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Symmetry–Moderated Wiener Index

Hossein Shabani, Ali Reza Ashrafi•

Department of Pure Mathematics, Faculty of Mathematical Sciences, University of Kashan, Kashan 87317–51167, I R Iran

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Abstract

The modified Wiener index is an algebraic modification of the classical Wiener index under symmetry group. This graph invariant was presented by Graovac and Pisanski in 1991. In this paper, the modified Wiener polynomial $\hat{W}(G,x)$ of a graph G is presented by which we extend some well–known results of the classical Wiener index to its modified version. Moreover, the modified Wiener polynomials of some classes of chemical graphs containing linear phenylene and its hexagonal squeeze, and the ortho–, meta– and para–polyphenylene chains are computed.

1. Introduction

Let $G = (V(G), E(G))$ be a simple connected graph with non–empty vertex set $V(G)$ and edge set $E(G)$. The distance $d_G(u,v)$ between vertices u and v of G is the length of a shortest path connecting u and v. The diameter of G, $d(G) = diam(G)$, is the maximum distances between vertices in G. The sum of all distances between pair of vertices in G is called the Wiener index of G and denoted by $W(G)$ [18]. Graovac and Pisanski in their seminal paper [4] applied the symmetry group of the graph under consideration to obtain an algebraic modification of the classical Wiener index. We encourage the interested readers to consult [12] for more information on the modified Wiener index and its relationship with representation theory of finite groups.

Suppose G is a graph, Γ is a subset of the automorphism group of G ($Aut(G)$) and λ is a real number. The λ*–distance number* of G is defined as

•Corresponding author (ashrafi@kashanu.ac.ir).

$$\delta_\lambda(G) = \frac{1}{|\Gamma||V(G)|}\sum_{g\in\Gamma}\sum_{u\in V(G)} d(u,g(u))^\lambda.$$

For $\lambda = 1$, $\delta_1(G) = \delta(G)$ is the ordinary distance number. The ***modified Wiener index*** is defined as $\hat{W}(G) = 1/2|V(G)|^2\ \delta(G)$ and the ***modified hyper–Wiener index*** [3] is defined as $\hat{WW}(G) = 1/2|V(G)|^2\ \delta(G) + 1/4|V(G)|^2\ \delta_2(G)$. In [16], the present authors computed the modified Wiener index of some graph operations. In this paper we continue our work by considering a polynomial version of this graph invariant.

Throughout this paper our notation is standard. We encourage the interested readers to consult papers [6,13,14] and references therein for more information on this topic.

2. Modified Wiener Polynomial

Hosoya [7] introduced the generating function $H(G,x)$ of distances in a given graph G and termed it the Wiener polynomial for $H(G,x)$. In an exact phrase, $H(G,x) = \sum_{k\ge 0} d(G,k)x^k$, where $d(G,k)$ denotes the number of pairs of vertices of the graph G whose distance is k. Some papers denote Hosoya polynomial as $W(G,x)$ and called it the Wiener polynomial. Similarly, we define the modified Wiener polynomial as follows:

Definition 1. Suppose G is a simple connected graph and Γ is a subgroup of $Aut(G)$. The "***modified Wiener polynomial***" of G is defined as

$$\hat{W}(G,x) = \frac{|V(G)|}{2|\Gamma|}\sum_{i=1}^{d(G)} \hat{d}(G,i)x^i,$$

where $\hat{d}(G,i) = \sum_{u\in V(G)} \hat{d}(u,i)$ and $\hat{d}(u,i) = \left|\{\{u,g(u)\} \mid g\in\Gamma \,\&\, d(u,g(u)) = i\}\right|$, $1 \le i \le d(G)$.

It is obvious that, the degree of the modified Wiener polynomial is $\le d(G)$. For a subset U of vertices of G, we assume that $\hat{d}(U,i) = \sum_{u\in U}\hat{d}(u,i)$, where $1 \le i \le d(G)$. Then we define the ***U–locally modified Wiener polynomial*** of G as

$$\hat{W}(U,x) = \frac{|U|}{2|\Gamma|}\sum_{i=1}^{d(G)} \hat{d}(U,i)x^i.$$

In the following lemma, an algebraic method for computing $\hat{W}(G,x)$ is presented.

Theorem 1. Suppse V_1, V_2, …, V_r are orbits of natural action of Γ on vertices of G. Then,

$$\hat{W}(G,x) = |V(G)|\sum_{k=1}^{r}\frac{\hat{W}(V_k,x)}{|V_k|}.$$

Indeed, if G is vertex transitive then $\hat{W}(G,x) = W(G,x)$.

Proof. It is easy to see that $\hat{d}(G,i) = \sum_{k=1}^{r}\hat{d}(V_k,i)$. Then,

$$\begin{aligned}\hat{W}(G,x) &= \frac{|V(G)|}{2|\Gamma|}\sum_{i=1}^{d(G)}\hat{d}(G,i)x^i = \frac{|V(G)|}{2|\Gamma|}\sum_{i=1}^{d(G)}\left(\sum_{k=1}^{r}\hat{d}(V_k,i)\right)x^i \\ &= \frac{|V(G)|}{2|\Gamma|}\sum_{k=1}^{r}\sum_{i=1}^{d(G)}\hat{d}(V_k,i)x^i = |V(G)|\sum_{k=1}^{r}\left(\frac{1}{2|\Gamma|}\sum_{i=1}^{d(G)}\hat{d}(V_k,i)x^i\right) \\ &= |V(G)|\sum_{k=1}^{r}\left(\frac{1}{|V_k|}\hat{W}(V_k,x)\right).\end{aligned}$$

If G is vertex transitive then for each i, $\hat{d}(G,i) = d(G,i)$. This proves the theorem. ■

Example 1. Let K_n and C_n be ***complete*** and ***cyclic graphs*** with n vertices. It is well known that the automorphism group of K_n is isomorphic to symmetric group $Sym(n)$ on n letters and the automorphism of C_n is isomorphic to dihedral group D_n of order $2n$ and these graphs are vertex transitive. Then, $\hat{W}(K_n,x) = \binom{n}{2}x$ and $\hat{W}(C_n,x) = n\sum_{i=1}^{n/2-1}x^i + \frac{n}{2}x$, where n is even and $\hat{W}(C_n,x) = n\sum_{i=1}^{(n-1)/2}x^i$, where n is odd.

Example 2. Let P_n be the ***path graph*** with n vertices and let S_n and W_n be ***star*** and ***wheel*** graphs with $n + 1$ vertices, where $n \geq 3$. The automorphism group of P_n is isomorphic to the cyclic group of order 2 and it has $\lceil n/2 \rceil$ orbits, where $\lceil x \rceil$ denotes the ceiling of x. Then

$$\hat{W}(P_n,x) = \begin{cases}\sum_{i=1}^{n/2}x^{2i-1} & n \text{ is even} \\ \sum_{i=1}^{(n-1)/2}x^{2i} & n \text{ is odd}.\end{cases}$$

The automorphism groups of S_n and W_n are isomorphic to *Sym*(n). These graphs have 2 orbits on vertices and so $\hat{W}(S_n,x)=\frac{n(n-1)}{2}x$ and $\hat{W}(W_n,x)=nx+\frac{n(n-3)}{2}x$.

Example 3. Let $K_{r,s}$ be the ***complete bipartite graph*** with vertex set $\{x_1, x_2, \ldots, x_r, y_1, y_2, \ldots, y_s\}$. If $r \neq s$, then the automorphism group of $K_{r,s}$ is isomorphic to $Sym(r) \times Sym(s)$. In this case, there are two orbits $\{x_1, x_2, \ldots, x_r\}$ and $\{y_1, y_2, \ldots, y_s\}$. Then $\hat{W}(K_{r,s},x)=\left(\binom{r}{2}+\binom{s}{2}\right)x^2$. In $r = s$ case, the automorphism group of $K_{r,r}$ is isomorphic to a semi–direct product of cyclic group of order 2 and $Sym(r) \times Sym(s)$. This graph is vertex transitive and so $\hat{W}(K_{r,r},x)=r^2x+r(r-1)x^2$.

Let g be an arbitrary automorphism of a graph G. Define the polynomial $\delta(g,x)$ as

$$\delta(g,x)=\frac{1}{|V(G)|}\sum_{u\in V(G)}x^{d(u,g(u))}.$$

For every subgroup Γ of $Aut(G)$, we define:

$$\delta(\Gamma,x)=\frac{1}{|\Gamma|}\sum_{g\in\Gamma}\delta(g,x).$$

The ***distance polynomial*** of a graph G is simply $\delta(\Gamma,x)=\delta(Aut(G),x)$.

Theorem 2. Let Γ be a subset of $Aut(G)$. The modified Wiener polynomial can be rewritten as

$$\hat{W}(G,x)=\frac{|V(G)|^2}{2}\delta(\Gamma,x).$$

Proof. Suppose that u is an arbitrary vertex of G. By definition, $\hat{d}(u,i)$ is equal to the number of automorphisms $g \in \Gamma$ such that $d(u,g(u)) = i$. Choose arbitrary vertices u and v of G in an orbit V_k such that $d(u,v) = i$. Therefore, all automorphisms which map u to v, have been considered in the set $\{\{u,g(u)\} \mid g\in\Gamma \,\&\, d(u,g(u))=i\}$. Now the repetition of x^i in $\sum_{g\in\Gamma}\sum_{u\in V(G)}x^{d(u,g(u))}$ is equal to $\hat{d}(G,i)$ and so we have:

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

This completes the proof. ■

Corollary 1. The modified Wiener polynomial satisfies the following conditions:

a) $\hat{W}'(G,1) = \hat{W}(G)$,

b) $\hat{W}'(G,1) + 1/2\hat{W}''(G,1) = \hat{WW}(G)$.

Proof. It is obtained directly from definition. ■

As in Theorem 2, for every subset *U* of *V*(*G*), we can rewrite the *U*–locally modified Wiener polynomial of *G* as

$$\hat{W}(U,x) = \frac{|U|}{2|\Gamma|}\sum_{g\in\Gamma}\sum_{u\in U} x^{d(u,g(u))}.$$

We can also define the ***U*–locally modified Wiener index** and ***U*–locally modified hyper–Wiener index** as:

$$\hat{W}(U) = \frac{|U|}{2|\Gamma|}\sum_{g\in\Gamma}\sum_{u\in U} d(u,g(u)) \text{ and } \hat{WW}(U) = 1/2\hat{W}(U) + \frac{|U|}{4|\Gamma|}\sum_{g\in\Gamma}\sum_{u\in U} d(u,g(u))^2.$$

Obviously, if Γ = *Aut*(*G*) and *U* is an orbit of *V*(*G*) then $\hat{W}(U) = W(U)$ and $\hat{WW}(U) = WW(U)$.

Corollary 2. If V_1, V_2, …, V_r are orbits of the action of Γ on *V*(*G*) then the modified Wiener index and the modified hyper–Wiener index can be computed by the following formulas:

a) $\hat{W}(G) = |V(G)|\sum_{k=1}^{r}\frac{W(V_k)}{|V_k|}$,

b) $\hat{WW}(G) = |V(G)|\sum_{k=1}^{r}\frac{WW(V_k)}{|V_k|}$.

3. Modified Wiener Polynomial of Some Chemical Graphs

Most calculations of this section are done for the families of graphs that can be viewed as fasciagraphs. For the introduction to polygraphs (i.e. fasciagraphs and rotagraphs) the interested readers are referred to the paper [1]. The idea there is to use the transfer matrix method to help calculate an invariant of a fasciagraph or rotagraphs. This method was first used for calculation of the matching polynomial but was later applied to some other graph invariant such as the Wiener index; see for instance [8,10].

In this section, the modified Wiener polynomial, modified Wiener index and modified hyper–Wiener index of linear phenylene and its hexagonal squeeze, ortho–, meta– and para–polyphenylene chains are computed. It is merit to mention here that the modified hyper–Wiener index is a symmetry version of so called topological index hyper–Wiener index was introduced by Klein et al.

3.1. Linear phenylene and its hexagonal squeeze

Phenylenes are polycyclic conjugated molecules with six– and four–membered rings, Figure 1. A phenylene *LP* is a planar 2–connected graph containing mutually congruent regular hexagons and mutually congruent squares, both with edges of equal length. Each square is joined to exactly two hexagons, whereas all hexagons are mutually disjoint. Each phenylene is in a one–to–one correspondence with a catacondensed benzenoid system called “hexagonal squeeze”, Figure 2, denoted by *LH* [5].

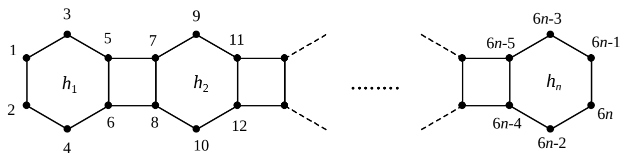

Figure 1. Linear phenylene LPh_n.

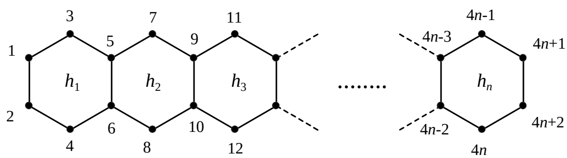

Figure 2. Linear hexagonal squeeze LH_n.

Theorem 3. Let n be a positive integer greater than 1. Then the modified Wiener polynomial of linear hexagonal squeeze of length n is equals to

$$\hat{W}(LH_n, x) = \frac{2n+1}{2(x-1)}\left(2x^{4n+2} + (2n+1)x^4 - (2n+1)x^3 - 2x^2\right).$$

Proof. In the molecular graph of LH_n, we have n hexagons, $n \geq 2$, and $|V(LH_n)| = 4n + 2$. One can easily prove that the automorphism group of this graph can be generated by two automorphisms

$$\alpha = (1,2)(3,4)\ldots(4n-1,4n)(4n+1,4n+2),$$
$$\beta = (1,4n+1)(3,4n-1)\ldots(2n-1,2n+3)(2n+1)(2,4n+2)(4,4n)\ldots(2n,2n+4)(2n+2).$$

It is clear that this group is isomorphic to $Z_2 \times Z_2$ and this group has exactly $n + 1$ orbits as follows:

$$V_i = \{2i - 1, 2i, 4n - 2i + 3, 4n - 2i + 4\};\ 1 \leq i \leq n + 1.$$

For $1 \leq i \leq n$, $|V_i| = 4$ and if i is even then $\hat{W}(V_i,x) = 2(x^{2n-2i+2} + x^{2n-2i+3} + x^3)$ and if i is odd, then $\hat{W}(V_i,x) = 2(x^{2n-2i+2} + x^{2n-2i+3} + x)$. For $i = n + 1$, $|V_{n+1}| = 2$ and so $\hat{W}(V_{n+1}, x) = \begin{cases} x & n \text{ is even} \\ x^3 & n \text{ is odd} \end{cases}$. By applying Theorem 2, the result is obtained. ■

By applying Corollary 1 of Theorem 2, the modified Wiener index and modified hyper–Wiener index of linear hexagonal squeezes can be computed by formulas $\hat{W}(LH_n) = 16n^3 + 28n^2 + 12n + 1$ and $\hat{WW}(LH_n) = 1/3(64n^4 + 128n^3 + 134n^2 + 49n + 3)$.

Theorem 4. Let $n > 1$ be a positive integer. Then the modified Wiener polynomial of the linear phenylene of length n is computed as follows:

$$\hat{W}(LPh_n, x) = \begin{cases} \dfrac{3n}{2(x-1)}\left(2x^{3n+1} + nx^4 - nx^3 + 2nx^2 - 2(n+1)x\right), & n \text{ is even}, \\ \dfrac{3n}{2(x-1)}\left(2x^{3n+1} + (n+1)x^4 - (n+1)x^3 + 2(n-1)x^2 - 2nx\right), & n \text{ is odd} \end{cases}.$$

Proof. The automorphism group of LPh_n can be generated by automorphisms α and β such that

$\alpha = (1,2)(3,4)\ldots(6n-3,6n-2)(6n-1,6n)$,

$\beta = (1,6n-1)(3,6n-3)\ldots(3n-1,3n+1)(2,6n)(4,6n-2)\ldots(3n,3n+2)$, n is even,

$\beta = (1,6n-1)(3,6n-3)\ldots(3n-2,3n+2)(3n)(2,6n)(4,6n-2)\ldots(3n-1,3n+3)(3n+1)$, n is odd. This group is isomorphic to $Z_2 \times Z_2$. It is clear that $V_i = \{2i - 1, 2i, 6n - 2i + 1, 6n - 2i + 2\}$, $1 \leq i \leq 3n/2$ (n is even) and $1 \leq i \leq (3n + 1)/2$ (n is odd) are orbits of this group under its natural action. For each n and each i, else n is odd and $i = (3n + 1)/2$, we have:

$$\hat{W}(V_i, x) = \begin{cases} 2(x^{3n-2i+1} + x^{3n-2i+2} + x^3), & i = 3k-1 \\ 2(x^{3n-2i+1} + x^{3n-2i+2} + x), & otherwise. \end{cases}$$

When n is odd and i = $(3n+1)/2$, $\hat{W}(V_{(3n+1)/2}, x) = 2x^3$. The result is now an immediate consequence of Theorem 2. ■

By applying Corollary 1 of Theorem 2, the modified Wiener and modified hyper–Wiener indices of linear chains can be computed as follows:

$$\hat{W}(LPh_n) = \begin{cases} \frac{27}{2}n^3 + \frac{33}{2}n^2 - 3n; & n \text{ is even}, \\ \frac{27}{2}n^3 + \frac{15}{2}n^2 + 6n; & n \text{ is odd}, \end{cases}$$

$$\hat{WW}(LPh_n) = \begin{cases} \frac{27}{2}n^4 + \frac{27}{2}n^3 + \frac{39}{2}n^2 - 3n; & n \text{ is even}, \\ \frac{27}{2}n^4 + \frac{27}{2}n^3 + \frac{21}{2}n^2 + \frac{21}{2}n; & n \text{ is odd}. \end{cases}$$

3.2. Linear polyphenylene chains

Any of numerous polymers in which the basic building block is a phenylene is called a polyphenylene. In fact, a polyphenylene is a graph obtained from a hexagonal cactus by expanding each of its cut–vertices to an edge. Here, a cactus graph is a connected graph in which no edge is contained in more than one cycle. In such graphs, each block is either a cycle or an edge. If all blocks of a cactus graph G are cycles of the same size m, then G is called an m–uniform cactus graph. A hexagonal cactus is a 6–uniform cactus.

An internal hexagon in a polyphenylene is called ortho–hexagon, meta–hexagon, or para–hexagon, Figure 3, if its cut–vertices are at distance 1, 2 or 3, respectively. If all internal hexagons in a polyphenylene chain are of the same type, say ortho, the chain is an ortho–chain. The meta– and para–chains can be defined analogously, Figure 4. We denote an ortho–, a meta– and a para–chain of length n by OP_n, MP_n and LP_n, respectively. We refer the interested readers to [2] for some results on this topic.

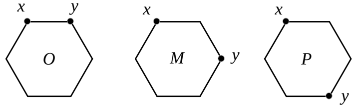

Figure 3. Ortho–, meta– and para–positions of atoms in benzene.

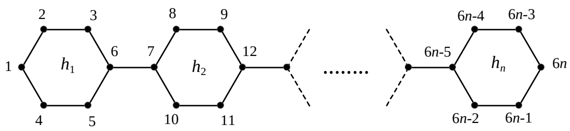

Figure 4. Para–polyphenylenes chain PP_n.

Suppose Γ is a group with subgroups H and K such that H is normal in Γ, $H \cap K = 1$ and $\Gamma = HK$. Then we say Γ is a **semi-direct product** of H by K and write $G = H{:}K$.

Theorem 5. Let $n > 1$ be a positive integer. Then the modified Wiener polynomial of para–polyphenylenes is equals to

$$\hat{W}(PP_n, x) = \begin{cases} \dfrac{3nx\left(x^{4n+4} + x^{4n+2} + x^{4n} + nx^6 - (n+1)x^4 + (n-1)x^2 - (n+1)\right)}{x^6 - x^4 + x^2 - 1}, & n \text{ is even,} \\ \dfrac{3nx\left(2x^{4n+4} + x^{4n} + x^{4n-2} - x^{4n-4} + (n-1)x^6 - nx^4 + (n-2)x^2 - n\right)}{x^6 - x^4 + x^2 - 1}, & n \text{ is odd}. \end{cases}$$

Proof. The molecular graph of a para–polyphenylenes is of the shape shown in Figure 4. Suppose $\alpha_i = (6i-4, 6i-2)(6i-3, 6i-1)$, $1 \le i \le n$. Then one can easily prove that all of a_i are graph automorphisms.

***Case I**: n is even*. For each i, $<\alpha_i> \cong Z_2$ and therefore the direct product of these groups is a normal subgroup of $Aut(PP_n)$. On the other hand, there will be another automorphism τ of order 2 and the automorphism group of PP_n is the semi-direct product $(Z_2 \times \cdots \times Z_2){:}<\tau>$, where $<\tau> \cong Z_2$. In fact, $\tau = \prod_{j=1}^{n/2} \gamma_j \eta_j \pi_j \mu_j \lambda_j \rho_j$, where $\gamma_j = (6i-5, 6n-6i)$, $\eta_j = (6i-4, 6n-6i+3)$, $\pi_j = (6i-3, 6n-6i+2)$, $\mu_j = (6i-2, 6n-6i+5)$, $\lambda_j = (6i-1, 6n-6i+4)$ and $\rho_j = (6i, 6n-6i+1)$.

For $1 \le i \le n/2$, the orbits of vertices are $V_{4i-3} = \{6i-5, 6n-6i+6\}$, $V_{4i-2} = \{6i-4, 6i-2, 6n-6i+3, 6n-6i+5\}$, $V_{4i-1} = \{6i-3, 6i-1, 6n-6i+2, 6n-6i+4\}$ and $V_{4i} = \{6i, 6n-6i+1\}$. Then for any i we have

$$\hat{W}(V_k, x) = \begin{cases} \frac{1}{2} x^{4n-2i+1} & k = 4t+1, 4t \\ x^{n-2i+1} + \frac{1}{2} x^2 & \textit{otherwise.} \end{cases}$$

The result follows from Theorem 2.

Case II: *n is odd*. Then $Aut(PP_n)$ has a subgroup H such that, H is the semi-direct product $K:<\omega>$, where $<\omega> \cong Z_2$, $\omega = \chi\prod_{j=1}^{(n-1)/2}\gamma_j\eta_j\pi_j\mu_j\lambda_j\rho_j$, $\chi = (3n-2,3n+3)(3n-1,3n)(3n+1,3n+2)$ and

$$K = <\alpha_1> \times <\alpha_2> \times \cdots \times <\alpha_{(n-1)/2}> \times <\alpha_{(n+3)/2}> \times \cdots \times <\alpha_n>..$$

Therefore, $Aut(PP_n) \cong <\alpha_{(n+1)/2}> \times H$. For $1 \le i \le (n-1)/2$, the orbits of the automorphism group on vertices are as in the case I. Note that, $V_{2n-1} = V_{2n+2}$ and $V_{2n+1} = V_{2n}$. Then for any i, we have:

$$\hat{W}(V_k, x) = \begin{cases} \frac{1}{2}x^{4n-2i+1}, & k = 4t+1, 4t \\ x^{n-2i+1} + \frac{1}{2}x^2, & \textit{otherwise.} \end{cases}$$

Now, the result is an immediate consequence of Theorem 2. ■

By Corollary 1, the modified Wiener and hyper–Wiener indices of linear chains can be computed and so

$$\hat{W}(PP_n) = \begin{cases} 18n^3 + 6n^2; & n \textit{ is even,} \\ 18n^3 + 6n^2 + 3n; & n \textit{ is odd,} \end{cases}$$

and

$$\hat{WW}(PP_n) = \begin{cases} 24n^4 + 9n^3 + \frac{3}{2}n^2; & n \textit{ is even,} \\ 24n^4 - 15n^3 - \frac{33}{2}n^2 + 3n; & n \textit{ is odd.} \end{cases}$$

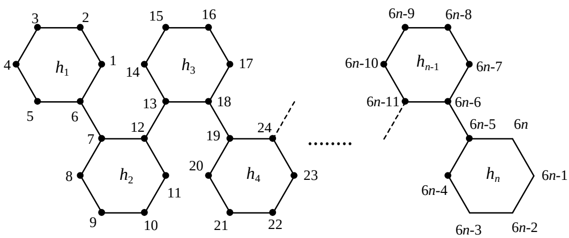

Figure 5. Ortho–polyphenylene chain OP_n.

Theorem 6. Let $n > 1$ be a positive integer. Then the modified Wiener polynomial of ortho–polyphenylene is equal to

$$\hat{W}(OP_n, x) = \begin{cases} \frac{3nx}{x^2-1}\left(3x^{4n} + x^{2n+4} - x^4 + 2x^3 - x^2 - 2x + 1\right) & n \text{ is even,} \\ \frac{3nx}{x^2-1}\left(3x^{4n} + x^{2n+4} + x^{2n+2} - x^{2n} - x^6 + 2x^3 - 2x - 2\right) & n \text{ is odd} \end{cases}.$$

Proof. The molecular graph of polyphenylene is depicted in Figure 5. There are n hexagons such that the i-th hexagon, $i = 1, \ldots, n$, is joined to the next and the previous one by an edge. The automorphism group of OP_n is generated by automorphisms $\alpha_1 = (1,5)(2,4)$, $\alpha_2 = (6n - 1,6n - 3)(6n,6n - 4)$ and $\beta = \prod_{i=1}^{3n}(i,6n-i+1)$. Therefore $Aut(OP_n)$ is isomorphic to dihedral group of order 8.

Suppose $A_i = \{i, 6n-i+1\}$. There are $3n - 2$ orbits as $V_1 = A_3$, $V_2 = A_4 \cup A_1$, $V_3 = A_5 \cup A_2$, $V_i = A_{i+2}$ and $i \leq 3n$-2. Then, $\hat{W}(V_2, x) = 4x^{2n+1} + 2x^2$, $\hat{W}(V_3, x) = 4x^{2n-1} + 2x^2$ and for other values i, except n is odd and $3n-4 \leq i \leq 3n-2$,

$$\hat{W}(V_i, x) = \begin{cases} x^{2n-4k+3} & i = 6k-7 \\ x^{2n-4k+5} & i = 6k-6 \\ x^{2n-4k+7} & i = 6k-5 \\ x^{2n-4k+5} & i = 6k-4 \\ x^{2n-4k+3} & i = 6k-3 \\ x^{2n-4k+1} & i = 6k-2 \end{cases}$$

and if n is odd then, $\hat{W}(V_{3n-4}, x) = \hat{W}(V_{3n-2}, x) = x$, $\hat{W}(V_{3n-3}, x) = x^3$.

Now, the result is an immediate consequence of Theorem 2. ■

Apply Corollary 1, the modified Wiener and hyper–Wiener indices of linear chains can be obtained as:

$$\hat{W}(LPh_n) = \begin{cases} 36n^3 + 12n^2 + 9n; & n \text{ is even,} \\ 36n^3 + 18n^2; & n \text{ is odd,} \end{cases}$$

and

$$\hat{WW}(LPh_n) = \begin{cases} 48n^4 + 30n^3 + 27n^2 + 15n; & n \text{ is even,} \\ 48n^4 + 36n^3 + 36n^2 + 24n; & n \text{ is odd.} \end{cases}$$

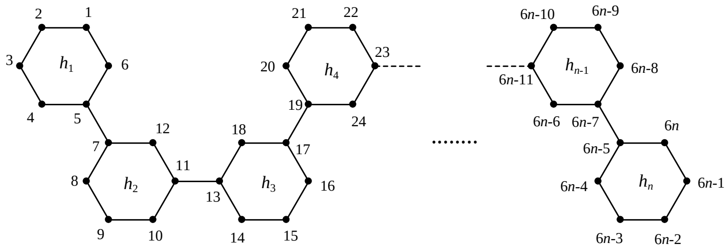

Figure 6. Meta–polyphenylene chain MP_n.

Theorem 7. Let $n > 1$ be a positive integer. Then the modified Wiener polynomial of a meta–polyphenylene is equals to

$$\hat{W}(MP_n, x) = \begin{cases} \frac{3nx}{x^2-1}\left(x^{3n+2} + x^{3n} + 2x^3 - x^2 - 2x - 1\right) & n \text{ is even,} \\ \frac{3nx}{x^2-1}\left(x^{3n+2} + x^{3n} - x^5 + x^3 - 2x\right) & n \text{ is odd} \end{cases}.$$

Proof. The molecular graph of a polyphenylene is depicted in Figure 6. There are n hexagons such that the i-th hexagon, $i = 1, \ldots, n$, is joined to the next and the previous one by an edge. The automorphism group of MP_n is generated by automorphisms $\alpha_1 = (1,3)(4,6)$, $\alpha_2 = (6n - 1, 6n - 3)(6n, 6n - 4)$ and $\beta = \prod_{i=1, i\neq 6k}^{3n}(i, 6n-i+1)\prod_{i=6k}^{[(n+1)/2]}(i, 6n-i+6)$. Therefore $Aut(MP_n)$ is isomorphic to dihedral group of order 8.

For any i, $(1 \le i \le 3n)$, let $A_i = \{i, 6n-i\}$ if $i \neq 6k$ and $A_i = \{i, 6n - i + 6\}$ if $i = 6k$, and if n is odd then for $i = 3n + 1$ let $A_{3n+1} = \{3n + 3\}$. Consider $V_1 = A_1$, $V_2 = A_2 \cup A_3$, $V_3 = A_4 \cup A_5$ and for other values of i, $V_i = A_{i+2}$. If n is even then, there are $3n - 2$ orbits and in other case there are $3n - 1$ orbits.

Therefore, $\hat{W}(V_1, x) = x^{3n+1}$, $\hat{W}(V_2, x) = 4x^{3n-1} + 2x^2$, $\hat{W}(V_3, x) = 4x^{3n-3} + 2x^2$, $\hat{W}(V_4, x) = x^{3n-5}$, and for other values i, except n is odd and $3n - 4 \le i \le 3n - 2$,

$$\hat{W}(V_i, x) = \begin{cases} x^{3n-i-2} & i = 6k-1 \\ x^{3n-i+1} & i = 6k \\ x^{3n-i} & i = 6k+1 \\ x^{3n-i-1} & i = 6k+2 \\ x^{3n-i-2} & i = 6k+3 \\ x^{3n-i+1} & i = 6k+4 \end{cases}$$

and if n is odd then, $\hat{W}(V_{3n-2},x)=\hat{W}(V_{3n-1},x)=0$ and $\hat{W}(V_{3n-3},x)=x^2$.
Now, the result is an immediate consequence of Theorem 2. ■

To calculate the modified Wiener hyper–Wiener indices of linear chains, it is enough to apply Corollary 1. We can see that

$$\hat{W}(MP_n)=\begin{cases}\frac{27}{2}n^3+9n^2+12n; & n \textit{ is even},\\ \frac{27}{2}n^3+9n^2-\frac{21}{2}n; & n \textit{ is odd},\end{cases}$$

and

$$\hat{WW}(MP_n)=\begin{cases}\frac{27}{2}n^4+\frac{81}{4}n^3+12n^2+18n; & n \textit{ is even},\\ \frac{27}{2}n^4+\frac{81}{4}n^3+12n^2-\frac{111}{4}n; & n \textit{ is odd}.\end{cases}$$

4. Conclusions

Finally, we compute different derivatives of the modified Wiener polynomial to extend the main results of [15] to the modified Wiener index. To do this, we assume that m is a positive integer. Then

$$\hat{W}^{(m)}(G):=\frac{1}{n!}\frac{d^m\left(x^{m-1}\hat{W}(G,x)\right)}{dx^m}\Bigg|_{x=1}$$

is a graph invariant with properties, $\hat{W}^{(1)}(G)=\hat{W}(G)$ and $\hat{W}^{(2)}(G)=\hat{WW}(G)$. For m = 3 we have:

$$\hat{W}^{(3)}(G):=\hat{WW}(G)-\frac{1}{6}\hat{W}(G)+\frac{|V(G)|}{12|\Gamma|}\sum_{u\in V(G)}\sum_{g\in\Gamma}d(u,g(u))^3.$$

which is related to the definition of Tratch–Stankevich–Zefirov index (*TSZ* index for short) [17,9] and so we let $\hat{TSZ}(G):=\hat{W}^{(3)}(G)$. We assume that n is a positive integer. The n^{th}–order modified Wiener index of G is defined as:

$$ {}^{n}\hat{W}(G) := \left. \frac{d^{n}\hat{W}(G,x)}{dx^{n}} \right|_{x=1} . $$

Obviously, ${}^{1}\hat{W}(G) = \hat{W}(G)$. We show that $\hat{W}^{(m)}(G)$ and ${}^{n}\hat{W}(G)$ can be calculated without the use of the modified Wiener polynomial.

Define the modified distance moments of a graph G as

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

where k is a positive integer. Then, we have:

$$ \hat{W}(G) = \hat{W}_{1}(G);\ W\hat{W}(G) = 1/2\hat{W}_{1}(G) + 1/2\hat{W}_{2}(G);\ T\hat{S}Z(G) = 1/3\hat{W}_{1}(G) + 1/2\hat{W}_{2}(G) + 1/6\hat{W}_{3}(G). $$

Let $(t)_n = t\,(t-1)\ldots(t-n+1)$ and $(t)^{(n)} = t\,(t+1)\ldots(t+n-1)$. The Stirling numbers of the first kind $s(n,k)$ and the unsigned Stirling numbers of the first kind, $c(n,k)$, are the coefficients in the expansions $(t)_n$ and $(t)^{(n)}$, respectively.

Theorem 8.

1) For any positive integer n, we have $\hat{W}^{(n)}(G) = \frac{1}{n!}\left(\sum_{k=1}^{n} c(n,k)\hat{W}_{k}(G)\right)$,

2) For any positive integer n and $1 \le n \le d(G)$, we have, ${}^{n}\hat{W}(G) = \sum_{k=1}^{n} s(n,k)\hat{W}_{k}(G)$,

The Stirling number of the second kind, $S(n,k)$, is the number of partitions of {1, …, n} into k non-empty parts. It is well-known that $t^{n} = \sum_{k=1}^{n} S(n,k)(t)_{k}$. A similar argument as in [15] shows that the following result holds.

Theorem 9. For any positive integer n,

$$ \hat{W}_{n}(G) = \sum_{k=1}^{n} S(n,k) \left. \frac{d^{k}(\hat{W}(G,x))}{dx^{k}} \right|_{x=1} . $$

The number of r-permutations of a collection of s distinct objects is denoted by $P(s,r)$. This number is equal to 0 when $r \ge s$ and otherwise $P(s,r) = s!/(s-r)!$. Obviously, $P(s,r) = (s)_r$.

In the following theorem the quantities $\hat{W}^{(n)}$ and ${}^{n}\hat{W}$ are computed.

Theorem 10. Suppose *G* is a graph. Then,

1) $\hat{W}^{(n)}(G) = \frac{1}{n!}\left(\sum_{k=1}^{diam(G)} P(n+k-1,n)\hat{d}(G,k)\right)$, where *n* is a positive integer,

2) ${}^{n}\hat{W}(G) = \sum_{k=n}^{diam(G)} P(k,n)\hat{d}(G,k)$, where $1 \le n \le diam(G)$.

Theorem 11. If $1 \le n \le d(G)$, then:

$$\hat{d}(G,n) = \frac{1}{n!}\sum_{k=0}^{d(G)-n} \frac{(-1)^k}{k!} \cdot x^k \frac{d^{n+k}(\hat{W}(G,x))}{dx^{n+k}}.$$

In this paper some new modifications of the modified Wiener index are presented. Also, it can be proved that if we define:

$$p(n,k) = \begin{cases} \frac{1}{n!}\frac{(-1)^k}{k!} & 0 \le k \le n \\ 0 & Otherwise \end{cases},$$

then we have the following orthogonality relations:

$$\sum_k P(n,k)p(k,m) = \delta_{n,m} \text{ and } \sum_k p(n,k)P(k,m) = \delta_{n,m}.$$

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