = Aut(\Gamma)$ and vertex set $V(\Gamma)$. Let $V_1, V_2, \ldots, V_k$ be all orbits of action G on $V(\Gamma)$. The partial modified Wiener index is

$$P\hat{W}(\Gamma) = \sum_{i=1}^{k} W(V_i). \tag{5}$$

Since, for every pair of vertices such as $x, y \in V_i$, the number of automorphisms which maps x to y is $|G|/|V_i|$, then

$$P\hat{W}(\Gamma) = \sum_{i=1}^{k} W(V_i) = \frac{1}{2|G|} \sum_{x \in V(\Gamma)} \sum_{\alpha \in G} |x^G| d(x, \alpha(x)). \tag{6}$$

Since, the elemnts of any orbit is less than or equal with the number of vertices, we can conclude that

$$P\hat{W}(\Gamma) \leq \hat{W}(\Gamma) \tag{7}$$

and equality holds if and only if Γ is vertex-transitive. Similar to the Wiener number, the partial modified Wiener number always is an integer while the Graovac-Pisanski number may be a rational number. If Γ is a non-vertex-transitive graph with orbits V_i's, then for every V_i $(1 \leq i \leq k)$ we have $1 \leq |V_i| \leq k$ and so

$$\frac{\hat{W}(\Gamma)}{P\hat{W}(\Gamma)} \in [\frac{n}{n-1}, n].$$

Theorem 2.1. *Let Γ is a graph with automorphism group $G = Aut(\Gamma)$ and vertex set $V(\Gamma)$. Let $V_1, V_2, \ldots, V_k$ be all orbits of action G on $V(\Gamma)$. Then*

$$P\hat{W}(\Gamma) = \frac{1}{2} \sum_{i=1}^{k} |V_i| D_{V_i}(u), \tag{8}$$

where $D_{V_i}(u) = \sum_{v \in V_i} d(u, v)$.

Proof. It is a well-known fact that the action of automorphism group on its orbit is transitive. Hence, for every pair of elements $x, y \in V_i$, $D_{V_i}(x) = D_{V_i}(y)$. Hence, we can conclude that for a vertex $u \in V_i$, we have

$$W(V_i) = \frac{1}{2} |V_i| D_{V_i}(u). \tag{9}$$

This completes the proof. □

Example 2.2. *A fullerene is a three connected cubic planar graph whose faces are pentagons and hexagons discoverd by H. Kroto and his team, see [4, 14]. The most stable cluster of fullerenes is C_{60}, a fullerene with exactly 60 carbon atoms, 12 pentagones and 20 hexagones, see Figure 1. It is well-known that this fullerene is vertex-transitive and thus*

$$\hat{W}(\Gamma) = P\hat{W}(\Gamma) = W(\Gamma).$$

Theorem 2.3. *Let Γ be a connected edge-transitive graph on n vertices. If Γ is not vertex-transitive, then there is a subset X on p vertices such that*

$$P\hat{W}(\Gamma) = \frac{1}{2}(pD_X(x) + (n-p)D_Y(y)). \tag{10}$$

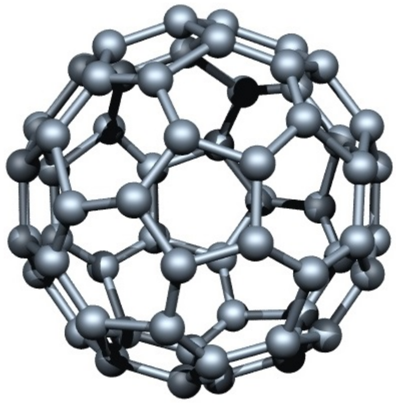

Figure 1. The fullerene graph C_{60}.

Proof. Since Γ is edge-transitive but not vertex-transitive, Γ is bipartite. Suppose $\Gamma = \Gamma(X, Y)$, where $|X| = p$, $|Y| = n - p$. Suppose $G = Aut(\Gamma)$, choose an arbitrary edge $e = xy$, where $x \in X$ and $y \in Y$. One can prove that $V(\Gamma) = x^G \cup y^G$. Hence, Eq.(6) yields the proof. $\square$

Example 2.4. *As an conclusion of above theorem, consider the star graph S_n on $n+1$ vertices. It is not difficult to see that this graph has two orbits a singleton orbit consist of the central vertex and the other vertices compose the second orbit. Hence, for the central vertex u, we have $D_{V_1}(u) = n$ and for the vertex v belong to the second orbit we have $D_{V_1}(v) = n(n-1)$. Thus*

$$P\hat{W}(\Gamma) = \frac{1}{2}(1 \times n + (n-1) \times n(n-1) = n(n^2 - 2n + 2).$$

Example 2.5. *Consider the path graph P_n on n vertices. It is not difficult to see that this graph has $\lfloor n/2 \rfloor$ orbits of order two. In the case that n is odd, there is also a singleton orbit $V_0 = \{x\}$. Two following cases hold:*

1. *n is odd. Suppose the orbits of the automorphism group action are $V_0, V_1, \cdots, V_{\lfloor n/2 \rfloor}$. It is not difficult to see that $W(V_i) = 2i,\ 1 \le i \le \lfloor n/2 \rfloor$ and thus*

$$P\hat{W}(\Gamma) = \sum_{i=1}^{\lfloor n/2 \rfloor} 2i = \frac{n-1}{2}\frac{n+1}{2} = \frac{n^2-1}{4}.$$

2. *n is even. In this case we have $\lfloor n/2 \rfloor$ orbits $U_1, U_2, \cdots, U_{\lfloor n/2 \rfloor}$, with $W(U_i) = 2i - 1$. This implies that*

$$P\hat{W}(\Gamma) = \sum_{i=1}^{\lfloor n/2 \rfloor} 2i - 1 = \frac{n^2}{4}.$$

References

[1] M. Deza, M. Dutour Sikirić and P. W. Fowler, Zigzags, railroads, and knots in fullerenes, *J. Chem. Inf. Comp. Sci.* 44(2004) 1282–1293.

[2] M. Dutour Sikirić , O. Delgado-Friedrichs and M. Deza, Space fullerenes: computer search for new Frank-Kasper structures, *Acta Crystallogr. A* 66 (2010) 602–615.
[3] S. Firouzian, M. Faghani, F. Koorepazan Moftakhar and A. R. Ashrafi, The hyper-Wiener and modified hyper-Wiener indices of graphs with an application on fullerenes, *Studia Ubb Chemia* 59 (2014) 163–170.
[4] P. W. Fowler and D. E. Manolopoulos, *An Atlas of Fullerenes*, Oxford Univ. Press, Oxford, 1995.
[5] M. Ghorbani, Fullerene graphs with pentagons and heptagons, *J. Math. Nanosci.* 3 (2013) 33–37.
[6] M. Ghorbani and T. Ghorbani, Computing the Wiener index of an infinite class of fullerenes, *Studia Ubb Chemia* 58 (1) (2013) 43-50.
[7] M. Ghorbani and M. Hakimi-Nezhaad, An algebraic study of non classical fullerenes, *Fuller. Nanotub. Car. N.* (2015), DOI: 10.1080/1536383X.2015.1090433.
[8] M. Ghorbani, M. Hakimi-Nezhaad and F. Abbasi-Barfaraz, An algebraic approach toWiener number, J. Appl. Math. Comput. 55 (2017) 629–643.
[9] M. Ghorbani and S. Klavžar, Modified Wiener index via canonical metric representation, and some fullerene patches, *Ars Math. Contemp.* 11 (2016) 247–254.
[10] A. Graovac and T. Pisanski, On the Wiener index of a graph, *J. Math. Chem.* 8 (1991) 53–62.
[11] I. Gutman and L. Šoltés, The range of the Wiener index and its mean isomer degeneracy, *Z. Naturforsch.* 46a (1991) 865–868.
[12] M. Hakimi-Nezhaad and M. Ghorbani, Differences between Wiener and modified Wiener indices, *J. Math. Nanosci.* 4 (2014) 19–25.
[13] F. Harary, *Graph Theory*, Addison-Wesley, Reading, Massachusetts, 1969.
[14] H. W. Kroto, J. R. Heath, S. C. ÓBrien, R. F. Curl and R. E. Smalley, C_{60}: buckminster fullerene, *Nature* 318 (1985) 162–163.
[15] H. J. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* 69 (1947) 17–20.