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Distance under Symmetry

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Abstract

Graovac and Pisanski [On the Wiener index of a graph, J. Math. Chem. **8** (1991) 53–62] applied an algebraic approach to generalize the Wiener index by symmetry group of the molecular graph under consideration. The aim of this paper is to continue this work and present some upper and lower bound for this graph invariant.

1 Introduction

Throughout this paper graph means simple connected graph. Suppose G is such a graph and $V(G)$ is its vertex set. The distance between the vertices $u, v \in V(G)$, $d(u, v)$, is defined as the number of edges in a shortest path connecting u and v. The sum of distances between all pairs of vertices in G is called the Wiener index of G [18]. This graph invariant found remarkable applications in chemistry [8].

Graovac and Pisanski [7] in a pioneering work applied the symmetry group of the graph under consideration to generalize the Wiener index. To the best of our knowledge, this paper is the only published paper in mathematics literature that combines the symmetry and topology of molecules to obtain a good correlation with some physico-chemical properties of molecules. To explain, we assume that G is a graph with automorphism group $\Gamma = Aut(G)$. Following [7], we define the **distance number of an**

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automorphism g, $\delta(g)$, to be the average of $d(u, g(u))$ overall vertices $u \in V(G)$ and $\delta(G) = \frac{1}{|\Gamma||V(G)|} \sum_{u \in V(G)} \sum_{g \in \Gamma} d(u, g(u))$. The **modified Wiener index** of G is defined as:

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

Suppose H is a group and X is a non empty set. A **group action** of H on X is a function $* : H \times X \to X$ given by $*(g, x) = g*x$ that satisfies the following two conditions:

1. for each $g, h \in H$ and $x \in X$, $(gh) * x = g * (h * x)$;
2. $e * x = x$, for every $x \in X$.

Suppose H acts on X and $g \in H$. The subset $Hx = \{gx|g \in H\}$ of X is called an **orbit** of the action. The action is said to be **transitive** if it has exactly one orbit. Define $Fix(g) = \{x \in X|g*x = x\}$. If t is the number of orbits then the **orbit counting lemma** [16] states that

$$t = \frac{1}{|H|} \sum_{g \in H} |Fix(g)|.$$

A graph G is called **vertex transitive** if the $Aut(G)$ has exactly one orbit on $V(G)$ under its natural action.

Throughout this paper we use the standard notations of group theory and graph theory. Suppose G and H are two graphs. The **Cartesian product** $G\Box H$ is a graph with vertex set $V(G) \times V(H)$ in such a way that vertices (a, b) and (x, y) are adjacent if and only if $a = x$ and $by \in E(H)$ or $b = y$ and $ax \in E(H)$, see [10] for details. Our notation is standard and taken from the standard books on these topics. The path, cycle and complete graphs with n vertices are denoted by P_n, C_n and K_n, respectively.

2 Main Results

A graph G is called asymmetric if its automorphism group is trivial. It is easy to see that the modified Wiener index of a graph G is equal to zero if and only if G is asymmetric. In [6, Corollary 2.3.3], it is proved that the most of finite graphs are having trivial automorphism group. To explain, we assume that 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 index of the most of graphs is zero.

A class function over the complex number $\mathbb{C}$ is a function f on a group H, such that f is constant on the conjugacy classes of H. By [11, p. 152], it is well-known that the set $CF(H,\mathbb{C})$ of all class functions constitutes a vector space over $\mathbb{C}$.

Suppose G is a connected graph and $\Gamma = Aut(G)$. For each automorphism $g \in \Gamma$, we define $\delta(g) = \frac{1}{|V(G)|} \sum_{x \in V(G)} d(x, g(x))$. This defines a mapping $\delta : \Gamma \to \mathbb{C}$. Then,

$$\hat{W}(G) = \frac{|V(G)|^2}{2|\Gamma|} \sum_{g \in \Gamma} \delta(g). \tag{1}$$

Theorem 1. δ is a class function and $\delta(g) = \delta(g^{-1})$, for each automorphism $g \in \Gamma$.

Proof. Suppose g_1 and g_2 are arbitrary elements of Γ. Then

$$\delta(g_1g_2) = \frac{1}{|V(G)|} \sum_{x \in V(G)} d(x, g_1g_2(x)).$$

Clearly, for each automorphism $g \in \Gamma$, $d(a,b) = d(g(a), g(b))$ and $g(V(G)) = V(G)$. Hence

$$\begin{aligned}
\delta(g_1g_2) &= \frac{1}{|V(G)|} \sum_{x \in V(G)} d(x, g_1g_2(x)) \\
&= \frac{1}{|V(G)|} \sum_{x \in V(G)} d(g_1^{-1}(x), g_2(x)) \\
&= \frac{1}{|V(G)|} \sum_{t \in V(G)} d(t, g_2g_1(t)) \\
&= \delta(g_2g_1).
\end{aligned}$$

Therefore $\delta(g_1g_2g_1^{-1}) = \delta(g_1^{-1}g_1g_2) = \delta(g_2)$, which implies that δ is a class function.

Apply our definition to prove $\delta(g) = \delta(g^{-1})$. We have

$$\begin{aligned}
\delta(g) &= \frac{1}{|V(G)|} \sum_{x \in V(G)} d(x, g(x)) \\
&= \frac{1}{|V(G)|} \sum_{x \in V(G)} d(g^{-1}(x), x) \\
&= \delta(g^{-1}),
\end{aligned}$$

proving the lemma. ∎

Suppose H is a group, V is a vector space over $\mathbb{C}$ and φ is a homomorphism from H into $GL(V)$, the set of all invertible n by n matrices on $\mathbb{C}$, $n = dimV$. The homomorphism φ is said to be a complex representation of H and the function χ from H into $\mathbb{C}$ given by

$\chi(g) = tr\varphi(g)$, $g \in H$, is called the complex character of H afforded by φ. If χ and γ are two complex class functions on H then their scalar product is defined as

$$\langle \chi, \gamma \rangle = \frac{1}{|H|} \sum_{g \in H} \chi(g)\overline{\gamma(g)}.$$

An irreducible complex character is a complex character χ such that $\langle \chi, \chi \rangle = 1$. It is well-known that the set of all irreducible complex characters of H constitute an orthonormal subset of $CF(H, \mathbb{C})$.

In Theorem 1, we proved that δ is a class function. Since $\delta(e) = 0$, δ is not a character of H. In the next theorem, we will prove that if $n > 1$ then the trivial character is a constituent of δ.

Theorem 2. Suppose G is a connected $n-$vertex graph, $\Gamma = Aut(G)$, t_1 denotes the number of orbits of Γ on $V(G)$ and t_2 is the number of orbits of Γ on $V(G) \times V(G)$ under natural actions of Γ on $V(G)$ and $V(G) \times V(G)$, respectively. Then,

1. $\langle \delta, \delta \rangle \geq 1 - \dfrac{2t_1}{n} + \dfrac{t_2}{n^2}$,
2. $\langle \delta, 1_G \rangle \geq n - \dfrac{t_1}{n}$, where 1_G denotes the trivial character of G.

Proof. Define $Fix_1(g)$ and $Fix_2(g)$, $g \in \Gamma$, to be the fixed sets of Γ under two actions, respectively. Then one can easily prove that $Fix_2(g) = Fix_1(g) \times Fix_1(g)$. We now apply the orbit$-$counting lemma to prove that

$$t_1 = \frac{1}{|\Gamma|} \sum_{g \in \Gamma} |Fix_1(g)| \quad \& \quad t_2 = \frac{1}{|\Gamma|} \sum_{g \in \Gamma} |Fix_1(g)|^2.$$

Since d is meter, $d(x, g(x)) = 0$ if and only of $g(x) = x$. Thus,

$$\delta(g) = \frac{1}{n} \sum_{x \in V(G)} d(x, g(x)) \geq 1 - \frac{|Fix_1(g)|}{n}$$

and so

$$\delta(g)^2 \geq 1 - \frac{2|Fix_1(g)|}{n} + \frac{|Fix_1(g)|^2}{n^2}.$$

Therefore,

$$\begin{aligned} < \delta, 1_G > &= \frac{1}{|\Gamma|} \textstyle\sum_{g \in \Gamma} \delta(g) \\ &\geq \frac{1}{|\Gamma|} \textstyle\sum_{g \in \Gamma} (1 - \frac{|Fix_1(g)|}{n}) \\ &= \frac{1}{|\Gamma|} (n|\Gamma| - t_1 \frac{|\Gamma|}{n}) \quad \text{(by orbit counting lemma)} \\ &= n - \frac{t_1}{n}. \end{aligned}$$

In a similar way,

$$\langle \delta, \delta \rangle = \frac{1}{|\Gamma|} \sum_{g \in \Gamma} \delta(g)^2 \geq 1 - \frac{2t_1}{n} + \frac{t_2}{n^2},$$

which completes the proof. ■

Suppose G is a graph with $V(G) = \{v_1, \ldots, v_n\}$ and as usual $\Gamma = Aut(G) = \{g_1, \ldots, g_m\}$. The matrix $\hat{D} = [\hat{d}_{ij}]$ is called the **modified distance matrix**, where $\hat{d}_{ij} = d(v_i, g_j(v_i))$, $1 \leq i \leq n$ and $1 \leq j \leq m$. Then the modified Wiener index of G is equal to:

$$\frac{n}{2m} \times \text{the summation of all entries in } \hat{D}.$$

Notice that $\delta(g_i)$ is the the average of the row corresponding to g_i. Define $\gamma : G \longrightarrow \mathbb{C}$ given by $\gamma(x) = \frac{1}{|\Gamma|} \sum_{g \in \Gamma} d(x, g(x))$.

Theorem 3. Suppose G is a connected $n-$vertex graph and $\Gamma = Aut(G)$. Then $\hat{W} \geq \frac{n}{2}(n - t_1)$, where t_1 denotes the number of orbits of Γ on $V(G)$. If G is vertex transitive then the equality is satisfied if and only if G is isomorphic to K_n.

Proof. Apply (1) and the orbit counting lemma, we have:

$$\begin{aligned} \hat{W}(G) = \frac{|V(G)|^2}{2|\Gamma|} \textstyle\sum_{g \in \Gamma} \delta(g) &= \frac{|V(G)|}{2|\Gamma|} \textstyle\sum_{g \in \Gamma} \sum_{x \in V(G)} d(x, g(x)) \\ &\geq \frac{|V(G)|}{2|\Gamma|}(n|\Gamma| - t_1|\Gamma|) \\ &= \frac{n}{2}(n - t_1) \end{aligned}$$

We now assume that G is a vertex transitive graph with n vertices. If G is a complete graph then it is clear that $\hat{W}(G) = \hat{W}(K_n) = \frac{n(n-1)}{2}$, as desired. Suppose $W(G) = \hat{W}(G) = \frac{n(n-1)}{2}$. By [7, Corollary 3.2], $W(K_n) = \hat{W}(K_n) = \frac{n(n-1)}{2}$ and so G is isomorphic to an $n-$vertex complete graph. ■

3 Applications

The aim of this section is to apply Theorem 1 and [7, Theorem 5.13] to compute the modified Wiener index of some known graphs.

In the following example, we calculate the character table of the automorphism group of some graphs together with their associated class functions. Suppose $\mathbb{Z}_n$, S_n and D_{2n} denote the cyclic group of order n, the symmetric group on n letters and the dihedral group of order $2n$. If H and K are subgroups of a group G such that H is normal,

$H \cap K = \{e\}$ and $G = HK$ then we say G is a semidirect product of H by K and in this case we write $G = H : K$.

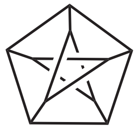

Figure 1: The Petersen Graph.

Example 4. In this example the class function δ together with the modified Wiener index of eight graphs are computed. These graphs are Petersen graph P_5, the dendrimer graph $D[2]$, the complete graph K_4, the complete bipartite graph $K_{3,3}$ and trees T_i, $1 \le i \le 4$. It is well-known that the automorphism group of the Petersen graph is isomorphic to the symmetric group S_5. This graph is depicted in Figure 1 and its character table together with class function δ_1 is recorded in Table 1.

Table 1: The Character Table of $Aut(P_5) \cong S_5$ and the Class Function δ_1.

	$1a$	$2a$	$2b$	$6a$	$3a$	$4a$	$5a$
χ_1	1	1	1	1	1	1	1
χ_2	1	-1	1	-1	1	-1	1
χ_3	4	-2	0	1	1	0	-1
χ_4	4	2	0	-1	1	0	-1
χ_5	5	1	1	1	-1	-1	0
χ_6	5	-1	1	-1	-1	1	0
χ_7	6	0	-2	0	0	0	1
δ_1	0	$\frac{6}{5}$	$\frac{6}{5}$	$\frac{6}{5}$	$\frac{9}{5}$	$\frac{9}{5}$	$\frac{3}{2}$

From Table 1, one can see that $\delta_1 = \frac{3}{2}\chi_1 - \frac{3}{10}\chi_5$ and $\hat{W}(P_5) = 75$. We now consider the dendrimer graph $D[2]$ that is depicted in Figure 2. Using GAP [17], one can easily show that $Aut(D[2]) \cong \mathbb{Z}_2 \times S_4$. On the other hand, from Table 2, we can calculate that $\delta_2 = \frac{11}{5}\chi_1 - \frac{4}{5}\chi_6 - \frac{1}{5}\chi_{10}$ and $\hat{W}(D[2]) = 110$.

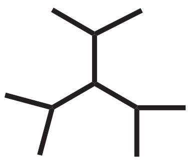

Figure 2: The Dendrimer Graph $D[2]$.

Table 2: The Character Table of $Aut(D[2]) \cong \mathbb{Z}_2 \times S_4$ and its Class Function.

	$1a$	$2a$	$2b$	$2c$	$2d$	$4a$	$2e$	$4b$	$3a$	$6a$
χ_1	1	1	1	1	1	1	1	1	1	1
χ_2	1	-1	1	-1	-1	1	1	-1	1	-1
χ_3	1	-1	1	-1	1	-1	-1	1	1	-1
χ_4	1	1	1	1	-1	-1	-1	-1	1	1
χ_5	2	-2	2	-2	0	0	0	0	-1	1
χ_6	2	2	2	2	0	0	0	0	-1	-1
χ_7	3	-1	-1	3	-1	1	-1	1	0	0
χ_8	3	-1	-1	3	1	-1	1	-1	0	0
χ_9	3	1	-1	-3	-1	-1	1	1	0	0
χ_{10}	3	1	-1	-3	1	1	-1	-1	0	0
δ_2	0	$\frac{2}{5}$	$\frac{4}{5}$	$\frac{6}{5}$	2	2	$\frac{12}{5}$	$\frac{12}{5}$	3	3

Table 3: The Character Table of $Aut(K_4)$ and its Class Function.

	$1a$	$2a$	$3a$	$2b$	$4a$
χ_1	1	1	1	1	1
χ_2	3	-1	0	-1	1
χ_3	2	0	-1	2	0
χ_4	3	1	0	-1	-1
χ_5	1	-1	1	1	-1
δ_3	0	$\frac{1}{2}$	$\frac{3}{4}$	1	1

It is well-known that the automorphism group of K_n is isomorphic to the symmetric group S_n and K_n is vertex transitive. By Table 3, $\delta_3 = \dfrac{3}{4}\chi_1 - \dfrac{1}{4}\chi_4$ and $\hat{W}(K_4) = W(K_4) = 6$. On the other hand, $Aut(K_{3,3}) \cong (S_3 \times S_3) : \mathbb{Z}_2$ and from Table 4 we can calculate that $\delta_4 = \dfrac{7}{6}\chi_1 + \dfrac{1}{6}\chi_4 - \dfrac{1}{3}\chi_9$ and $\hat{W}(K_{3,3}) = 21$. This shows that the number of constituents of the class function δ is independent from the vertex transitivity of the graph under consideration.

We now consider four trees T_1, T_2, T_3 and T_4. A simple calculation by GAP shows that $Aut(T_1) \cong S_4$, $Aut(T_2) \cong D_{12}$ and $Aut(T_3) \cong \mathbb{Z}_2 \times S_4$ and $Aut(T_4) \cong (S_3 \times S_3) : \mathbb{Z}_2$. Suppose δ_5, δ_6, δ_7 and δ_8 denotes their class function according to Theorem 1, respectively.

Table 4: The Character Table of $Aut(K_{3,3})$ and its Class Function.

	$1a$	$2a$	$2b$	$3a$	$6a$	$2c$	$4a$	$6b$	$3b$
χ_1	1	1	1	1	1	1	1	1	1
χ_2	1	-1	1	1	-1	-1	1	-1	1
χ_3	1	-1	1	1	-1	1	-1	1	1
χ_4	1	1	1	1	1	-1	-1	-1	1
χ_5	2	0	-2	2	0	0	0	0	2
χ_6	4	-2	0	1	1	0	0	0	-2
χ_7	4	0	0	-2	0	-2	0	1	1
χ_8	4	0	0	-2	0	2	0	-1	1
χ_9	4	2	0	1	-1	0	0	0	-2
δ_4	0	$\frac{2}{3}$	$\frac{4}{3}$	1	$\frac{5}{3}$	1	1	1	2

Table 5: The Character Table of $Aut(T_1)$ and the Class Function δ_5.

	$1a$	$2a$	$3a$	$2b$	$4a$
χ_1	1	1	1	1	1
χ_2	1	-1	1	1	-1
χ_3	3	-1	0	-1	1
χ_4	2	0	-1	2	0
χ_5	3	1	0	-1	-1
δ_5	0	$\frac{4}{5}$	$\frac{6}{5}$	$\frac{8}{5}$	$\frac{8}{5}$

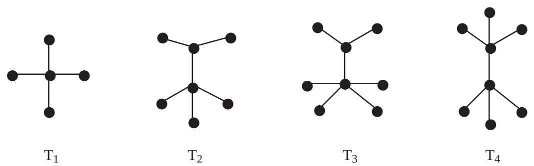

Figure 3: The Graphs T_1, T_2, T_3 and T_4.

Table 6: The Character Table of $Aut(T_2)$ and its Class Function.

	$1a$	$2a$	$3a$	$2b$	$2c$	$6a$
χ_1	1	1	1	1	1	1
χ_2	1	-1	1	-1	1	-1
χ_3	1	-1	1	1	-1	1
χ_4	1	1	1	-1	-1	-1
χ_5	2	0	-1	-2	0	1
χ_6	2	0	-1	2	0	-1
δ_6	0	$\frac{4}{7}$	$\frac{6}{7}$	$\frac{4}{7}$	$\frac{8}{7}$	$\frac{10}{7}$

Table 7: The Character Table of $Aut(T_3)$ and the Class Function δ_7.

	$1a$	$2a$	$3a$	$2b$	$4a$	$2c$	$2d$	$6a$	$2e$	$4b$
χ_1	1	1	1	1	1	1	1	1	1	1
χ_2	1	-1	1	1	-1	-1	1	-1	-1	1
χ_3	1	-1	1	1	-1	1	-1	1	1	-1
χ_4	1	1	1	1	1	-1	-1	-1	-1	-1
χ_5	2	0	-1	2	0	-2	0	1	-2	0
χ_6	2	0	-1	2	0	2	0	-1	2	0
χ_7	3	-1	0	-1	1	-3	1	0	1	-1
χ_8	3	-1	0	-1	1	3	-1	0	-1	1
χ_9	3	1	0	-1	-1	-3	-1	0	1	1
χ_{10}	3	1	0	-1	-1	3	1	0	-1	-1
δ_7	0	$\frac{1}{2}$	$\frac{3}{4}$	1	1	$\frac{1}{2}$	1	$\frac{5}{4}$	$\frac{3}{2}$	$\frac{3}{2}$

Suppose $O_{T_1}, O_{T_2}, O_{T_3}$ and O_{T_4} denote the orbits of the automorphism groups of these trees, respectively. Our calculations with GAP show that

$$\begin{aligned} O_{T_1} &= [[1],[2,4,3,5]], \\ O_{T_2} &= [[1],[2,3],[4],[5,7,6]], \\ O_{T_3} &= [[1],[2],[3,4],[5,7,6,8]], \\ O_{T_4} &= [[1,4,5,7,6,8],[2,3]]. \end{aligned}$$

From Tables 5, 6, 7 and 8, we can calculate that $\hat{W}(T_1) = 15$, $\hat{W}(T_2) = 21$, $\hat{W}(T_3) = 32$ and $\hat{W}(T_4) = 56$ and the class functions $\delta_5, \delta_6, \delta_7$ and δ_8 can be computed as follows:

$$\begin{aligned} \delta_5 &= \frac{6}{5}\chi_1 - \frac{2}{5}\chi_5, \\ \delta_6 &= \frac{6}{7}\chi_1 - \frac{2}{7}\chi_4 - \frac{2}{7}\chi_6, \\ \delta_7 &= \chi_1 - \frac{1}{4}\chi_4 - \frac{1}{4}\chi_{10}, \\ \delta_8 &= \frac{7}{4}\chi_1 - \frac{3}{4}\chi_4 - \frac{1}{4}\chi_9. \end{aligned}$$

Table 8: The Character Table of $Aut(T_4)$ and the Class Function δ_8.

	$1a$	$2a$	$2b$	$3a$	$6a$	$2c$	$4a$	$6b$	$3b$
χ_1	1	1	1	1	1	1	1	1	1
χ_2	1	-1	1	1	-1	-1	1	-1	1
χ_3	1	-1	1	1	-1	1	-1	1	1
χ_4	1	1	1	1	1	-1	-1	-1	1
χ_5	2	0	-2	2	0	0	0	0	2
χ_6	4	-2	0	1	1	0	0	0	-2
χ_7	4	0	0	-2	0	-2	0	1	1
χ_8	4	0	0	-2	0	2	0	-1	1
χ_9	4	2	0	1	-1	0	0	0	-2
δ_8	0	$\frac{1}{2}$	1	$\frac{3}{4}$	$\frac{5}{4}$	$\frac{5}{2}$	$\frac{5}{2}$	$\frac{5}{2}$	$\frac{3}{2}$

Our calculations given Example 4, and some other calculations with GAP [17] and MAGMA [1] suggest the following conjecture:

Conjecture 5: For each graph G, the class function δ is a rational combination of the trivial character χ_1 and at most two other irreducible characters of $Aut(G)$.

For the sake of completeness, we mention here a result of Graovac and Pisanski [7] about modified Wiener index of the Cartesian product of graphs.

Theorem 6. (Graovac and Pisanski [7, Theorem 5.13]) Suppose G and H are connected graphs such that each orbit of the action of $Aut(G \times H)$ on $V(G) \times V(H)$ has the form $A \times B$, where A is an orbit for the action of $Aut(G)$ on $V(G)$ and B is an orbit for the action of $Aut(H)$ on $V(H)$. Then

$$\hat{W}(G\Box H) = |V(G)|^2\hat{W}(H) + |V(H)|^2\hat{W}(G).$$

If S is a $q-$element set and d is a positive integer then the **Hamming graph** $H(d,q)$ is defined to be the graph with vertex set S^d. Two vertices of $H(d,q)$ are adjacent if and only if they differ in precisely one coordinate. It is well-known that the Hamming graph $H(d,q)$ is isomorphic to the Cartesian product of d complete graphs K_q. A Hamming graph with $q = 2$ is called a hypercube, denoted by Q_d. Since the Hamming graph is vertex transitive, the Wiener and modified Wiener indices coincide in this case. A tedious calculations show that $\hat{W}(K_{n_1}\Box\cdots\Box K_{n_r}) = \sum_{i=1}^{r}\binom{n_i}{2}\frac{n_1n_2\cdots n_r}{n_i}$. By substituting $n_1 = n_2 = \cdots = n_r = q$ and $d = r$, we have $\hat{W}(H(d,q)) = d\binom{q}{2}q^{d-1}$ and $\hat{W}(Q_d) = d2^{d-1}$.

A C_4-**grid** is a Cartesian product of two paths. The Cartesian product of a path and a cycle and two cycles are called C_4-**nanotube** and C_4-**nanotorus**, respectively. In the following, the modified Wiener indices of these graphs are calculated.

Example 7. In this example the modified Wiener index of a C_4-grid, C_4-nanotube and C_4-nanotorus are computed. We recall that the symmetry group of a path P_n is a cyclic group of order two with the following non identity element g:

$$g = \begin{cases} (1\ n)(2\ n-1)\cdots(\frac{n-1}{2}\ \frac{n+3}{2}) & n\ is\ odd \\ (1\ n)(2\ n-1)\cdots(\frac{n}{2}\ \frac{n+2}{2}) & n\ is\ even \end{cases}$$

On the other hand, the group of all symmetries of a regular polygon, including both rotations and reflections is isomorphic to a dihedral group of order $2n$, denote by D_{2n}. We mention here that there is a typographical error in [7, Example 5.6] for computing $\hat{W}(P_n)$. One can easily prove that:

$$\hat{W}(P_n) = \hat{W}(C_n) = \begin{cases} \frac{n^3}{8} & n\ is\ even \\ \frac{n^3-n}{8} & n\ is\ odd \end{cases} \tag{2}$$

Apply (2) and [7, Theorem 5.13] to prove the following equality:

$$
\begin{aligned}
\hat{W}(C_m \square P_n) &= \hat{W}(P_m \square P_n) = \hat{W}(C_m \square C_n) \\
&= |V(C_m)|^2 \hat{W}(C_n) + |V(C_n)|^2 \hat{W}(C_m) \\
&= \begin{cases}
\dfrac{m^2 n^2}{8}(n+m) & m \textit{ and } n \textit{ are even} \\
\dfrac{mn}{8}(mn^2 + n(m^2-1)) & m \textit{ is odd and } n \textit{ is even} \\
\dfrac{mn}{8}(m(n^2-1) + nm^2) & n \textit{ is odd and } m \textit{ is even} \\
\dfrac{mn}{8}(m(n^2-1) + n(m^2-1)) & m \textit{ and } n \textit{ are odd}
\end{cases}
\end{aligned}
$$

A cubic graph G is called $3-$connected, if there does not exist a set of two vertices whose removal disconnects the graph. A fullerene graph is a planar, cubic and $3-$connected graph such that all faces are pentagons or hexagons. The importance of fullerene graphs is for its applications in fullerene chemistry. The fullerene era was started after pioneering work of Kroto and his team [14]. The mathematical properties of fullerene graphs are a new branch of nanoscience started by pioneering work of Fowler and his team [4, 15]. We encourage the interested readers to consult papers [12, 13] and references therein for more information on this topic.

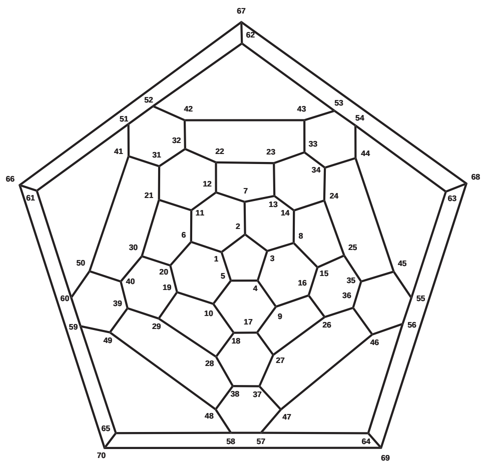

Figure 4: The Fullerene Graph C_{70}.

Example 8. Datta, Banerje and Mukherjee [2], constructed the IPR fullerenes C_{50+10n}, $n \geq 1$, with exactly $50 + 10n$ carbon atoms. In this example, the modified Wiener index this class of fullerenes is calculated, see Figures 4 and 5. We first notice that the symmetry

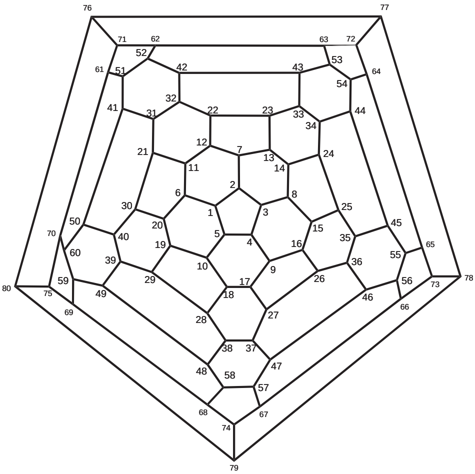

Figure 5: The Fullerene Graph C_{80}.

group of the fullerene C_{50+10n} has D_{5h} point group symmetry and so it is isomorphic to the dihedral group D_{20}.

We first label this fullerene graph by a method given by Fripertinger [5]. We apply HyperChem [9] and TopoCluj [3] to calculate the adjacency and distance matrices of molecular graphs. Suppose permutations A_1, A_2 and A_3 are defined as follows:

$A_1 := (2,\ 5)(3,\ 4)(7,\ 10)(8,\ 9)(11,\ 20)(12,\ 19)(13,\ 18)(14,\ 17)(15,16)\cdots(10n+31,10n+40)(10n+32,10n+39)(10n+33,10n+38)(10n+34,10n+37)(10n+35,10n+36)(10n+42,10n+45)(10n+43,10n+44)(10n+47,10n+50)(10n+48,10n+49)$,

$A_2 := (1,2,3,4,5)(6,7,8,9,10)(11,13,15,17,19)(12,14,16,18,20)\cdots(10n+31,10n+33,10n+35,10n+37,10n+39)(10n+32,10n+34,10n+36,10n+38,10n+40)(10n+41,10n+42,10n+43,10n+44,10n+45)(10n+46,10n+47,10n+48,10n+49,10n+50)$,

$A_3 := (1,10n+46)(2,10n+47)(3,10n+48)(4,10n+49)(5,10n+50)(6,10n+41)(7,10n+42)(8,10n+43)(9,10n+44)(10,10n+45)(11,10n+31)(12,10n+32)(13,10n+33)(14,10n+34)(15,10n+35)(16,10n+36)(17,10n+37)(18,10n+38)(19,10n+39)(20,10n+40)(21,10n+21)\cdots(30,10n+30)\cdots(5n+11,5n+31)(5n+12,5n+32)(5n+13,5n+33)(5n+14,5n+34)(5n+15,5n+35)(5n+16,5n+36)(5n+17,5n+37)(5n+18,5n+38)(5n+19,5n+39)(5n+20,5n+40)$.

A simple calculation shows that the permutations A_1, A_2 and A_3 are automorphisms of the fullerene C_{50+10n}. Since the group $\langle A_1, A_2, A_3\rangle$ has order 20, $Aut(C_{50+10n}) \cong \langle A_1, A_2, A_3\rangle \cong D_{20}$. Define $x = A_2A_3$ and $y = A_1$. Then $x^{10} = y^2 = e$ and $yxy^{-1} = x^{-1}$ and so by [11, p. 183], the representatives of the conjugacy classes of D_{20} are $e, x, x^2, x^3, x^4, x^5, y, xy$. In Table 9, the class functions $\delta'(g) = |V(G)|\delta(g)$ on each conjugacy class of dihedral group D_{20} are computed.

Table 9: The Class Functions $\delta'(g) = |V(G)|\delta(g)$ on each Conjugacy Class.

		n **is Even**		
Conjugacy Classes	$1a$	$2a$	$5a$	$5b$
	0	$50n + 154$	$40n + 140$	$80n + 240$
Conjugacy Classes	$2b$	$2c$	$10a$	$10b$
	$5n^2 + 50n + 140$	$5n^2 + 76n + 286$	$5n^2 + 70n + 240$	$5n^2 + 90n + 390$
		n **is Odd**		
Conjugacy Classes	$1a$	$2a$	$5a$	$5b$
	0	$50n + 154$	$40n + 140$	$80n + 240$
Conjugacy Classes	$10a$	$2b$	$10b$	$2c$
	$5n^2 + 60n + 175$	$5n^2 + 74n + 281$	$5n^2 + 80n + 305$	$5n^2 + 100n + 475$

Apply Theorem 1 and calculations given Table 9, to prove that

$$\hat{W}(C_{50+10n}) = \begin{cases} \frac{25}{2}n^3 + \frac{745}{2}n^2 + \frac{5285}{2}n + \frac{10925}{2} & n \textit{ is odd} \\ \frac{25}{2}n^3 + \frac{745}{2}n^2 + 2640n + 5450 & n \textit{ is even} \end{cases}$$

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References

[1] W. Bosma, J. Cannon, C. Playoust, The Magma algebra system. I. The user language. Computational algebra and number theory, *J. Symb. Comput.* **24** (1997) 235–265.

[2] K. Datta, M. Banerje, A. K. Mukherjee, Strongly subspectral pairs in C_{50+10n} and C_{60+12n} fullerenes via a common generic graph, *Phys. Chem. Chem. Phys.* **1** (1999) 2919–2922.

[3] M. D. Diudea, O. Ursu, L. C. Nagy, *TOPOCLUJ*, Babes Bolyai Univ., Cluj, 2002.

[4] P. W. Fowler, D. E. Manolopoulos, *An Atlas of Fullerenes*, Oxford Univ. Press, Oxford, 1995.

[5] H. Fripertinger, The cycle index of the symmetry group of the fullerene C_{60}, *MATCH Commun. Math. Comput. Chem.* **33** (1996) 121–138.

[6] C. Godsil, G. Royle, *Algebraic Graph Theory*, Springer, New York, 2001.

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

[8] I. Gutman, L. Šoltés, The range of the Wiener index and its mean isomer degeneracy, *Z. Naturforsch.* **46a** (1991) 865–868.

[9] HyperChem package Release 7.5 for Windows, Hypercube Inc., Florida, USA, 2002.

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

[11] G. James, M. Liebeck, *Representations and Characters of Groups*, Cambridge Univ. Press, New York, 2001.

[12] F. Koorepazan–Moftakhar, A. R. Ashrafi, Z. Mehranian, Symmetry and PI polynomials of C_{50+10n} fullerenes, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 425–436.

[13] F. Koorepazan–Moftakhar, A. R. Ashrafi, Fullerenes: Topology and symmetry, in: I. Gutman (Ed.), *Topics in Chemical Graph Theory*, Univ. Kragujevac, Kragujevac, 2014, pp. 163–176.

[14] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, R. E. Smalley, C_{60}: Buckminsterfullerene, *Nature* **318** (1985) 162–163.

[15] W. Myrvold, B. Bultena, S. Daugherty, B. Debroni, S. Girn, M. Minchenko, J. Woodcock, P. W. Fowler, FuiGui: a graphical user interface for investigating conjectures about fullerenes, *MATCH Commun. Math. Comput. Chem.* **58** (2007) 403–422.

[16] P. M. Neumann, A lemma that is not Burnside's, *Math. Sci.* **4** (1979) 133–141.

[17] The GAP Team, Group, *GAP – Groups, Algorithms, and Programming, Version 4.5.5*; 2012, (`http://www.gap-system.org`).

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