Modified Wiener index via canonical metric representation, and some fullerene patches*

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Abstract

A variation of the classical Wiener index, the modified Wiener index, that was introduced in 1991 by Graovac and Pisanski, takes into account the symmetries of a given graph. In this paper it is proved that the computation of the modified Wiener index of a graph G can be reduced to the computation of the Wiener indices of the appropriately weighted quotient graphs of the canonical metric representation of G. The computation simplifies in the case when G is a partial cube. The method developed is applied to two infinite families of fullerene patches.

Keywords: modified Wiener index, canonical metric representation, partial cubes, fullerene patches, nanocones.

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1 Introduction

The Wiener index is a central graph invariant in chemical graph theory as well as in metric graph theory, in the latter often being equivalently studied as the average distance. Several variations of the Wiener index were also extensively investigated, including the hyper-Wiener index and the terminal Wiener index. In 1991, Graovac and Pisanski [3]

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introduced the *modified Wiener index* with an idea to design a chemically applicable topological index which adequately takes into account the symmetries of a graph. The index received less attention than it deserves, but was studied recently by Koorepazan-Moftakhar and Ashrafi [13] where bounds on this graph invariant were obtained and exact values for some fullerenes.

Ten years after the seminal paper [3] an additional variation of the Wiener index was proposed in [15] and three years later named in [6] by the same term—the modified Wiener index. In the same paper the so-called variable Wiener index was also introduced; see the recent survey of Liu and Liu [14] on the variable Wiener index and related indices, especially on the related terminology. As it happens, also Graovac (see [16]) used the term modified Wiener index for the variation from [6, 15]. 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. Anyhow, in this paper the term modified Wiener index is reserved for the original invariant. If the theory of this index will be more extensively developed in the future (for instance, it would be interesting to see how the invariant performs in the QSAR modelling for predicting physico-chemical properties of molecules), then the research community might wish to find a new name for it (to be honest, the terms "modified" and "variable" are not very descriptive), a possibility would be to call it the *Graovac-Pisanski index*.

We proceed as follows. In the next section concepts needed are formally introduced. The main result and its specialization to partial cubes are presented and proved in Section 3. In the final section we give closed expressions for the modified Wiener index of two infinite families of nanocones. These chemical graphs belong to the family of the so-called fullerene patches [4, 5].

2   Preliminaries

We denote the set $\{1, \ldots, n\}$ with $[n]$. Unless stated otherwise, graphs considered are simple and connected. The distance $d_G(u, v)$ between vertices u and v of G is the usual shortest-path distance. A subgraph of a graph is called *isometric* if the distance between any two vertices of the subgraph is independent of whether it is computed in the subgraph or in the entire graph.

The *Wiener index* $W(G)$ of G is the sum of distances between all pairs of vertices of G. A *weighted graph* (G, w) is a graph $G = (V(G), E(G))$ together with the weight function $w : V(G) \to \mathbb{R}_0^+$. The Wiener index $W(G, w)$ of (G, w), first introduced in [10], is:

$$W(G, w) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} w(u)\, w(v)\, d_G(u, v)\,.$$

Note that if $w \equiv 1$ then $W(G, w) = W(G)$.

The *modified Wiener index* $\widehat{W}(G)$ of G was introduced in [3] as

$$\widehat{W}(G) = \frac{|V(G)|}{2|\mathrm{Aut}(G)|} \sum_{u \in V(G)} \sum_{\alpha \in \mathrm{Aut}(G)} d_G(u, \alpha(u))\,,$$

where $\mathrm{Aut}(G)$ is the automorphism group of G. Roughly speaking, the modified Wiener index measures how far the vertices of a graph are moved on the average by its automorphisms.

The *Cartesian product* $G \square H$ of graphs G and H is the graph with vertex set $V(G) \times V(H)$, where the vertex (g, h) is adjacent to the vertex (g', h') whenever $gg' \in E(G)$ and $h = h'$, or $g = g'$ and $hh' \in E(H)$.

If G is a graph, then the Djoković-Winkler's relation Θ is defined on $E(G)$ as follows: if $e = xy \in E(G)$ and $f = uv \in E(G)$, then $e\Theta f$ if $d(x, u) + d(y, v) \neq d(x, v) + d(y, u)$. Relation Θ is reflexive and symmetric, hence its transitive closure Θ^* is an equivalence relation. The partition of $E(G)$ induced by Θ^* is called the Θ^*-*partition* of $E(G)$. Let G be a graph and let $\{F_1, \ldots, F_k\}$ be the Θ^*-partition of $E(G)$. For any $j \in [k]$, let G/F_j be the graph whose vertex set consists of the connected components of the graph $G - F_j$, two components C and C' being adjacent if there exists an edge $uv \in F_j$ such that $u \in C$ and $v \in C'$. Further, for any $j \in [k]$ let $\alpha_j : G \to G/F_j$ be the mapping that assigns to each vertex of G the component of $G - F_j$ to which it belongs. Now, the *canonical metric representation* of G is the (isometric) mapping $\alpha = (\alpha_1, \ldots, \alpha_k) : G \to G/F_1 \square \cdots \square G/F_k$. This mapping is due to Graham and Winkler [2]. The fundamental property of α from [2] that is essential for us is that $\alpha(G)$ is an isometric subgraph of $G/F_1 \square \cdots \square G/F_k$.

3 The main result

Our main result (Theorem 3.1) asserts that $\widehat{W}(G)$ can be computed from the weighted Wiener indices of a collection of smaller graphs—the graphs of the canonical metric representation of G. Before stating the result we need to introduce the appropriate weighting functions.

Let G be a connected graph, let $V_1, \ldots, V_t$ be the orbits under the action of $\mathrm{Aut}(G)$ on $V(G)$, and let $F_1, \ldots, F_k$ be the Θ^*-classes of G. For any $i \in [t]$ and any $j \in [k]$ define $w_{ij} : V(G/F_j) \to \mathbb{R}_0^+$ by setting

$$w_{ij}(C) = |V_i \cap C|, \; C \in V(G/F_j) \,.$$

We are now ready for the main result.

Theorem 3.1. *Let G be a connected graph of order n and let $V_1, \ldots, V_t$ be the orbits under the action of $\mathrm{Aut}(G)$ on $V(G)$. If $F_1, \ldots, F_k$ are the Θ^*-classes of G, and G/F_j ($j \in [k]$) and w_{ij} ($i \in [t]$, $j \in [k]$) are as above, then*

$$\widehat{W}(G) = n \sum_{i=1}^{t} \frac{1}{|V_i|} \sum_{j=1}^{k} W(G/F_j, w_{ij}) \,.$$

Proof. We first recall from [3, p. 57] that the modified Wiener index can be equivalently written as $\widehat{W}(G) = n \sum_{i=1}^{t} (W(V_i)/|V_i|)$. Hence we can write

$$\widehat{W}(G) = n \sum_{i=1}^{t} \frac{1}{|V_i|} \sum_{\{x,y\} \subseteq V_i} d_G(x, y) \,.$$

As already mentioned above, the canonical metric representation α is an isometry. Moreover, it is well-known (cf. for instance [7, Proposition 5.1]) that the distance function is additive on the Cartesian product operation, that is, $d_{G \square H} = d_G + d_H$. These facts yield

the first equality in the following computation:

$$
\begin{aligned}
\widehat{W}(G) &= n \sum_{i=1}^{t} \frac{1}{|V_i|} \sum_{\{x,y\} \subseteq V_i} \sum_{j=1}^{k} d_{G/F_j}(\alpha_j(x), \alpha_j(y)) \\
&= n \sum_{i=1}^{t} \frac{1}{|V_i|} \left(\sum_{j=1}^{k} \sum_{\{x,y\} \subseteq V_i} d_{G/F_j}(\alpha_j(x), \alpha_j(y)) \right) \\
&= n \sum_{i=1}^{t} \frac{1}{|V_i|} \sum_{j=1}^{k} \left(\frac{1}{2} \sum_{x \in V_i} \sum_{y \in V_i} d_{G/F_j}(\alpha_j(x), \alpha_j(y)) \right) \\
&= n \sum_{i=1}^{t} \frac{1}{|V_i|} \sum_{j=1}^{k} W(G/F_j, w_{ij}).
\end{aligned}
$$

To see the truth of the last equality, note that a pair of vertices $x \in V_i \cap C$ and $y \in V_i \cap C'$, where C, C' are components of $G - F_j$, contributes $d_{G/F_j}(\alpha_j(x), \alpha_j(y))$ to the summation. For each such pair of vertices the contribution is the same and there are $w_{ij}(C) \cdot w_{ij}(C')$ such pairs. □

We note that a result parallel to Theorem 3.1 was earlier proved in [9] for the Wiener index, see [1, 17] for applications of this result. It was recently further generalized twofold: to vertex-weighted graphs and to partitions coarser that the Θ^*-partition [11].

An important case containing many chemical graphs is the class of graphs isometrically embeddable into hypercubes; these graphs are known as *partial cubes*. It is well known that these graphs are precisely the connected bipartite graphs for which the relation Θ is transitive. Moreover, if F is an arbitrary Θ-class (or, equivalently, an arbitrary Θ^*-class) of G, then $G - F$ consists of two connected components. It therefore follows that for partial cubes Theorem 3.1 can be simplified as follows:

Corollary 3.2. *Let G be a partial cube of order n and let $V_1, \dots, V_t$ be the orbits under the action of $\mathrm{Aut}(G)$ on $V(G)$. If $F_1, \dots, F_k$ are the Θ-classes of G, and $n_{ij} = |V_i \cap C_j|$, $n'_{ij} = |V_i \cap C'_j|$ $(i \in [t], j \in [k])$, where C_j and C'_j are the connected components of $G - F_j$, then*

$$
\widehat{W}(G) = n \sum_{i=1}^{t} \frac{1}{|V_i|} \sum_{j=1}^{k} n_{ij} \cdot n'_{ij}.
$$

4 Modified Wiener index of two families of fullerene patches

To illustrate the applicability of Theorem 3.1 and Corollary 3.2 we determine in this section the modified Wiener index of two families of nanocones.

4.1 $\widehat{W}$ of nanocones NCH(n)

The nanocones NCH(n), $n \geq 1$, are defined as follows. NCH(1) is isomorphic to the 6-cycle ("H" in the name stands for "hexagon"), while for $n \geq 2$, the nanocone NCH(n) is obtained from NCH($n - 1$) by adding an additional outer ring of hexagons to it. The construction should be clear from Fig. 1 where NCH(4) is shown. (These nanocones are in chemical graph theory also known as the coronene/circumcoronene series.)
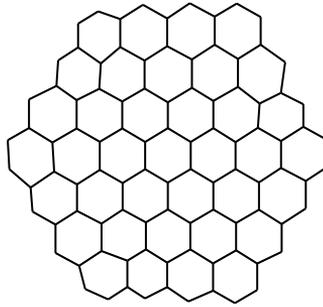
Figure 1: The nanocone NCH(4)

It is well-known that the nanocones NCH(n) are partial cubes (cf. [12]). Using Corollary 3.2 we can thus obtain the next result, a sketch of its proof being given in the rest of the subsection.

Theorem 4.1. *If $n \geq 1$, then $\widehat{W}(\mathrm{NCH}(n)) = 3n^3(10n^2 - 1)$.*

NCH(n) contains n concentric cycles (that is, the cycles iteratively added when the graphs is built from NCH(1)), call them the *layers* of NCH(n) and denote with $L_1, \ldots, L_n$. Clearly, $|L_i| = 12i - 6$, $1 \leq i \leq n$. Consequently, $|V(\mathrm{NCH}(n))| = \sum_{i=1}^{n}(12i - 6) = 6n^2$.

The Θ-classes of NCH(n) are its orthogonal cuts, in Fig. 2 the horizontal cuts of NCH(4) are shown. In general, the cuts are in three directions and hence NCH(n) contains $3(2n - 1)$ Θ-classes.
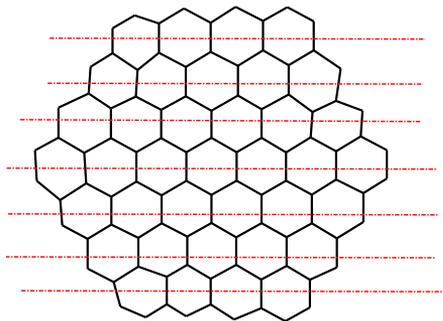

Figure 2: Horizontal Θ-classes of NCH(4)

To apply Corollary 3.2 we also need to know the symmetries of NCH(n); we claim that the automorphism group of NCH(n) is isomorphic to the dihedral group D_{12} of order 12. To simplify the notation set $\Gamma = \mathrm{Aut}(\mathrm{NCH}(n))$. Let α be the rotation of NCH(n) for $60°$, and let β be the reflection of NCH(n) over the central vertical line. Clearly, $\Gamma \geq \langle \alpha, \beta \rangle$. On the other hand, if x is any vertex of the middle hexagon of NCH(n), then its orbit x^{Γ} is formed by the vertices of the middle hexagon and its stabilizer Γ_x consists of the identity and the reflection over the line through x and its antipode on the inner cycle. Hence

$|\Gamma| = |x^{\Gamma}| \times |\Gamma_x| = 12$. Since $\alpha^6 = \beta^2 = 1$ and $\beta^{-1}\alpha\beta = \alpha^{-1}$, we conclude that Γ is indeed isomorphic to D_{12}. Note furthermore that each orbit of the action of Γ is a subset of some layer L_i, $i \in [n]$. Moreover, the layer L_i contains $i - 1$ orbits of size 12 and one orbit of size 6.

For a graph G set

$$\widehat{w}(G) = \widehat{W}(G)/|V(G)|,$$

so that $\widehat{W}(\mathrm{NCH}(n)) = 6n^2 \widehat{w}(\mathrm{NCH}(n))$. Using the above description of orbits, Corollary 3.2, and considering the contributions of the vertices from L_n, a straightforward (but somehow lengthy) computation yields the recurrence

$$\widehat{w}(\mathrm{NCH}(1)) = \frac{9}{2},$$

$$\widehat{w}(\mathrm{NCH}(n)) = \widehat{w}(\mathrm{NCH}(n-1)) + 15n(n-1) + \frac{9}{2}, \quad n \geq 2.$$

The solution of this recurrence is $\widehat{w}(\mathrm{NCH}(n)) = 5n^3 - \frac{n}{2}$ and Theorem 4.1 follows.

4.2 $\widehat{W}$ of nanocones NCP(n)

The nanocones NCP(n), $n \geq 1$, are defined analogously as the nanocones NCH(n), except that now we start with a pentagon (hence the letter "P" in NCP) and then adding rings of hexagons to it. More precisely, NCP(1) is isomorphic to the 5-cycle, while for $n \geq 2$ the nanocone NCP(n) is obtained from NCP($n-1$) by adding an additional outer ring of hexagons to it. See Fig. 3 for NCP(4).
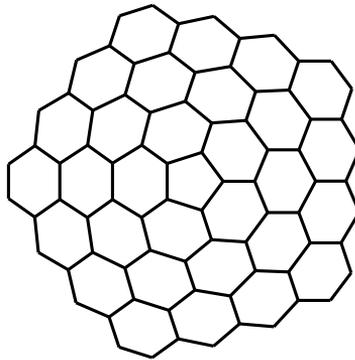

Figure 3: The nanocone NCP(4)

Since nanocones NCP(n) are not partial cubes, we cannot apply Corollary 3.2 for them, hence we need to use the more general Theorem 3.1 to get:

Theorem 4.2. *If $n \geq 1$, then $\widehat{W}(\mathrm{NCP}(n)) = 5n^3(11n^2 - 2)/3$.*

In the rest of this subsection we give a sketch of the proof of this result.

Just as for NCH(n), let us denote with $L_1, \ldots, L_n$ the *layers* of NCP(n). Since $|L_i| = 10i - 5$, $i \in [n]$, we get that $|V(\mathrm{NCP}(n))| = \sum_{i=1}^{n} 10i - 5 = 5n^2$. The Θ^*-classes of NCP(n) can be described as follows. One class, say F, consists of the edges of the inner

5-cycle together with the edges of the cuts propagating from them, see the left-hand side of Fig. 4. (The right-hand side of the figure shows the graph $\mathrm{NCP}(4) - F$.) All the other Θ^*-classes of $\mathrm{NCP}(n)$ are the orthogonal cuts across hexagons. Since each additional layer defines five such cuts, the total number of Θ^*-classes is $1 + 5(n-1) = 5n - 4$.
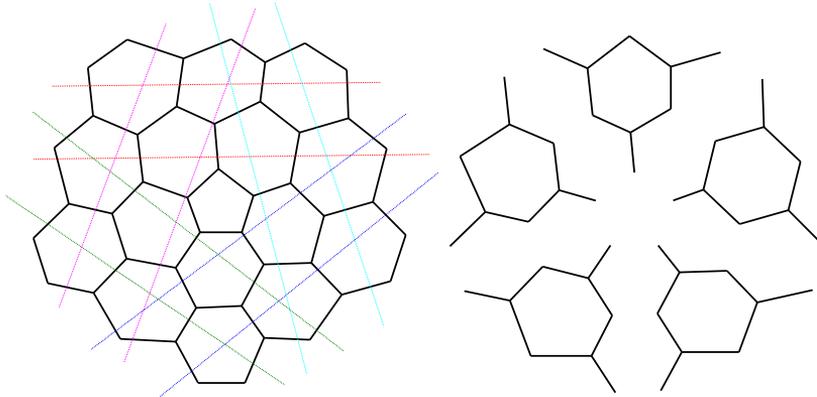

Figure 4: Θ^*-classes of NCP(3)

Similarly as for $\mathrm{NCH}(n)$, the automorphism group of $\mathrm{NCP}(n)$ is isomorphic to the dihedral group D_{10} of order 10. Set $\Gamma = \mathrm{Aut}(\mathrm{NCP}(n))$, let α be the rotation of $\mathrm{NCP}(n)$ for $72°$, and let β be the reflection of $\mathrm{NCP}(n)$ over the central vertical line. Clearly, $\Gamma \geq \langle \alpha, \beta \rangle$. On the other hand, if x is any vertex of the middle pentagon of $\mathrm{NCP}(n)$, then its orbit x^Γ is formed by the vertices of the middle pentagon and its stabilizer Γ_x consists of the identity and the reflection over the line through x and the midpoint of the edge opposite to x. Hence $|\Gamma| = |x^\Gamma| \times |\Gamma_x| = 10$. Since $\alpha^5 = \beta^2 = 1$ and $\beta^{-1}\alpha\beta = \alpha^{-1}$, we conclude that Γ is isomorphic to D_{10}. Furthermore, the layer L_i, $i \in [n]$, contains $i - 1$ orbits of size 10 and one orbit of size 5. Using Theorem 3.1 and considering the contributions of the vertices from L_n, a straightforward computation yields

$$
\begin{aligned}
\widehat{w}(NCP(1)) &= 3, \\
\widehat{w}(NCP(n)) &= \widehat{w}(NCP(n-1)) + 11n(n-1) + 3, \ \ n \geq 2.
\end{aligned}
$$

The solution of this recurrence is $\widehat{w}(NCP(n)) = (11n^3 - 2n)/3$ and Theorem 4.2 follows.

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