STUDIA UBB CHEMIA, LIX, 4, 2014 (p. 163-170)
(RECOMMENDED CITATION)

THE HYPER-WIENER AND MODIFIED HYPER-WIENER INDICES OF GRAPHS WITH AN APPLICATION ON FULLERENES

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ABSTRACT. Graovac and Pisanski have proposed an algebraic approach for generalizing the Wiener index by automorphism group of the graph under consideration. In this paper we introduce a new modification of the hyper-Wiener index. The hyper-Wiener and modified hyper-Wiener indices of two infinite classes of fullerenes are presented.

Keywords: *Wiener index, hyper-Wiener index, modified hyper-Wiener index, fullerene*.

INTRODUCTION

Throughout this paper, graph means connected graphs without loops and multiple edges. Suppose G is such a graph, with the vertex set $V(G)$. The distance between the vertices $u, v \in V(G)$ is denoted by $d(u, v)$ and it is defined as the number of edges in a shortest path connecting them. The Wiener index, $W(G)$, equals the sum of distances between all pairs of vertices in G [1]. This graph invariant found remarkable applications in chemistry [1,2]. The hyper-Wiener index of acyclic graphs was introduced by Milan Randić in 1993. Then Klein, Lukovits and Gutman [3], generalized Randić's definition for all connected graphs, as a generalization of the Wiener index. It is defined as

$$WW(G) = 1/2W(G) + 1/2\sum_{\{x,y\}} d(x,y)^2.$$

We refer to [4,5] for mathematical properties and chemical meaning of this topological index. It merits to mention the matrix-based version of some distance-based topological indices, introduced by Diudea [6-9]. To explain,

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we assume that D and W are Distance and Wiener matrices of a given graph G of order n. The distance matrix is an $n \times n$ matrix in which the ij^{th} entry is the length of a shortest path connecting the i^{th} and j^{th} vertices of the graph under consideration. The Wiener matrix is another $n \times n$ matrix such that its ij^{th} entry is defined as the number of paths containing the (i, j)-path. These matrices can be taken as the basis for calculating W (as the half-sum of matrix entries), whereas Distance-Path D_p and Wiener-Path W_p can be used to calculate the hyper-Wiener index. D_p counts the internal paths of the path ij while W_p the external paths containing the path ij. In a tree graph, the sum of all internal paths equals the sum of external paths (as established in [3]) while, in cyclic graphs, W_p is not defined, thus D_p being the only matrix enabling the calculation of hyper-Wiener index. We encourage the interested readers to consult the mentioned papers by Diudea and references therein for more information on this topic.

Graovac and Pisanski [10] in a pioneering work proposed an algebraic approach for generalizing the Wiener index by automorphism group of the graph under consideration. To explain, we assume that G is a graph with automorphism group $\Gamma = Aut(G)$. The modified Wiener index of G is defined as:

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

They introduced this generalization of the classical Wiener index to consider the symmetry structure of the graph G. Define in a similar way the modified hyper-Wiener index of G as follows:

$$\hat{WW}(G) = \frac{1}{2}\hat{W}(G) + \frac{|V(G)|}{4|\Gamma|} \sum_{u \in V(G), \alpha \in \Gamma} d(u, \alpha(u))^2.$$

Throughout this paper we use standard notations of graph theory. The path, cycle, star and complete graphs with n vertices are denoted by P_n, C_n, S_n and K_n, respectively.

MODIFIED HYPER-WIENER INDICES OF PATH, CYCLE, STAR AND COMPLETE GRAPHS

It is easy to see that the modified Wiener index of a graph G is equal to zero if and only if $Aut(G)$ is a trivial group. The same is true for the modified hyper-Wiener index of G. On the other hand, it is well-known that most of the finite graphs have trivial automorphism groups. In an exact phrase, suppose α_n and β_n denote the number of n-vertex graphs and n-vertex graphs with trivial automorphism group, respectively. Then,

$$\lim_{n\to\infty}\frac{\alpha_n}{\beta_n}=1.$$

This means that the modified Wiener and hyper-Wiener indices of most of graphs are zero.

From now on, we consider some well-known graphs like path, cycle, star and complete graph on n vertices. On the other hand, the hyper-Wiener index of n-vertex path P_n, the n-vertex cycle C_n and the n-vertex star S_n can be computed by the following formula:

$$WW(P_n)=\frac{1}{24}(n^4+2n^3-n^2-2n);\ WW(S_n)=\frac{1}{2}(n-1)(3n-4),$$

$$WW(C_n)=\begin{cases}\dfrac{n^2(n+1)(n+2)}{48} & 2|n\\[2mm] \dfrac{n(n^2-1)(n+3)}{48} & 2\nmid n\end{cases}.$$

We recall that the symmetry group of a path P_n is a cyclic group of order two and its non-identity element g is as follows:

$$g=\begin{cases}(1\ \ n)(2\ \ n-1)\ldots\left(\dfrac{n+3}{2}\right)\left(\dfrac{n-1}{2}\ \ \dfrac{n+3}{2}\right) & n \text{ is odd}\\[2mm] (1\ \ n)(2\ \ n-1)\ldots\left(\dfrac{n}{2}\ \ \dfrac{n+2}{2}\right) & n \text{ is even}\end{cases}.$$

On the other hand the group of all symmetries of a regular polygon, including both rotations and reflections is called the dihedral group. This group has the order $2n$ and is denoted by D_{2n}.

Assume that n is odd. Then we have:

$$\begin{aligned}\widehat{W}(P_n) &= \frac{|V(G)|}{2|Aut(G)|}\sum_{u\in V(G),g\in Aut(G)} d(u,g(u))\\ &= \frac{n}{4}\times 2\times\left[d(1,n)+d(2,n-1)+\cdots+d\left(\frac{n-1}{2},\frac{n+3}{2}\right)\right]\\ &= \frac{n}{2}\times[(n-1)+(n-3)+\cdots+2]\\ &= \frac{n^3-n}{8};\text{ when } n \text{ is odd.}\end{aligned}$$

$$
\begin{aligned}
\widehat{W}(P_n) &= \frac{|V(G)|}{2|Aut(G)|}\sum_{u\in V(G),g\in Aut(G)} d(u,g(u)) \\
&= \frac{n}{4}\times 2\times\left[d(1,n)+d(2,n-1)+\cdots+d\left(\frac{n}{2},\frac{n+2}{2}\right)\right] \\
&= \frac{n}{2}\times[(n-1)+(n-3)+\cdots+1] \\
&= \frac{n^3}{8}\text{; when } n \text{ is even.}
\end{aligned}
$$

This corrects the calculation of modified Wiener index given [10]. If n is odd then the modified hyper-Wiener index can be calculated in the following form:

$$
\begin{aligned}
\widehat{WW}(P_n) &= \frac{1}{2}\times\frac{n^3-n}{8}+\frac{n}{8}\times 2\times(2^2+4^2+\cdots+(n-1)^2) \\
&= \frac{n^3-n}{16}+\frac{n^4-n^2}{24} \\
&= \frac{n^4}{24}+\frac{n^3}{16}-\frac{n^2}{24}-\frac{n}{16},
\end{aligned}
$$

and if n is even then we have,

$$
\begin{aligned}
\widehat{WW}(P_n) &= \frac{1}{2}\times\frac{n^3}{8}+\frac{n}{8}\times 2\times(1^2+3^2+\cdots+(n-1)^2) \\
&= \frac{n^3}{16}+\frac{n^2}{24}(n^2-1).
\end{aligned}
$$

To compute the modified hyper-Wiener index of cycle graph C_n, we apply calculation of the modified Wiener index of C_n given [Example 5.7, 10] as follows:

$$
\widehat{W}(C_n) = \begin{cases} \frac{n^3}{8} & n \text{ is even} \\ \frac{n^3-n}{8} & n \text{ is odd} \end{cases}.
$$

By a method similar to the case of P_n, we have:

$$
\widehat{WW}(C_n) = \begin{cases} \frac{1}{48}n^4+\frac{1}{16}n^3+\frac{1}{24}n^2 & n \text{ is even} \\ \frac{1}{48}n^4+\frac{1}{16}n^3-\frac{1}{48}n^2-\frac{1}{16}n & n \text{ is odd} \end{cases}.
$$

It is clear that if $u,v \in K_n$ then $d(u,v) = 1$ and so between graphs with exactly n vertices, the complete graph K_n has the minimum hyper–Wiener index. Hence for every n–vertex graph G,

$$WW(G) \geq WW(K_n) = \binom{n}{2}.$$

On the other hand, it is easy to see that the symmetry group of K_n is isomorphic to the symmetric group S_n and so

$$\widehat{W}(K_n) \;=\; \hat{W}W(K_n) = \frac{n^2}{2} - \frac{n}{2}.$$

Since graphs with trivial automorphism group have zero hyper-Wiener index, the complete group K_n does not have the minimum value of hyper-Wiener index in the set of all n-vertex graphs.

We end this section by calculation of the modified hyper-Wiener index of S_n. Suppose $X = \{1, \ldots, k\}$. We denote by Sym_k the set of all permutations of X. Sym_k forms a group under composition of functions. It is well-known that the symmetry group of the star graph is isomorphic to Sym_{n-1}. So,

$$\widehat{W}(S_n) = \frac{|V(S_n)|}{2|Aut(S_n)|} \sum_{u \in V(S_n), g \in Aut(S_n)} d\big(u, g(u)\big) = \frac{n}{2(n-1)!} \sum_i i \times n_i.$$

Define $A = \big\{\big(u, g(u)\big) \big| u \in \{1, \ldots, n-1\}, g \in Aut(S_n) = Sym_{n-1},\ g(u) \neq u\}$ and note that in the star graph all pairs of vertices are in distance 0, 1 or 2. By the structure of star graph, we have $d(u, g(u)) = 2$ and so $|A| = (n-1)! - (n-2)! = (n-2)(n-2)!$. Therefore,

$$\widehat{W}(S_n) = (n-1) \times \frac{n}{2(n-1)!} \times 2 \times (n-2)(n-2)! = n(n-2),$$

$$\begin{aligned}
\hat{W}W(S_n) &= \frac{1}{2} \hat{W}(S_n) + \frac{|V(S_n)|}{4|Aut(S_n)|} \sum_{u \in V(S_n), g \in Aut(S_n)} d(u, g(u))^2 \\
&= \frac{n(n-2)}{2} + \frac{n}{4(n-1)!} \times 4 \times (n-1) \times |A| \\
&= \frac{n(n-2)}{2} + n(n-2) = \frac{3}{2} n(n-2).
\end{aligned}$$

FULLERENE GRAPHS

A graph G is called 3-regular or cubic, if the degree of each vertex is three. G is said to be 3-connected, if there does not exist a set of two vertices whose removal disconnects the graph. A planar, cubic and 3-connected graph is called a fullerene graph if all faces are pentagons and hexagons. The importance of fullerene graphs is for applications in fullerene chemistry. This new topic has been developed after pioneering work of Kroto and his team [11]. The mathematical properties of fullerene graphs are a new branch of nanoscience started by pioneering work of Fowler *et al*. [12,13]. We encourage the reader to consult the papers [14-16] and references therein for more information on this topic.

In [17-20], the symmetry and topology of some infinite classes of fullerenes are investigated. The aim of this section is to continue our last works on two fullerene series C_{50+10n} and C_{60+12n} (Figures 1 and 2, respectively) by computing the modified Wiener and hyper-Wiener indices. We first notice that the symmetry group of the fullerene C_{50+10n} has D_{5h} point group symmetry and so it is isomorphic to the dihedral group D_{20}. The fullerene graphs C_{60+12n} have D_{6d} point group symmetry that is isomorphic to the dihedral group D_{24}, when n is odd. If n is even, these fullerenes have the point group symmetry D_{6h} isomorphic to $Z_2 \times Z_2 \times Sym_3$, the symmetry group on three symbols. By this information, we apply HyperChem [21] and TopoCluj [22] to calculate

$$WW(C_{72}) = 47178, WW(C_{84}) = 75564, \widehat{WW}(C_{72}) = 52056, \widehat{WW}(C_{84}) = 84042.$$

On the other hand, some of the present authors [23], proved a matrix method for calculation of the Wiener index of some classes of fullerenes. By applying this method, one can see that:

$$WW\left(C_{50+10n}\right) = \begin{cases} \frac{25}{6}n^4 + \frac{400}{3}n^3 + \frac{9635}{6}n^2 + \frac{31625}{3}n + 14515 & n \text{ is odd} \\ \frac{25}{6}n^4 + \frac{400}{3}n^3 + \frac{9635}{6}n^2 + \frac{31715}{3}n + 14710 & n \text{ is even} \end{cases},$$

$$WW\left(C_{60+12n}\right) = \begin{cases} 6n^4 + 204n^3 + 2628n^2 + 20076n + 21924 & n \text{ is odd} \\ 6n^4 + 204n^3 + 2628n^2 + 20136n + 22362 & n \text{ is even} \end{cases}.$$

Figure 1. The Case of $n = 9$ in C_{50+10n}.

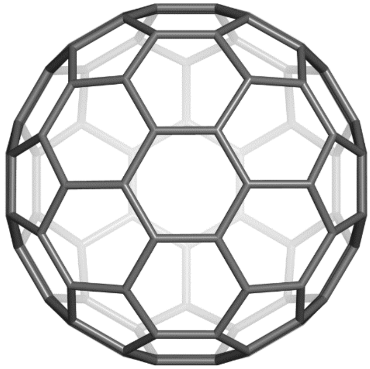

Figure 2. The Case of $n = 9$ in C_{60+12n}.

We now use the automorphism group of these fullerenes to compute their modified hyper-Wiener indices. A simple case by case calculation for pairs of vertices at distance i can provide the following formulas for the modified hyper-Wiener indices of C_{50+10n} and C_{60+12n} fullerenes:

$$\widehat{WW}\left(C_{50+10n}\right) = \begin{cases} \frac{25}{6}n^4 + \frac{725}{6}n^3 + \frac{5320}{3}n^2 + \frac{60745}{6}n + \frac{37575}{2} & n \text{ is odd} \\ \frac{25}{6}n^4 + \frac{725}{6}n^3 + \frac{5350}{3}n^2 + \frac{30335}{3}n + 18475 & n \text{ is even} \end{cases},$$

$$\widehat{WW}\left(C_{60+12n}\right) = \begin{cases} 6n^4 + 183n^3 + 3069n^2 + 18075n + 32775 & n \text{ is odd} \\ 6n^4 + 183n^3 + 3093n^2 + 18606n + 34830 & n \text{ is even} \end{cases}.$$

Our calculation, on fullerene graphs of small order suggests the following conjecture:

CONJECTURE

If F is a fullerene graph then $\frac{WW(F)}{\widehat{WW}(F)} \leq 3$.

ACKNOWLEDGMENTS

The first author is partially supported by the Payame Noor University. We are indebted to Professor Mircea V. Diudea for his suggestions and helpful remarks.

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