A METHOD FOR COMPUTING THE EDGE-HYPER-WIENER INDEX OF PARTIAL CUBES AND AN ALGORITHM FOR BENZENOID SYSTEMS

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The edge-hyper-Wiener index of a connected graph G is defined as $WW_e(G) = \frac{1}{2} \sum_{\{e,f\} \subseteq E(G)} d(e,f) + \frac{1}{2} \sum_{\{e,f\} \subseteq E(G)} d(e,f)^2$. We develop a method for computing the edge-hyper-Wiener index of partial cubes, which constitute a large class of graphs with a lot of applications. It is also shown how the method can be applied to trees. Furthermore, an algorithm for computing the edge-hyper-Wiener index of benzenoid systems is obtained. Moreover, the algorithm is used to recalculate already known closed formulas for the edge-Wiener index and the edge-hyper-Wiener index of linear poly-acenes. Finally, the method is presented on a benzenoid system with more complicated structure.

1. INTRODUCTION

The hyper-Wiener index is a distance-based graph invariant, used as a structure descriptor for predicting physicochemical properties of organic compounds (often those significant for pharmacology, agriculture, environment-protection etc.). It was introduced in 1993 by M. Randić [15] and has been extensively studied in many papers. Randić's original definition of the hyper-Wiener index was applicable just to trees and therefore, the hyper-Wiener index was later defined for all graphs [14]. The hyper-Wiener index is closely related to the well known Wiener index [19], which is one of the most popular molecular descriptors. Moreover, it is also

connected to the Hosoya polynomial [**6**], since the relationship between them was proved in [**2**].

In [**11**] a method for computing the hyper-Wiener index of partial cubes was developed and later it was applied to some chemical graphs [**3, 13, 20**]. Partial cubes constitute a large class of graphs with a lot of applications and includes, for example, many families of chemical graphs (benzenoid systems, trees, phenylenes, cyclic phenylenes, polyphenylenes). For more details about these graphs see [**5**].

The Wiener index and the hyper-Wiener index are based on the distances between pairs of vertices in a graph and therefore, similar concepts have been introduced for distances between pairs of edges under the names the edge-Wiener index [**7**] and the edge-hyper-Wiener index [**8**], respectively. However, the authors in [**7, 8**] suggested several possible definitions and our definitions are there referred to as the first edge-Wiener index and the first edge-hyper Wiener index. With other words, the edge-hyper-Wiener index of a graph G is just the hyper-Wiener index of the line graph $L(G)$ and a similar result holds for the edge-Wiener index. For some recent studies on the edge-hyper-Wiener index see [**1, 16, 17, 18**].

In this paper we develop a method for computing the edge-hyper-Wiener index of partial cubes. Our main result is parallel to the result from [**11**]. However, the present method is a bit more difficult and the proof requires some additional insights. We use the cut method to reduce the problem of calculating the edge-hyper-Wiener index of partial cubes to the problem of calculating the edge-Wiener index and the contributions of pairs of Θ-classes (for more information about the cut method see [**12**]). As an example, we describe how the method can be used on trees. In the case of polycyclic molecules the calculation of the edge-hyper-Wiener index by the definition is not easy, especially if one is interested in finding general expressions of homologous series. Therefore, using the main result and the results from [**9**], we develop an algorithm for computing the edge-hyper-Wiener index of benzenoid systems, which is much more efficient than the calculation by the definition. This algorithm is then used to obtain closed formulas for the edge-Wiener index and the edge-hyper-Wiener index of linear polyacenes. Finally, the algorithm is used also an a benzenoid system with more complicated (branched) structure.

2. PRELIMINARIES

Unless stated otherwise, the graphs considered in this paper are connected. We define $d(x, y)$ to be the usual shortest-path distance between vertices $x, y \in V(G)$. The distance $d(e, f)$ between edges e and f of graph G is defined as the distance between vertices e and f in the line graph $L(G)$. Here we follow this convention because in this way the pair $(E(G), d)$ forms a metric space.

The *Wiener index* and the *edge-Wiener index* of a connected graph G are defined

in the following way:

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v), \qquad W_e(G) = \sum_{\{e,f\} \subseteq E(G)} d(e,f).$$

On the other hand, for edges $e = ab$ and $f = xy$ of a graph G it is also legitimate to set

$$\widehat{d}(e,f) = \min\{d(a,x), d(a,y), d(b,x), d(b,y)\}.$$

Replacing d with $\widehat{d}$, we obtain another variant of the edge-Wiener index:

$$\widehat{W}_e(G) = \sum_{\{e,f\} \subseteq E(G)} \widehat{d}(e,f).$$

Obviously, if e and f are two different edges of G, then $d(e,f) = \widehat{d}(e,f) + 1$. Therefore, for any G it holds

(1)
$$W_e(G) = \widehat{W}_e(G) + \binom{|E(G)|}{2}.$$

The *hyper-Wiener index* and the *edge-hyper-Wiener index* of G are defined as:

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} d(u,v) + \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} d(u,v)^2,$$

$$WW_e(G) = \frac{1}{2} \sum_{\{e,f\} \subseteq E(G)} d(e,f) + \frac{1}{2} \sum_{\{e,f\} \subseteq E(G)} d(e,f)^2.$$

It is easy to see that for any connected graph G it holds $W_e(G) = W(L(G))$ and $WW_e(G) = WW(L(G))$.

Two edges $e_1 = u_1 v_1$ and $e_2 = u_2 v_2$ of graph G are in relation Θ, $e_1 \Theta e_2$, if

$$d_G(u_1, u_2) + d_G(v_1, v_2) \neq d_G(u_1, v_2) + d_G(u_1, v_2).$$

Note that this relation is also known as Djoković-Winkler relation. The relation Θ is reflexive and symmetric, but not necessarily transitive. We denote its transitive closure (i.e. the smallest transitive relation containing Θ) by Θ^*.

The *hypercube Q_n* of dimension n is defined in the following way: all vertices of Q_n are presented as n-tuples $(x_1, x_2, \ldots, x_n)$ where $x_i \in \{0, 1\}$ for each $1 \leq i \leq n$ and two vertices of Q_n are adjacent if the corresponding n-tuples differ in precisely one coordinate. Therefore, the *Hamming distance* between two tuples x and y is the number of positions in x and y in which they differ.

A subgraph H of a graph G is called an *isometric subgraph* if for each $u, v \in V(H)$ it holds $d_H(u,v) = d_G(u,v)$. Any isometric subgraph of a hypercube is called a

partial cube. For an edge ab of a graph G, let W_{ab} be the set of vertices of G that are closer to a than to b. We write $\langle S \rangle$ for the subgraph of G induced by $S \subseteq V(G)$. The following theorem puts forth two fundamental characterizations of partial cubes:

Theorem 2.1. *[5] For a connected graph G, the following statements are equivalent:*

(i) *G is a partial cube.*

(ii) *G is bipartite, and $\langle W_{ab} \rangle$ and $\langle W_{ba} \rangle$ are convex subgraphs of G for all $ab \in E(G)$.*

(iii) *G is bipartite and $\Theta = \Theta^*$.*

Is it also known that if G is a partial cube and E is a Θ-class of G, then $G - E$ has exactly two connected components, namely $\langle W_{ab} \rangle$ and $\langle W_{ba} \rangle$, where $ab \in E$. For more information about partial cubes see [**5**].

3. THE EDGE-HYPER-WIENER INDEX OF PARTIAL CUBES

In this section a method for computing the edge-hyper-Wiener index of partial cubes is developed. For this purpose, we need some auxiliary results. We start with the following definition.

Definition 3.2. *Let G be a partial cube and let E_k be a Θ-class of G. Furthermore, let U and U' be the connected components of the graph $G - E_k$. If $e, f \in E(G)$, we define*

$$\delta_k(e, f) = \begin{cases} 1; & e \in E(U) \,\&\, f \in E(U') \text{ or } e \in E(U') \,\&\, f \in E(U), \\ 0; & \text{otherwise.} \end{cases}$$

The following lemma is crucial for our main theorem.

Lemma 3.3. *Let G be a partial cube with Θ-classes $E_1, \ldots, E_d$. If $e, f \in E(G)$, then it holds*

$$\widehat{d}(e, f) = \sum_{k=1}^{d} \delta_k(e, f).$$

Proof. Let a and x be end-vertices of e and f, respectively, such that $d(a, x) = \widehat{d}(e, f)$. Also, let b and y be the remaining end-vertices of e and f, respectively. Furthermore, let P be a shortest path between a and x. Obviously, $|E(P)| = \widehat{d}(e, f)$. For every $k \in \{1, \ldots, d\}$ we define

$$F_k = E_k \cap E(P).$$

Let $k \in \{1, \ldots, d\}$ and let U and U' be the connected components of the graph $G - E_k$ such that $a \in V(U)$. Now we can show that $|F_k| = \delta_k(e, f)$. We consider the following two cases.

1. $F_k = \emptyset$

   In this case, since no edge of P is in E_k, it follows that path P is completely contained in U or U'. Hence, $\delta_k(e, f) = 0 = |F_k|$ and the statement is true.

2. $F_k \neq \emptyset$

   In this case, since no two edges in a shortest path are in relation Θ (see [**5**]), it follows $|F_k| = 1$. Let uv be the edge in F_k. Without loss of generality suppose that $V(U) = W_{uv}$ and $V(U') = W_{vu}$. Obviously, $a \in V(U)$ and $x \in V(U')$. We first show that $b \in V(U) = W_{uv}$. If $b \in W_{vu}$, then $d(b, v) < d(b, u) = d(a, u) + 1$ (the equality holds since G is bipartite) and therefore, $d(b, v) \leq d(a, u)$. Hence, $\widehat{d}(e, f) < |E(P)|$, which is a contradiction. In a similar way we can show that $y \in V(U')$. Therefore, $e \in E(U)$ and $f \in E(U')$. It follows that $\delta_k(e, f) = 1 = |F_k|$.

We have proved that $|F_k| = \delta_k(e, f)$ for any $k \in \{1, \ldots, d\}$. Therefore,

$$\widehat{d}(e, f) = |E(P)| = \sum_{k=1}^{d} |E_k \cap E(P)| = \sum_{k=1}^{d} |F_k| = \sum_{k=1}^{d} \delta_k(e, f),$$

which completes the proof.

$\square$

To prove the main result, we need to introduce some additional notation. If G is a graph with Θ-classes $E_1, \ldots, E_d$, we denote by U_k and U_k' the connected components of the graph $G - E_k$, where $k \in \{1, \ldots, d\}$. For any $k, l \in \{1, \ldots, d\}$ set

$$
\begin{aligned}
M_{kl}^{11} &= E(U_k) \cap E(U_l), \\
M_{kl}^{10} &= E(U_k) \cap E(U_l'), \\
M_{kl}^{01} &= E(U_k') \cap E(U_l), \\
M_{kl}^{00} &= E(U_k') \cap E(U_l').
\end{aligned}
$$

Also, for $k, l \in \{1, \ldots, d\}$ and $i, j \in \{0, 1\}$ we define

$$m_{kl}^{ij} = |M_{kl}^{ij}|.$$

Lemma 3.4. *Let G be a partial cube and let d be the number of its Θ-classes. Then*

$$\sum_{e \in E(G)} \sum_{f \in E(G)} \widehat{d}(e, f)^2 = 2\widehat{W}_e(G) + 4 \sum_{k=1}^{d-1} \sum_{l=k+1}^{d} \left(m_{kl}^{11} m_{kl}^{00} + m_{kl}^{10} m_{kl}^{01} \right).$$

Proof. Using Lemma 3.3 we obtain

$$
\sum_{e \in E(G)} \sum_{f \in E(G)} \widehat{d}(e, f)^2 = \sum_{e \in E(G)} \sum_{f \in E(G)} \left(\sum_{k=1}^{d} \delta_k(e, f) \right)^2
$$

$$
= \sum_{e \in E(G)} \sum_{f \in E(G)} \sum_{k=1}^{d} \sum_{l=1}^{d} \delta_k(e, f) \delta_l(e, f)
$$

$$
= \sum_{k=1}^{d} \sum_{l=1}^{d} \left(\sum_{e \in E(G)} \sum_{f \in E(G)} \delta_k(e, f) \delta_l(e, f) \right)
$$

$$
= \sum_{k=1}^{d} \sum_{e \in E(G)} \sum_{f \in E(G)} \delta_k(e, f)
$$

$$
+ \sum_{k=1}^{d} \sum_{\substack{l=1 \\ l \neq k}}^{d} \left(\sum_{e \in E(G)} \sum_{f \in E(G)} \delta_k(e, f) \delta_l(e, f) \right)
$$

$$
= \sum_{e \in E(G)} \sum_{f \in E(G)} \sum_{k=1}^{d} \delta_k(e, f)
$$

$$
+ 2 \sum_{k=1}^{d} \sum_{\substack{l=1 \\ l \neq k}}^{d} \left(\frac{1}{2} \sum_{e \in E(G)} \sum_{f \in E(G)} \delta_k(e, f) \delta_l(e, f) \right)
$$

$$
= \sum_{e \in E(G)} \sum_{f \in E(G)} \widehat{d}(e, f) + 2 \sum_{k=1}^{d} \sum_{\substack{l=1 \\ l \neq k}}^{d} \left(m_{kl}^{11} m_{kl}^{00} + m_{kl}^{10} m_{kl}^{01} \right),
$$

where the last equality follows from the obvious fact that $\delta_k(e, f) \delta_l(e, f) = 1$ if and only if $\delta_k(e, f) = 1$ and $\delta_l(e, f) = 1$. Hence,

$$
\sum_{e \in E(G)} \sum_{f \in E(G)} \widehat{d}(e, f)^2 = 2 \widehat{W}_e(G) + 4 \sum_{k=1}^{d-1} \sum_{l=k+1}^{d} \left(m_{kl}^{11} m_{kl}^{00} + m_{kl}^{10} m_{kl}^{01} \right)
$$

and we are done.

$\square$

Now everything is prepared for the main result of the paper.

Theorem 3.5. *Let G be a partial cube and let d be the number of its Θ-classes. Then*

$$
(2) \qquad WW_e(G) = 2W_e(G) + \sum_{k=1}^{d-1} \sum_{l=k+1}^{d} \left(m_{kl}^{11} m_{kl}^{00} + m_{kl}^{10} m_{kl}^{01} \right) - \binom{|E(G)|}{2}.
$$

Proof. We first notice that

$$
\sum_{e \in E(G)} \sum_{f \in E(G)} d(e,f)^2 \;=\; \sum_{e \in E(G)} \sum_{\substack{f \in E(G) \\ f \neq e}} d(e,f)^2
$$

$$
= \sum_{e \in E(G)} \sum_{\substack{f \in E(G) \\ f \neq e}} \left(\widehat{d}(e,f) + 1 \right)^2
$$

$$
= \sum_{e \in E(G)} \sum_{\substack{f \in E(G) \\ f \neq e}} \widehat{d}(e,f)^2 + 2 \sum_{e \in E(G)} \sum_{\substack{f \in E(G) \\ f \neq e}} \widehat{d}(e,f)
$$

$$
+ \sum_{e \in E(G)} \sum_{\substack{f \in E(G) \\ f \neq e}} 1.
$$

Using Lemma 3.4 we thus get

$$
\sum_{e \in E(G)} \sum_{f \in E(G)} d(e,f)^2 \;=\; 2\widehat{W}_e(G) + 4 \sum_{k=1}^{d-1} \sum_{l=k+1}^{d} \left(m_{kl}^{11} m_{kl}^{00} + m_{kl}^{10} m_{kl}^{01} \right)
$$

$$
+ \; 4\widehat{W}_e(G) + |E(G)| \cdot (|E(G)| - 1).
$$

Therefore, using also Equation 1, we obtain

$$
WW_e(G) \;=\; \frac{1}{4} \sum_{e \in E(G)} \sum_{f \in E(G)} d(e,f) + \frac{1}{4} \sum_{e \in E(G)} \sum_{f \in E(G)} d(e,f)^2
$$

$$
= \; \frac{1}{2} W_e(G) + \frac{1}{2} \widehat{W}_e(G) + \sum_{k=1}^{d-1} \sum_{l=k+1}^{d} \left(m_{kl}^{11} m_{kl}^{00} + m_{kl}^{10} m_{kl}^{01} \right)
$$

$$
+ \; \widehat{W}_e(G) + \frac{|E(G)| \cdot (|E(G)| - 1)}{4}
$$

$$
= \; 2W_e(G) + \sum_{k=1}^{d-1} \sum_{l=k+1}^{d} \left(m_{kl}^{11} m_{kl}^{00} + m_{kl}^{10} m_{kl}^{01} \right) - \frac{|E(G)| \cdot (|E(G)| - 1)}{2}
$$

and the proof is complete.

$\square$

As already mentioned, trees are partial cubes (it is easy to see that in a tree any two distinct edges are not in relation Θ and therefore, Θ is a transitive relation, see also [5]). Moreover, a Θ-class in a tree is just a single edge. Therefore, for a tree T with edges $e_1, \ldots, e_m$, Theorem 3.5 reduces to

$$
WW_e(T) = 2W_e(T) + \sum_{k=1}^{m-1} \sum_{l=k+1}^{m} m_1(e_k, e_l) m_2(e_k, e_l) - \binom{m}{2},
$$

where $m_1(e_k, e_l)$ and $m_2(e_k, e_l)$ are the number of edges in the two extremal connected components of the graph $T - \{e_k, e_l\}$, see Figure 1.
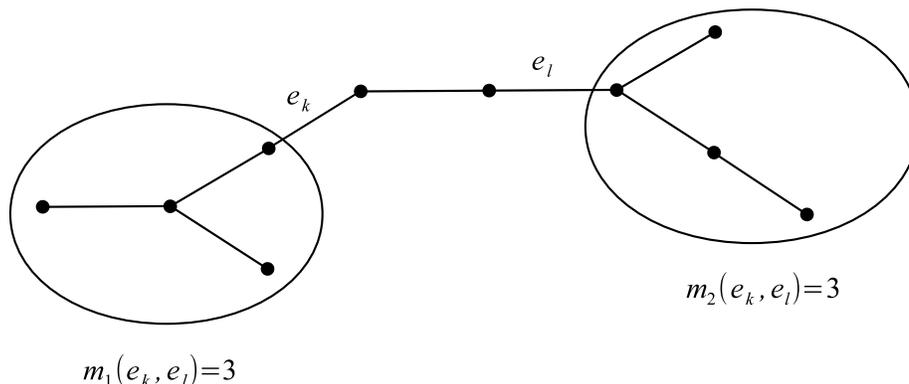

Figure 1: A tree with two extremal components with respect to e_k and e_l.

4. ALGORITHM FOR BENZENOID SYSTEMS

Let $\mathcal{H}$ be the hexagonal (graphite) lattice and let Z be a cycle on it. Then a *benzenoid system* is induced by the vertices and edges of $\mathcal{H}$, lying on Z and in its interior. These graphs are the molecular graphs of the benzenoid hydrocarbons, a large class of organic molecules. For more information about benzenoid systems see [**4**].

An *elementary cut* C of a benzenoid system G is a line segment that starts at the center of a peripheral edge of a benzenoid system G, goes orthogonal to it and ends at the first next peripheral edge of G. By C we sometimes also denote the set of edges that are intersected by the corresponding elementary cut. Elementary cuts in benzenoid systems have been described and illustrated by numerous examples in several earlier articles.

The main insight for our consideration is that every Θ-class of a benzenoid system G coincide with exactly one of its elementary cuts. Therefore, it is not difficult to check that all benzenoid systems are partial cubes.

In the case of benzenoid systems, Theorem 3.5 provides a particular simple procedure for computing the edge-hyper-Wiener index:

1. We first compute the edge-Wiener index using the procedure described in [**9**], which we briefly repeat: the edge set of a benzenoid system G can be naturally partitioned into sets E_1, E_2, and E_3 of edges of the same direction. For $i \in \{1, 2, 3\}$, set $G_i = G - E_i$. Then the connected components of the graph G_i are paths. The quotient graph T_i, $1 \leq i \leq 3$, has these paths as

vertices, two such paths (i.e. components of G_i) P' and P'' being adjacent in T_i if some edge in E_i joins a vertex of P' to a vertex of P''. It is known that T_1, T_2 and T_3 are trees. We next extend the quotient trees T_1, T_2, T_3 to weighted trees (T_i, w_i), (T_i, w_i'), (T_i, w_i, w_i') as follows:

- for $C \in V(T_i)$, let $w_i(C)$ be the number of edges in the component C of G_i;
- for $E = C_1 C_2 \in E(T_i)$, let $w_i'(E)$ be the number of edges between components C_1 and C_2.

Then the edge-Wiener index of a benzenoid system G can be computed as

$$(3) \quad W_e(G) = \sum_{i=1}^{3} \left(\widehat{W}_e(T_i, w_i') + W_v(T_i, w_i) + W_{ve}(T_i, w_i, w_i') \right) + \binom{|E(G)|}{2}.$$

To efficiently compute all the terms in Equation 3, some additional notation is needed. If T is a tree and $e \in E(T)$, then the graph $T - e$ consists of two components that will be denoted by $C_1(e)$ and $C_2(e)$. For a vertex-edge weighted tree (T, w, w') and $e \in E(T)$ set

$$n_i(e) = \sum_{u \in V(C_i(e))} w_i(u) \qquad \text{and} \qquad m_i(e) = \sum_{e \in E(C_i(e))} w_i'(e).$$

Using this notation we recall the following results (see [9]):

$$\begin{aligned} W_v(T, w) &= \sum_{e \in E(T)} n_1(e) n_2(e), \\ \widehat{W}_e(T, w') &= \sum_{e \in E(T)} m_1(e) m_2(e), \\ W_{ve}(T, w, w') &= \sum_{e \in E(T)} \big(n_1(e) m_2(e) + n_2(e) m_1(e) \big). \end{aligned}$$

2. Let us denote the second term in Equation 2 by $WW_e^*(G)$, i.e.

$$WW_e^*(G) = \sum_{k=1}^{d-1} \sum_{l=k+1}^{d} \left(m_{kl}^{11} m_{kl}^{00} + m_{kl}^{10} m_{kl}^{01} \right).$$

To compute this term we proceed as follows. Let C_k and C_l be two distinct elementary cuts (Θ-classes) of a benzenoid system G such that $l > k$. Then there are two different cases, since the elementary cuts can intersect or not - see Figure 2.

By a_{kl}, b_{kl}, c_{kl}, and d_{kl} we denote the number of edges in the corresponding components of $G - C_k - C_l$. Then the contribution of the pair C_k, C_l to $WW_e^*(G)$ will be denoted by $f(C_k, C_l)$ and we obtain
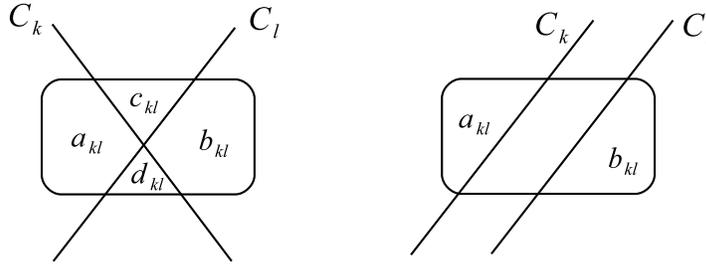
Figure 2: Two different positions of two elementary cuts.

$$f(C_k, C_l) = \begin{cases} a_{kl}b_{kl} + c_{kl}d_{kl}, & C_k \text{ and } C_l \text{ intersect} \\ a_{kl}b_{kl}, & \text{otherwise.} \end{cases}$$

Therefore, term $WW_e^*(G)$ for a benzenoid system G with d elementary cuts can be computed as

$$WW_e^*(G) = \sum_{k=1}^{d-1} \sum_{l=k+1}^{d} f(C_k, C_l).$$

Algorithm 1: Edge-Hyper-Wiener Index of Benzenoid Systems

Input : Benzenoid system G with m edges
Output: $WW_e(G)$
1   $C_1, \ldots, C_d \leftarrow$ `calculateElementaryCuts` (G)
2   $(T_1, T_2, T_3) \leftarrow$ `calculateQuotientTrees` (G)
3   **for** $i = 1$ to 3 **do**
4     $(w_i, w_i') \leftarrow$ `calculateWeights` (T_i, G)
5     $X_{i,1} \leftarrow W_v(T_i, w_i)$
6     $X_{i,2} \leftarrow W_e(T_i, w_i')$
7     $X_{i,3} \leftarrow W_{ve}(T_i, w_i, w_i')$
8     $Y_i \leftarrow X_{i,1} + X_{i,2} + X_{i,3}$
9   **end**
10   $W_e(G) \leftarrow Y_1 + Y_2 + Y_3 + \binom{m}{2}$
11   $WW_e^*(G) \leftarrow 0$
12   **for** $k = 1$ to $d - 1$ **do**
13   **for** $l = k + 1$ to d **do**
14       $f_{k,l} \leftarrow$ `calculateContriCuts` (C_k, C_l)
15       $WW_e^*(G) \leftarrow WW_e^*(G) + f_{k,l}$
16   **end**
17   **end**
18   $WW_e(G) \leftarrow 2W_e(G) + WW_e^*(G) - \binom{m}{2}$

Finally, we arrive to the algorithm for the computation of the edge-hyper-Wiener index of benzenoid systems. For a given benzenoid system G we first compute its elementary cuts using a procedure called `calculateElementaryCuts` and then the quotient trees T_i using a procedure `calculateQuotientTrees`. For each T_i we first compute the vertex weights w and the edge weights w' using a procedure `calculateWeights`. When the edge-Wiener index is calculated, we sum up all the contributions of pairs of elementary cuts - procedure `calculateContriCuts`. Furthermore, Theorem 3.5 is applied to obtain the final result. The algorithm is shown in the previous page.

5. CLOSED FORMULAS FOR LINEAR POLYACENES

In this section we derive closed formulas for the edge-Wiener index and the edge-hyper-Wiener index of linear polyacenes using the procedure described in the previous section. If $h \geq 1$, then *linear polyacene* L_h is formed of h linearly connected hexagons, see Figure 3. Recall that for $h = 1, 2, 3, 4, 5$ the graph L_h represents benzene, naphthalene, anthracene, naphthacene, and pentacene (see [4]).
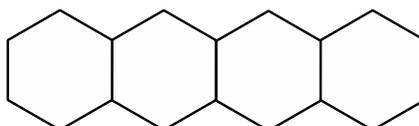

Figure 3: Linear polyacene L_4.

Although closed formulas for linear polyacenes were previously obtained in [10, 8], it can be computed by hand that $W_e(L_3) = 350$ and $WW_e(L_3) = 812$, but these results do not coincide with the mentioned results.

To obtain closed formulas, we first compute the edge-Wiener index. The corresponding weighted quotient trees for L_h are depicted in Figure 4.
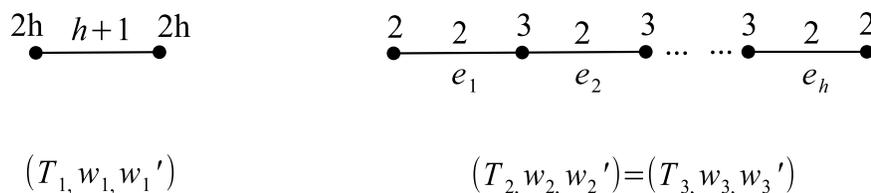

Figure 4: Weighted quotient trees for linear polyacene L_h.

Obviously,

$$W_v(T_1, w_1) = 4h^2, \quad \widehat{W}_e(T_1, w_1') = 0, \quad W_{ve}(T_1, w_1, w_1') = 0.$$

To compute the corresponding Wiener indices of the second tree, we first notice that for the edge e_i, $i \in \{1, \ldots, h\}$ it holds:

$$
\begin{aligned}
n_1(e_i) &= 3(i-1) + 2 = 3i - 1, \\
n_2(e_i) &= 3(h-i) + 2 = 3h - 3i + 2, \\
m_1(e_i) &= 2(i-1) = 2i - 2, \\
m_2(e_i) &= 2(h-i) = 2h - 2i.
\end{aligned}
$$

Therefore, after an elementary calculation we obtain

$$
\begin{aligned}
W_v(T_2, w_2) &= \sum_{i=1}^{h} (3i-1)(3h-3i+2) = \frac{1}{2}h(3h^2 + 3h + 2), \\
\widehat{W}_e(T_2, w_2') &= \sum_{i=1}^{h} (2i-2)(2h-2i) = \frac{2}{3}h(h^2 - 3h + 2), \\
W_{ve}(T_2, w_2, w_2') &= \sum_{i=1}^{h} \Big((3i-1)(2h-2i) + (2i-2)(3h-3i+2) \Big) \\
&= 2(h-1)h^2.
\end{aligned}
$$

Also, one can easily see the the number of edges in L_h is

$$
(4) \qquad\qquad |E(L_h)| = 5h + 1.
$$

Hence, Equation 3 implies that for any $h \geq 1$ it holds

$$
(5) \qquad\qquad W_e(L_h) = \frac{1}{6}h(50h^2 + 69h + 43).
$$

Next, we have to compute $WW_e^*(L_h)$. Let $B, C_1, C_2, \ldots, C_h, D_1, D_2, \ldots, D_h$ be the elementary cuts of L_h, where $h \geq 1$. See Figure 5.
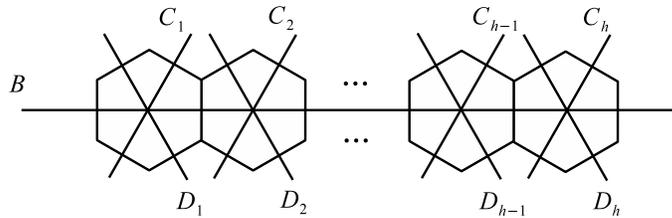

Figure 5: Elementary cuts of L_h.

To obtain the final result, we need to calculate the contributions $f(\cdot, \cdot)$ of all the pairs of elementary cuts. Therefore, the number of edges in specific components (parts) of a graph is shown in Table 1.

Pair of elementary cuts	Part a	Part b	Part c	Part d
B, C_k $(k = 1, \ldots, h)$	$2k - 1$	$2h - 2k + 1$	$2h - 2k$	$2k - 2$
B, D_k $(k = 1, \ldots, h)$	$2k - 2$	$2h - 2k$	$2h - 2k + 1$	$2k - 1$
C_k, C_l $(k < l)$	$5k - 3$	$5h - 5l + 2$	/	/
D_k, D_l $(k < l)$	$5k - 3$	$5h - 5l + 2$	/	/
C_k, D_l $(k < l)$	$5k - 3$	$5h - 5l + 2$	/	/
C_k, D_l $(k > l)$	$5l - 3$	$5h - 5k + 2$	/	/
C_k, D_k $(k = 1, \ldots, h)$	$5k - 4$	$5h - 5k + 1$	0	0

Table 1: Number of edges in the connected components.

Firstly, we sum up all the contributions of the pairs B, C_k, where $k = 1, \ldots, h$, and we obtain

$$\sum_{k=1}^{h} \Big((2k-1)(2h-2k+1) + (2h-2k)(2k-2) \Big) = \frac{1}{3}h(4h^2 - 6h + 5).$$

The same result is obtained for the pairs B, D_k, $k = 1, \ldots, h$. Secondly, we sum up all the contributions of the pairs C_k, C_l, $k < l$, and we get

$$\sum_{k=1}^{h-1} \sum_{l=k+1}^{h} (5k-3)(5h-5l+2) = \frac{1}{24}h(25h^3 - 70h^2 + 83h - 38).$$

It is easy to notice that the same result is obtained for the pairs D_k, D_l $(k < l)$, for the pairs C_k, D_l $(k < l)$ and for the pairs C_k, D_l $(k > l)$. Finally, we sum up all the contributions of the pairs C_k, D_k, $k = 1, \ldots, h$, and we obtain

$$\sum_{k=1}^{h} (5k-4)(5h-5k+1) = \frac{1}{6}h(25h^2 - 45h + 26).$$

By summing up the contributions of all the pairs of elementary cuts from Table 1 we then calculate

(6)
$$WW_e^*(L_h) = \frac{1}{6}h(25h^3 - 29h^2 + 14h + 8).$$

Finally, using Theorem 3.5, Equation 5, Equation 6, and Equation 4 we deduce that for any $h \geq 1$ it holds

$$WW_e(L_h) = \frac{1}{6}h(25h^3 + 71h^2 + 77h + 79).$$

6. AN ADDITIONAL EXAMPLE

In this final section we present our method for computing the edge-hyper Wiener index on a benzenoid system with more complicated (branched) structure. Therefore, let G be a benzenoid system from Figure 6. We can see that G has 25 edges. To compute the edge-Wiener index, we consider the following weighted quotient trees from Figure 7.
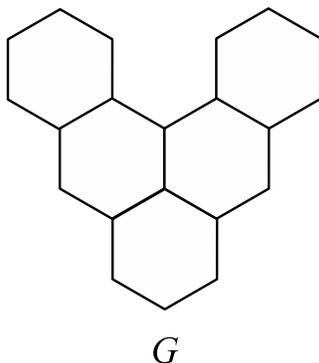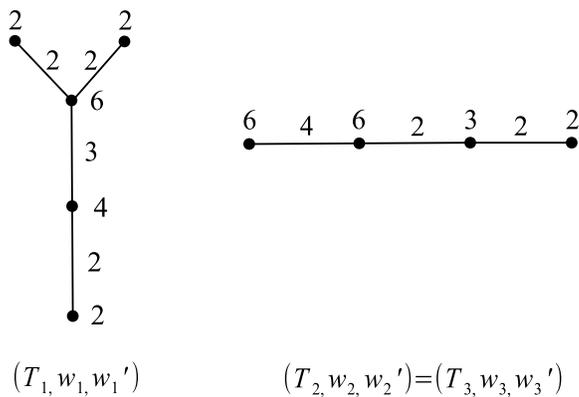

Figure 6: Benzenoid system G.

$$(T_{1,}\, w_{1,}\, w_1{}') \qquad (T_{2,}\, w_{2,}\, w_2{}') = (T_{3,}\, w_{3,}\, w_3{}')$$

Figure 7: Weighted quotient trees.

One can easily compute the following:

$$W_v(T_1, w_1) = 144, \qquad \widehat{W}_e(T_1, w_1') = 8, \qquad W_{ve}(T_1, w_1, w_1') = 86,$$
$$W_v(T_2, w_2) = 156, \qquad \widehat{W}_e(T_2, w_2') = 8, \qquad W_{ve}(T_2, w_2, w_2') = 80,$$

$$W_v(T_3, w_3) = 156, \qquad \widehat{W}_e(T_3, w'_3) = 8, \qquad W_{ve}(T_3, w_3, w'_3) = 80.$$

Hence, by Equation 3 we get

$$W_e(G) = (144 + 8 + 86) + (156 + 8 + 80) + (156 + 8 + 80) + 300 = 1026.$$

To compute $WW_e^*(G)$, we need to determine the contributions of pairs of elementary cuts. The elementary cuts of G will be denoted by B_1, B_2, B_3, B_4, C_1, C_2, C_3, D_1, D_2, D_3, see Figure 8.
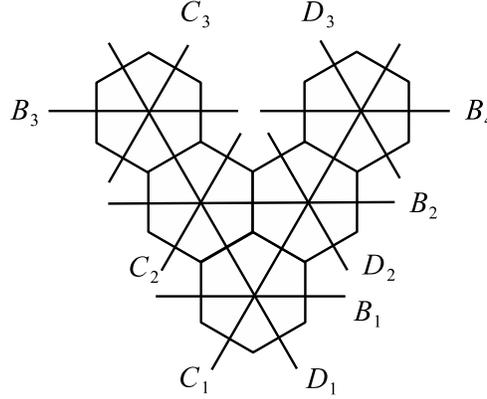

Figure 8: Elementary cuts of G.

The contributions of pairs of elementary cuts are given in Table 2. Some cases are omitted since elementary cuts C_1, C_2, C_3 and D_1, D_2, D_3 are symmetric.

Pair	$f(\cdot,\cdot)$	Pair	$f(\cdot,\cdot)$	Pair	$f(\cdot,\cdot)$	Pair	$f(\cdot,\cdot)$
B_1, B_2	28	B_1, C_3	4	B_4, C_2	14	C_2, D_1	40
B_1, B_3	4	B_2, C_1	36	B_4, C_3	4	C_2, D_2	49
B_1, B_4	4	B_2, C_2	42	C_1, C_2	42	C_2, D_3	14
B_2, B_3	16	B_2, C_3	16	C_1, C_3	12	C_3, D_1	14
B_2, B_4	16	B_3, C_1	12	C_2, C_3	32	C_3, D_2	14
B_3, B_4	4	B_3, C_2	32	C_1, D_1	25	C_3, D_3	4
B_1, C_1	14	B_3, C_3	20	C_1, D_2	40		
B_1, C_2	14	B_4, C_1	5	C_1, D_3	14		

Table 2: Contributions of pairs of elementary cuts.

Summing up all the contributions of all the pairs we obtain

$$WW_e^*(G) = 884.$$

Finally, by Theorem 3.5 it follows

$$WW_e(G) = 2 \cdot 1026 + 884 - 300 = 2636.$$

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