Applied Mathematics and Computation 281 (2016) 223–232

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Combination of distance and symmetry in some molecular graphs

F. Koorepazan-Moftakhar [a,b], A.R. Ashrafi [a,b,*]

[a] Department of Pure Mathematics, Faculty of Mathematical Sciences, University of Kashan, Kashan 87317-53153, Islamic Republic of Iran
[b] Institute of Nanoscience and Nanotechnology, University of Kashan, Kashan 87317-53153, Islamic Republic of Iran

ARTICLE INFO

Keywords:
Wiener index
Modified Wiener index
Automorphism group
(3, 6)-fullerene

ABSTRACT

Suppose G is a connected graph or a union of connected graphs and Γ is a subgroup of $Aut(G)$. The modified Wiener index of G with respect to Γ can be defined as follows:

$$\hat{W}_{\Gamma}(G) = \frac{|V(G)|}{2|\Gamma|} \sum_{u \in V(G)} \sum_{g \in \Gamma} d(u, g(u)).$$

In this article, this graph invariant for the cycle C_n with respect to all subgroups of $Aut(C_n)$ is computed. As consequences, the modified Wiener indices of some molecular graphs like (3, 6)- and (5, 6)-fullerenes with respect to a subgroup of their symmetry groups are computed. Some open questions are also presented.

© 2016 Elsevier Inc. All rights reserved.

1. Introduction

Throughout this paper all graphs are assumed to be simple and connected or disconnected with isomorphic components. A chemical graph is a simple graph in which the vertices are atoms and edges are the chemical bonds. The name "chemical graph" used in literature after pioneering work of Balaban [3]. A graph G is called 3-connected, if it has more than three vertices and remains connected whenever fewer than three vertices are removed. A (3, 6)-fullerene is a 3-connected planar cubic graph whose faces are only triangles and hexagons [1]. Note that by our definition, a (3, 6)-fullerene has to be a polyhedral graph and so it does not have a pair of fused triangles. This is the definition that all chemists would accept for a (3, 6)-fullerene. For the main mathematical properties of fullerenes, we refer to the famous book of Fowler and Manolopoulos [7] and the interesting paper [8].

A topological index is a graph invariant applicable in chemistry. The Wiener index is the oldest distance-based topological index. To define, we assume that G is a chemical graph and x, y are two vertices in G. The distance between x and y, $d(x, y)$, is the length of a shortest path connecting them. The sum of all distances between distinct vertices of G is called the Wiener index of G and denoted by $W(G)$ [23]. In the same paper, Wiener was introduced another graph invariant nowadays named "Wiener polarity index". This index is defined as the number of unordered pairs of vertices $\{u, v\}$ of G such that the shortest distance $d(u, v)$ between u and v is 3. For more information on this topic we refer the interested readers to [6,20].

In literature, there are hundreds published papers devoted to the mathematical properties of the Wiener index. Hriňáková et al. [12], established congruence relations for some families of graphs with a tree-like structure, whose vertices and edges

* Corresponding author. Tel.: +98 3155912367.
E-mail address: ashrafi_1385@yahoo.co.in, ashrafi@kashanu.ac.ir (A.R. Ashrafi).

http://dx.doi.org/10.1016/j.amc.2016.01.065
0096-3003/© 2016 Elsevier Inc. All rights reserved.

represent some graphs of prescribed type and congruence. Lin [17] characterized the trees with the maximal Wiener index in $\mathbb{MT}_{n,k}$, where $\mathbb{MT}_{n,k}$ denotes the set of all trees of order n with exactly k vertices of maximum degree. A vertex of degree ≥ 3 in a tree T is called a branching vertex. Lin [19] also characterized the extremal Wiener index of trees with a given number of vertices of even degree and in [18], the lower and upper bounds of the Wiener index of an n-vertex tree with given number of branching vertices were obtained. Knor et al. [15] proved that the Wiener index of any bipartite graph G is always greater than the Wiener index of $con(G)$, where the common neighborhood graph $con(G)$ has the same vertex set as G and two vertices of $con(G)$ are adjacent if they have a common neighbor in G. Kelenc et al. [14], considered some other modifications of the Wiener index into account

Before we can proceed further in our investigation, some algebraic concepts were fixed. Graovac and Pisanski [11], proposed a distance-symmetry-based graph invariant for a chemical graph by considering a subgroup of its full automorphism group. They named this topological index "Modified Wiener Index". To define, we first notice that the largest possible symmetry group for a given molecule M is the full automorphism group of the chemical graph of M. Suppose G is a connected chemical graph and Γ is a subgroup of $Aut(G)$. Then the modified Wiener index of G with respect to Γ can be defined as follows:

$$\hat{W}_\Gamma(G) = \frac{|V(G)|}{2|\Gamma|} \sum_{u\in V(G)} \sum_{g\in\Gamma} d(u, g(u)).$$

If we define $\delta(g) = \frac{1}{|V(G)|} \sum_{u\in V(G)} d(u, g(u))$ then $\hat{W}_\Gamma(G) = \frac{|V(G)|^2}{2|\Gamma|} \sum_{g\in\Gamma} \delta(g)$.

The present authors [16], presented a representation theoretical method for computing modified Wiener index of a graph. In [2], the authors applied the same approach to calculate the modified Wiener index of some graph operations. Ghorbani and Klažar [10] extended the method of orthogonal cuts for computing modified Wiener index of some fullerene patches.

Throughout this paper C_n denotes a cycle of length n. The cyclic group of order n, the dihedral group of order $2n$ and the symmetric group on n symbols are denoted by Z_n, D_{2n} and S_n, respectively. Our calculations are done with the aid of GAP [22] and Sage [21]. Suppose H is a group and $\mathbb{C}$ denotes the complex field. A function $\gamma : H \longrightarrow \mathbb{C}$ is called a class function, if $\gamma(x) = \gamma(g^{-1}xg)$, for each $x, g \in H$. Our other notations are standard and can be taken from the standard books of graph and group theory.

2. Main results

In this section, the modified Wiener indices of cycles, complete and star graphs under all subgroups of the full automorphism group are computed. We first compute a formula for the modified Wiener index of a non-connected graph with non-isomorphic components.

Lemma 2.1. *Suppose $G_1, \ldots, G_n$ are disjoint non-isomorphic graphs and $G = G_1 \cup \cdots \cup G_n$. Then,*

$$\delta(g) = \frac{1}{|V(G_1 \cup \cdots \cup G_n)|} \sum_{i=1}^{n} |V(G_i)|\delta(g_i).$$

Proof. We first prove the case of $n = 2$. To do this, we assume that G and H are two disjoint and non-isomorphic graphs. Then $Aut(G\cup H) \cong Aut(G) \times Aut(H)$ and so we have:

$$\begin{aligned}
\delta(g) &= \frac{1}{|V(G\cup H)|} \sum_{x\in V(G\cup H)} d(x, g(x)) \\
&= \frac{1}{|V(G\cup H)|} \left[\sum_{x\in V(G)} d(x, g(x)) + \sum_{x\in V(H)} d(x, g(x)) \right] \\
&= \frac{1}{|V(G\cup H)|} \left[\sum_{x\in V(G)} d(x, g_1(x)) + \sum_{x\in V(H)} d(x, g_2(x)) \right] \\
&= \frac{1}{|V(G\cup H)|} [|V(G)|\delta(g_1) + |V(H)|\delta(g_2)].
\end{aligned}$$

We now apply an inductive argument to complete the proof. □

We now calculate the modified Wiener index of complete graphs. To proceed, we assume that Γ is a subgroup of $Aut(K_n) \cong S_n$. Then $\hat{W}_\Gamma(K_n) = \frac{n}{2|\Gamma|} \sum_{g\in\Gamma, x\in V(K_n)} d(x, g(x)) = \frac{n}{2}(n-t)$, where t denotes the number of orbits of Γ in its natural action on vertices. On the other hand, we assume that Γ_1 and Γ_2 are conjugate subgroups of $Aut(K_n) \cong S_n$ with t_1 and t_2 orbits, respectively. Then obviously $t_1 = t_2$ and so their modified Wiener indices are the same. In the next lemma, we prove that in general the modified Wiener indices of conjugate subgroups of $Aut(G)$ are the same.

Lemma 2.2. *Suppose G is a graph and $\Gamma_1, \Gamma_2 \subseteq Aut(G)$. If Γ_1 and Γ_2 are conjugate then $\hat{W}_{\Gamma_1}(G) = \hat{W}_{\Gamma_2}(G)$.*

Download English Version:

https://daneshyari.com/en/article/4625860

Download Persian Version:

https://daneshyari.com/article/4625860

Daneshyari.com