A Congruence Relation for the Wiener Index of Graphs with a Tree–Like Structure

Katarína Hriňáková [a], Martin Knor [a], Riste Škrekovski [b,c,d], Aleksandra Tepeh [d,e]

[a] *Slovak University of Technology in Bratislava, Faculty of Civil Engineering, Department of Mathematics, Radlinského 11, 813 68, Bratislava, Slovakia,*
hrinakova@math.sk , knor@math.sk

[b] *Faculty of Information Studies, 8000 Novo Mesto, Slovenia,*
[c] *FAMNIT, University of Primorska, 6000 Koper, Slovenia,*
[d] *Faculty of Mathematics and Physics, University of Ljubljana, 1000 Ljubljana,*
skrekovski@gmail.com

[e] *Faculty of Electrical Engineering and Computer Science, University of Maribor, Smetanova ulica 17, 2000 Maribor, Slovenia,*
aleksandra.tepeh@gmail.com

(Received January 27, 2014)

Abstract

The Wiener index, defined as the sum of distances between all unordered pairs of vertices in a graph, is one of the most popular molecular descriptors. Congruence relations for the Wiener index for specific families of trees were studied by several authors. Namely, in [Gutman, Rouvray, Comput. Chem. 14 (1990) 29–32] it is shown that Wiener indices of any two trees on the same number of vertices and with 1-factor are congruent modulo 4. Recently, the author of [Lin, MATCH Commun. Math. Comput. Chem. 70 (2013) 575–582] generalized this result to trees with path factors and [Gutman, Xu, Liu, to appear in Filomat] generalized it to even much larger class of graphs. We continue this work by establishing congruence relations for various large families of graphs with a tree-like structure, whose “vertices” and “edges” represent some graphs of prescribed type and congruence.

1 Introduction

All graphs considered in this paper are finite, simple and connected. Let G be a graph. Its vertex and edge sets are denoted by $V(G)$ and $E(G)$, respectively. Let $u, v \in V(G)$.

The length of a shortest path in G between u and v is denoted by $d_G(u, v)$ (or by $d(u, v)$ when no confusion is likely).

The oldest topological index related to molecular branching is the Wiener index [14], which was introduced in 1947. It is defined as the sum of distances between all (unordered) pairs of vertices of G,

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v).$$

The Wiener index plays an important role in organic chemistry and has been extensively studied. At first it was used for predicting the boiling point of paraffins [13], but later strong correlation between the Wiener index and the chemical properties of a compound was found. Nowadays this index is a tool used for preliminary screening of drug molecules [1]. The Wiener index also predicts binding energy of protein-ligand complex at a preliminary stage. Besides applications in chemistry it was studied also from a purely graph-theoretical point of view. More details can be found in some of the many surveys [2, 4, 7, 11, 15].

In [14], Wiener proved that for a tree T

$$W(T) = \sum_{e=ij \in E(T)} n_e(i) n_e(j),$$

where $n_e(i)$ and $n_e(j)$ are the orders of the components of $T - ij$. In analogy to this result, we have the following vertex version [9].

Theorem 1. *Let T be a tree on n vertices. Then*

$$W(T) = \sum_{v \in V(T)} \sum_{1 \le i < j \le p} n(T_i)\, n(T_j) + \binom{n}{2},$$

where $T_1, T_2, \ldots, T_p$ are the components of $T - v$.

In addition, Gutman and Škrekovski [9] generalized this result by proving that for a connected graph G, $W(G) = \sum_{v \in V(G)} B(v) + \binom{n}{2}$. This formula shows that the Wiener index is related to the *betweenness centrality* $B(v)$ of the vertices $v \in V(G)$, a quantity used in theory of social networks, which measures the number of times a vertex lies on a shortest path between two other vertices.

If a tree contains a small number of *branching vertices* (i.e., vertices of degree at least three) it is suitable to apply the theorem of Doyle and Graver [3]. Some applications of this formula were elaborated in [5, 10].

Theorem 2 (Doyle and Graver). *Let T be a tree on n vertices. Then*

$$W(T) = \binom{n+1}{3} - \sum_{v \in V(T)} \sum_{1 \le i < j < k \le p} n(T_i)\, n(T_j)\, n(T_k)\,,$$

where $T_1, T_2, \ldots, T_p$ are the components of $T - v$.

It was of interest to several authors to obtain congruence relations for the Wiener index. The first result of this kind was proved by Gutman and Rouvray [8]. They established the congruence relation for the Wiener index of trees with perfect matchings.

Theorem 3 (Gutman and Rouvray). *Let T and T' be two trees on the same number of vertices. If both T and T' have perfect matchings, then $W(T) \equiv W(T') \pmod 4$.*

A *segment* of a tree is its path-subtree whose terminal vertices are branching or pendant vertices. Dobrynin, Entringer and Gutman [2] obtained a congruence relation for the Wiener index in the class of *k-proportional trees*. Trees of this class have the same order, the same number of segments, and the lengths of all segments are proportional to the coefficient k. More precisely, if $l_1, l_2, \ldots, l_m$ and $l'_1, l'_2, \ldots, l'_m$ are the lengths of the segments of the trees T and T', respectively, then $l_i = kr_i$ and $l'_i = kr'_i$, $1 \le i \le m$, where r_i and r'_i are positive integers.

Theorem 4 (Dobrynin, Entringer and Gutman). *Let T and T' be two k-proportional trees. Then*

$$W(T) \equiv W(T') \pmod{k^3}.$$

Theorem 3 was recently generalized by Lin in [12] by establishing the congruence relation for the Wiener index of trees containing T-factors. A graph G has a *T-factor* if there exist m ($m = |V(G)|/r$) vertex disjoint trees $T_1, T_2, \ldots, T_m$ such that $V(G) = V(T_1) \cup V(T_2) \cup \cdots \cup V(T_m)$ and each T_i is isomorphic to a tree T on r vertices. If T is a path on r vertices, we say that the graph G has a P_r-factor. In this sense the well-known perfect matching (or 1-factor) is a P_2-factor.

It is well known that for a path on n vertices, $W(P_n) = \binom{n+1}{3}$. Lin observed that for an arbitrary tree T on n vertices with a P_r-factor, each summand of $\sum_{1 \le i<j<k \le p} n(T_i)\, n(T_j)\, n(T_k)$ contains the factor r for any (branching) vertex $v \in V(T)$. Consequently, using Theorem 2 he obtained that $W(T) \equiv \binom{n+1}{3} \pmod r$. In addition, he proved that $W(T) \equiv \binom{n+1}{3} \pmod{2r}$ in the case when r is even. As a corollary, we obtain the main result of [12]:

Theorem 5 (Lin). *If T and T' are two trees on the same number of vertices, both with P_r-factors, then*

$$W(T) \equiv W(T') \pmod{r} \quad \textit{for odd } r,$$

and

$$W(T) \equiv W(T') \pmod{2r} \quad \textit{for even } r.$$

Recently Gutman, Xu and Liu [6] showed that the first congruence in the above result is a special case of a much more general result on the Szeged index and as a consequence for the Wiener index they obtained the following result (compare with Corollary 13).

Theorem 6 (Gutman, Xu and Liu). *Let Γ_0 be the union of connected graphs $G_1, G_2, \ldots, G_p$, $p \geq 2$, each of order $r \geq 2$, all blocks of which are complete graphs. Denote by Γ a graph obtained by adding $p-1$ edges to Γ_0 so that the resulting graph is connected. Then*

$$W(\Gamma) \equiv \sum_{i=1}^{p} W(G_i) \pmod{r}.$$

Here we give a straightforward argument for both congruences from Theorem 5, and in the next two sections we describe how the idea of that proof can be generalized to show that the Wiener index is in the same congruence class modulo r (or $2r$ when r is even) for larger families $\mathcal{G} = \mathcal{G}(\mathcal{H}, \mathcal{F})$ of graphs with a tree-like structure, whose "vertices" are graphs from a given set $\mathcal{H}$ all of congruent order, and "edges" are from a given set of graphs $\mathcal{F}$ also all of congruent order (see the beginning of Section 2 for precise definitions of these notions).

Proof of Theorem 5. Let T be a tree on n vertices having a P_r-factor. For an edge $uv \in E(T)$, denote by T_u and T_v the connected components of $T - \{uv\}$, such that $u \in V(T_u)$ and $v \in V(T_v)$.

Let ij be an edge connecting vertices from different copies of P_r of the P_r-factor. Then $|V(T_i)| = ar$ and $|V(T_j)| = br$ for some integers a and b such that $(a+b)r = n$. Let T' be a tree obtained from T by replacing the edge ij by an edge $i'j$, where i' is a neighbour of i in T_i. Note that $W(T) = W(T_i) + W(T_j) + \sum d_T(x,y)$, and $W(T') = W(T_i) + W(T_j) + \sum d'_T(x,y)$, where the sum in both cases is taken over all $x \in V(T_i)$ and $y \in V(T_j)$. Observe that for $x \in T_i$ the difference between $d_T(x,i')$ and $d_T(x,i)$ is either 1 or -1. Let s be the number of vertices in $V(T_i)$ for which $d_T(x,i') - d_T(x,i) = 1$. We derive

$$\begin{aligned} W(T') - W(T) &= \sum_x \sum_y \Big(d_{T'}(x,y) - d_T(x,y) \Big) = \sum_x \sum_y \Big(d_T(x,i') - d_T(x,i) \Big) \\ &= |T_j| \sum_x \Big(d_T(x,i') - d_T(x,i) \Big) \\ &= br(s - (ar - s)) = 2brs - abr^2, \end{aligned}$$

where $x \in V(T_i)$ and $y \in V(T_j)$.

Hence $W(T') \equiv W(T) \pmod{r}$, and clearly $W(T') \equiv W(T) \pmod{2r}$ in the case when r is even. It is left to the reader to observe that by replacing edges sequentially as described above, one can always construct a path on n vertices which is in the same congruence class modulo r as T. Hence the result follows. $\square$

The generalizations of the above proof are given in Theorems 10 and 17. From them we infer some interesting consequences, for example Corollary 11, where $\mathcal{H}$ is composed of cycles, and $\mathcal{F}$ of paths. In Corollaries 12 and 18, $\mathcal{H}$ is a set of trees and $\mathcal{F}$ is composed of edges (paths of length 1). When all graphs of $\mathcal{H}$ are isomorphic to a given tree T and $\mathcal{F}$ contains only edges, (i.e., we consider graphs with T-factors), we get Corollaries 14 and 20. And, as a particular case, when this prescribed tree T is a path, we obtain Lin's Theorem.

2 Congruence modulo r

In this section we generalize the first part of Theorem 5. However, the notation introduced here will be used also in the next section.

Let r and t be integers, $r \geq 2$ and $0 \leq t < r$. We will choose three things. First, let $\mathcal{H} = \{H_1, H_2, \ldots, H_\ell\}$ be a set of connected graphs, such that for all i, $1 \leq i \leq \ell$, we have $|V(H_i)| \equiv r - t \pmod{r}$. Second, let $\mathcal{F} = \{F_1, F_2, \ldots, F_{\ell-1}\}$ be a set of connected graphs, such that for all j, $1 \leq j \leq \ell - 1$, we have $|V(F_j)| \equiv t + 2 \pmod{r}$. Third, for every F_j, choose vertices $v_j^1, v_j^2 \in V(F_j)$ (we remark that chosen vertices v_j^1 and v_j^2 are not necessarily distinct). Now, when these three items are chosen, namely $\mathcal{H}$, $\mathcal{F}$ and pairs of vertices in graphs of $\mathcal{F}$, identify the vertices v_j^i, $1 \leq i \leq 2$ and $1 \leq j \leq \ell$, with some vertices of $H_1 \cup H_2 \cup \cdots \cup H_\ell$ so that each v_j^i will be identified with exactly one vertex of $H_1 \cup H_2 \cup \cdots \cup H_\ell$ (if $v_j^1 = v_j^2$ then this vertex will be identified with two vertices of $H_1 \cup H_2 \cup \cdots \cup H_\ell$). After this identification the resulting graph may be disconnected. Denote by $\mathcal{G} = \mathcal{G}(\mathcal{H}, \mathcal{F})$ the class of those graphs obtained by this identification process, which are connected.

In Fig. 1 we have one graph G of $\mathcal{G}$ for given parameters r, t and ℓ, and for given sets $\mathcal{H}$, $\mathcal{F}$ and $\{v_j^1, v_j^2\}_{j=1}^{\ell-1}$. The vertices of H_j's are depicted by full circles in Fig. 1 and the edges of H_i's are thick. Observe that $|V(H_1)| \equiv |V(H_2)| \equiv |V(H_3)| \equiv |V(H_4)| \equiv 7-3 \pmod 7$ and $|V(F_1)| \equiv |V(F_2)| \equiv |V(F_3)| \equiv 3+2 \pmod 7$.

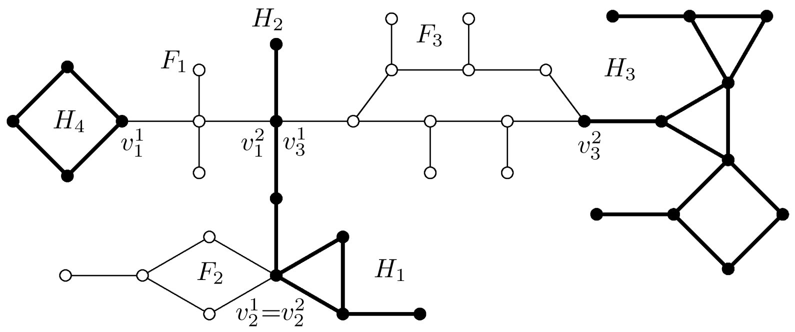

Figure 1: A graph of $\mathcal{G}$ for $r = 7$, $t = 3$, $\ell = 4$ and given H_i's, F_j's and v_j^k's.

In the definition above, there are ℓ graphs in $\mathcal{H}$, $\ell - 1$ graphs in $\mathcal{F}$, and each graph of $\mathcal{F}$ connects two graphs of $\mathcal{H}$. Since the resulting structures (graphs in $\mathcal{G}$) are connected, if we contract every H_i to a single vertex and we consider F_j's as edges joining pairs of these contracted vertices, then the resulting graph is a tree. In this way, $H_1, H_2, \ldots, H_\ell$ can be regarded as *supervertices*, $F_1, F_2, \ldots, F_{\ell-1}$ as *superedges*, and the corresponding graph is called an *associated supergraph*. For example, for the graph depicted in Fig. 1 the associated supergraph is the claw $K_{1,3}$ with central supervertex H_2 and pendant supervertices H_1, H_3 and H_4.

Now we define a representative graph $\Gamma_{\mathcal{G}}$ for $\mathcal{G}$ (recall that in $\Gamma_{\mathcal{G}}$ we fixed $\mathcal{H}$, $\mathcal{F}$ and $\{v_j^1, v_j^2\}_{j=1}^{\ell-1}$). For every i, $1 \leq i \leq \ell$, choose one vertex of $V(H_i)$ and denote it by u_i. Then $\Gamma_{\mathcal{G}}$ is obtained from $H_1 \cup \cdots \cup H_\ell \cup F_1 \cup \cdots \cup F_{\ell-1}$ by identifying v_i^1 with u_i and v_i^2 with u_{i+1}. Observe that the associated supergraph for $\Gamma_{\mathcal{G}}$ is a path of length $\ell - 1$ with the ordering of supervertices $(H_1, H_2, \ldots, H_\ell)$. Moreover, H_i is connected with H_{i+1} by the superedge F_i, $1 \leq i \leq \ell - 1$.

Roughly speaking, our main results state that it does not matter how we provide the identification, the Wiener index of all graphs in $\mathcal{G}$ is in the same congruence class modulo r. We obtain this by showing that every graph from $\mathcal{G}$ is in the same congruence class modulo r as $\Gamma_{\mathcal{G}}$.

First, we will consider the following operation: Let $G \in \mathcal{G}$. Choose j, $1 \leq j \leq \ell - 1$, and k, $1 \le k \le 2$. Assume that the vertex v_j^k of F_j was identified with a vertex, say u, of H_a. So detach v_j^k from this vertex. This will disconnect G to two components, say G^1 and G^2. Assume that $u \in V(G^1)$. Choose $u' \in V(H_1) \cup \cdots \cup V(H_\ell)$ such that $u' \in V(G^1)$, identify v_j^k with u' and denote the resulting graph by G'. If $u' \in V(H_b)$, then we denote this operation by $[H_a, F_j, H_b]$.

We show that the operation defined above preserves the modularity by r.

Lemma 7. *Let $G, G' \in \mathcal{G}$, where G' was obtained from G by the operation $[H_a, F_j, H_b]$ as described above. Then $W(G) \equiv W(G') \pmod r$.*

Proof. Due to the tree structure of G, the graphs G^1 and G^2 are connected and satisfy

$$|V(G^1)| \equiv r - t \pmod r \quad \text{and} \quad |V(G^2 - v_j^k)| \equiv 0 \pmod r.$$

However, the graph $G^2 - v_j^k$ may be disconnected. For this reason, denote $W_{-w}(G^2) = \sum d_{G^2}(u,v)$, where the sum is taken over all two-element subsets of $G^2 - w$. Since both $V(G)$ and $V(G')$ are disjoint unions of $V(G^1)$ and $V(G^2 - v_j^k)$, we have

$$\begin{aligned} W(G) &= W(G^1) + W_{-v_j^k}(G^2) + \sum d_G(x,y) \quad \text{and,} \\ W(G') &= W(G^1) + W_{-v_j^k}(G^2) + \sum d_{G'}(x,y), \end{aligned} \tag{1}$$

where the sums are taken over all $x \in V(G^1)$ and $y \in V(G^2 - v_j^k)$. Here all the shortest paths from x to y must contain v_j^k in both G and G'. Therefore, for a fixed $x \in V(G^1)$ there is $d_x \in \mathbb{Z}$ (where $d_x = d_{G'}(x,u') - d_G(x,u)$), such that for an arbitrary $y \in V(G^2 - v_j^k)$ we have $d_{G'}(x,y) = d_G(x,y) + d_x$. Since $|V(G^2 - v_j^k)| \equiv 0 \pmod r$, we have

$$\sum_x \Big(\sum_y d_{G'}(x,y) \Big) = \sum_x \Big(\sum_y \big(d_G(x,y) + d_x \big) \Big) \equiv \sum_x \Big(\sum_y d_G(x,y) \Big) \pmod r,$$

where $x \in V(G^1)$ and $y \in V(G^2 - v_j^k)$. By (1), $W(G) \equiv W(G') \pmod r$. $\square$

Let $G \in \mathcal{G}$ and $1 \le j \le \ell - 1$. Assume that in the process of obtaining G, v_j^1 was identified with $u_a \in V(H_a)$ and v_j^2 was identified with $u_b \in V(H_b)$. Now detach u_a from v_j^1 and detach u_b from v_j^2, identify u_a with v_j^2 and identify u_b with v_j^1, and denote the resulting graph by G'. We say that G' was obtained from G by *reversing* the superedge F_j.

Let $G \in \mathcal{G}$. In the next lemma we show that by a sequence of operations $[H_a, F_j, H_b]$, the graph G can be transformed to a graph $G^\times$ which is either identical with $\Gamma_\mathcal{G}$, or can be obtained from $\Gamma_\mathcal{G}$ by reversing of some superedges F_j.

Lemma 8. *Let $G \in \mathcal{G}$. By a sequence of operations $[H_a, F_j, H_b]$ the graph G can be transformed to a graph from $\mathcal{G}$, denote it by $G^\times$, such that the associated supergraph for $G^\times$ is a path with F_i connecting H_i with H_{i+1}, $1 \le i \le \ell - 1$, where one of v_i^1 and v_i^2 is identified with u_i, while the other vertex is identified with u_{i+1}.*

Proof. Let $G \in \mathcal{G}$. First we transform G to G', where the associated supergraph for G' is the path $(H_1, H_2, \dots, H_\ell)$.

Assume that we already have a subpath $(H_1, H_2, \dots, H_i)$ in the associated supergraph S. Due to the tree structure, there is a unique path from H_i to H_{i+1} in S. Denote by F_a the last edge of this path and denote by H_b the end vertex of F_a which is different from H_{i+1}. Consequently, provide the operation $[H_b, F_a, H_i]$. Observe that after this operation we have the subpath $(H_1, H_2, \dots, H_i, H_{i+1})$ in the associated supergraph. Hence, repeating this procedure we obtain the required graph $G' \in \mathcal{G}$.

Now we transform G' to G'', where the associated supergraph for G'' is the path $(H_1, H_2, \dots, H_\ell)$, analogously as in the associated supergraph for G', but in G'' the supervertices H_i and H_{i+1} are connected by the superedge F_i.

Assume that we already have a subpath with superedges $(H_1, F_1, H_2, F_2, \dots \dots, F_{i-1}, H_i)$ in the associated supergraph S. Suppose that F_i does not connect H_i with H_{i+1} in S, but instead it connects H_j with H_{j+1} for some j, $j > i$. For every k, $i \le k < j$, denote by $F_{k'}$ the superedge connecting H_k with H_{k+1} in S (see Fig. 2). Now provide the operation $[H_j, F_i, H_i]$. This attaches F_i to H_i (see Fig. 2). Consequently, provide $[H_{j-1}, F_{(j-1)'}, H_{j+1}]$, $[H_{j-2}, F_{(j-2)'}, H_j]$, $\dots$, $[H_i, F_{i'}, H_{i+2}]$. Finally, provide $[H_{j+1}, F_i, H_{i+1}]$ (see Fig. 2). After these steps we have a subpath with edges $(H_1, F_1, H_2, F_2, \dots, F_{i-1}, H_i, F_i, H_{i+1})$ in the associated supergraph. Hence, repeating this procedure we obtain the required graph $G'' \in \mathcal{G}$.

Finally, providing $[H_i, F_i, H_i]$ we can attach the corresponding vertex v_i^j to u_i, and providing $[H_{i+1,}F_i, H_{i+1}]$ we can attach v_i^{3-j} to u_{i+1}. Hence, repeating this procedure we can transform G'' to a graph $G^\times$, such that the associated supergraph for $G^\times$ is a path $(H_1, F_1, H_2, F_2, \dots, F_{\ell-1}, H_\ell)$, where one of v_j^1 and v_j^2 is identified with u_i, while the pther vertex is identified with u_{i+1}. $\square$

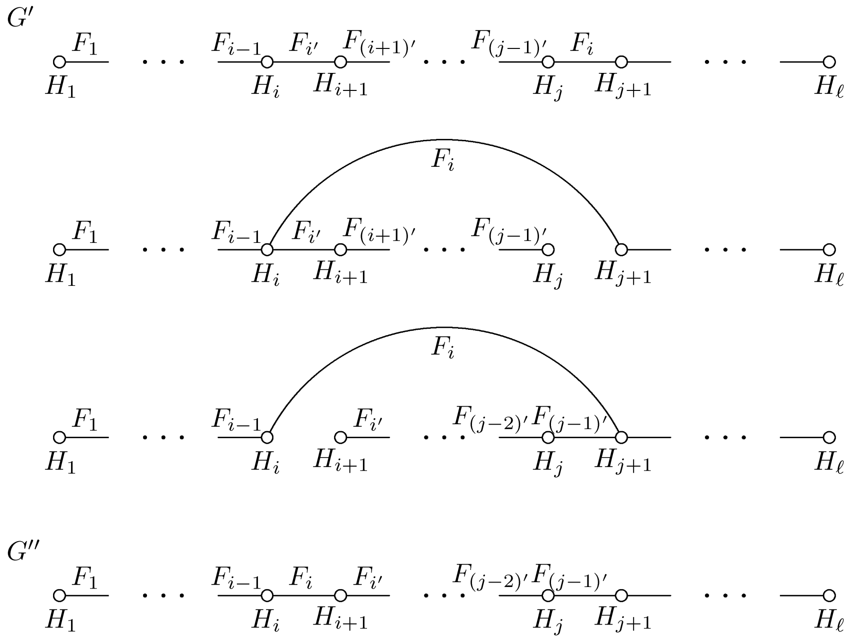

Figure 2: Sequence of supergraphs during the process of obtaining G'' from G'.

In the next lemma we show that for the graph $G^\times$ from Lemma 8 it holds $W(G^\times) \equiv W(\Gamma_{\mathcal{G}}) \pmod{r}$.

Lemma 9. *Let $G \in \mathcal{G}$ and $1 \leq j \leq \ell - 1$. Let G' be obtained from G by reversing the superedge F_j. Then $W(G) \equiv W(G') \pmod{r}$.*

PROOF. Assume that v_j^1 was identified with $u_a \in V(H_a)$ and v_j^2 was identified with $u_b \in V(H_b)$ in G. Let G^1 and G^2 be the connected components obtained after detaching the vertex v_j^1 from u_a and v_j^2 from u_b, such that $u_a \in V(G^1)$ and $u_b \in V(G^2)$.

Having two vertices of $V(G)$, their distance in G differs from that in G' only if one of the vertices is in $F_j - \{v_j^1, v_j^2\}$ and the other is in $V(G^1) \cup V(G^2)$. Hence,

$$W(G) - W(G') = \sum \Big(d_G(x,y) - d_{G'}(x,y)\Big) + \sum \Big(d_G(y,z) - d_{G'}(y,z)\Big),$$

where the first sum is taken over all $x \in V(G^1)$ and $y \in V(F_j - \{v_j^1, v_j^2\})$, while the second sum is taken over all $y \in V(F_j - \{v_j^1, v_j^2\})$ and $z \in V(G^2)$. Since all the paths from x to y (from y to z, respectively) must pass through u_a (through u_b, respectively), we have

$$\begin{aligned} W(G) - W(G') &= |V(G^1)| \sum \Big(d_G(u_a,y) - d_{G'}(u_a,y)\Big) \\ &+ |V(G^2)| \sum \Big(d_G(y,u_b) - d_{G'}(y,u_b)\Big), \end{aligned}$$

where the sums are taken over all $y \in V(F_j - \{v_j^1, v_j^2\})$. Since G' was obtained from G

by reversing F_j, we have $d_G(u_a, y) = d_{F_j}(v_j^1, y) = d_{G'}(y, u_b)$ and $d_{G'}(u_a, y) = d_{F_j}(y, v_j^2) = d_G(y, u_b)$.

This yields

$$W(G) - W(G') = \Big(|V(G^1)| - |V(G^2)|\Big) \sum \Big(d_{F_j}(v_j^1, y) - d_{F_j}(y, v_j^2)\Big).$$

Since $|V(G^1)| \equiv |V(G^2)| \equiv r - t \pmod{r}$, we have $W(G) \equiv W(G') \pmod{r}$, as required.

□

By Lemmas 7, 8 and 9, for every $G \in \mathcal{G}$ it holds $W(G) \equiv W(\Gamma_{\mathcal{G}}) \pmod{r}$. Hence, we have the main result of this section:

Theorem 10. *Let $G_1, G_2 \in \mathcal{G}$. Then $W(G_1) \equiv W(G_2) \pmod{r}$.*

Probably the most interesting case appears when all the superedges are paths. This yields the following corollaries of Theorem 10:

Corollary 11. *Let $H_1, H_2, \ldots, H_\ell$ be a collection of cycles with lengths congruent to $r - t \pmod{r}$. Further, let $F_1, F_2, \ldots, F_{\ell-1}$ be a collection of paths of lengths congruent to $t + 1 \pmod{r}$. Finally, let $\mathcal{G}$ be a class of connected graphs obtained by identifying each end vertex of F_j's with exactly one vertex of $H_1 \cup H_2 \cup \cdots \cup H_\ell$ so that the resulting graph is connected. Then for every $G_1, G_2 \in \mathcal{G}$ we have $W(G_1) \equiv W(G_2) \pmod{r}$.*

Corollary 12. *Let $H_1, H_2, \ldots, H_\ell$ be a collection of trees with numbers of vertices congruent to $r - t \pmod{r}$. Further, let $F_1, F_2, \ldots, F_{\ell-1}$ be a collection of paths of lengths congruent to $t + 1 \pmod{r}$. Finally, let $\mathcal{G}$ be a class of connected graphs obtained by identifying each end vertex of F_j's with exactly one vertex of $H_1 \cup H_2 \cup \cdots \cup H_\ell$ so that the resulting graph is connected. Then for every $G_1, G_2 \in \mathcal{G}$ we have $W(G_1) \equiv W(G_2) \pmod{r}$.*

Another interesting case appears when all the superedges are simple edges.

Corollary 13. *Let $H_1, H_2, \ldots, H_\ell$ be a collection of connected graphs with numbers of vertices congruent to $0 \pmod{r}$. Let $\mathcal{G}$ be a class of connected graphs obtained by adding $\ell - 1$ edges to $H_1 \cup H_2 \cup \cdots \cup H_\ell$. Then for every $G_1, G_2 \in \mathcal{G}$ we have $W(G_1) \equiv W(G_2) \pmod{r}$.*

For graphs having T-factors we have the following corollary, which also follows from Theorem 6.

Corollary 14. *Let T be a tree with r vertices. Further, let G_1 and G_2 be trees with the same number of vertices, both having a T-factor. Then $W(G_1) \equiv W(G_2) \pmod{r}$.*

We remark that an instance of Corollary 14 when T is a path on r vertices, r being odd, is exactly the first part of Theorem 5.

3 Congruence modulo $2r$ when r is even

In this section we generalize the second part of Theorem 5. However, there are some limitations in this case.

First, an analogue of Theorem 10 does not necessarily hold if some graph of $\mathcal{H}$ is not a tree even if $t = 0$ and $\ell = 2$. To demonstrate this, let r be even, $r \geq 4$, $\ell = 2$, $t = 0$, H_1 is a path on r vertices, H_2 is a cycle of length $r - 1$ with one pendant vertex attached, F_1 is an edge, and v_1^1 and v_1^2 are the end vertices of F_1. Denote by u the vertex of degree 3 in H_2. In G the edge F_1 joins an end vertex of H_1 with u, while in G' the edge F_1 joins an end vertex of H_1 with a neighbour of u on the cycle, see Fig. 3 for the case $r = 4$. Then $W(G') = W(G) + r$, and so $W(G') \not\equiv W(G) \pmod{2r}$. (For the case $r = 2$ it suffices to consider the same graph as for $r = 6$.)

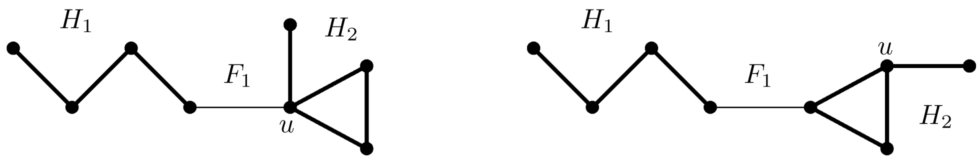

Figure 3: The graphs G and G' demonstrating that an analogue of Theorem 10 is not true if some graph in $\mathcal{H}$ is not a tree.

Next, an analogue of Theorem 10 does not necessarily hold if $t > 0$ even if $\ell = 2$ and H_1, H_2 and F_1 are all paths. To demonstrate this, let r be even, $r \geq 4$, $\ell = 2$, $t = 1$, H_1 and H_2 are paths on $r - 1$ vertices, F_1 is a path on 3 vertices, and v_1^1 and v_1^2 are different end vertices of F_1. Denote by u_1 and u_2 the central vertices of H_1 and H_2, respectively. In G the end vertices of F_1 are identified with u_1 and u_2, while in G' the end vertices of F_1 are identified with u_1 and a neighbour of u_2, see Fig. 4 for the case $r = 4$. Then

$W(G') = W(G) + r$, and so $W(G') \not\equiv W(G) \pmod{2r}$. (For the case $r = 2$ it suffices to consider the same graph as for $r = 6$.)

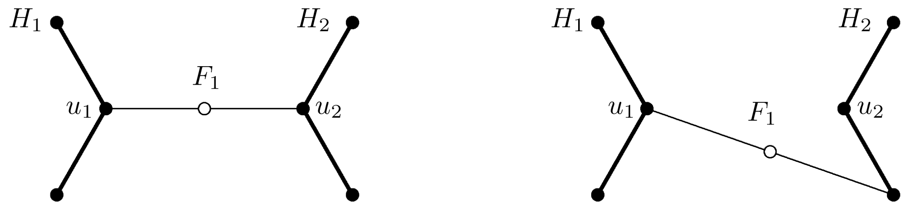

Figure 4: The graphs G and G' demonstrating that an analogue of Theorem 10 is not true if $t > 0$.

In the light of the above examples we restrict ourselves to trees and to $t = 0$. Hence, let r be an even number, $r \geq 2$. Analogously as in Section 2, we choose three things. First, let $\mathcal{H} = \{H_1, H_2, \ldots, H_\ell\}$ be a set of trees, such that for all i, $1 \leq i \leq \ell$, we have $|V(H_i)| \equiv r \pmod{r}$. Second, let $\mathcal{F} = \{F_1, F_2, \ldots, F_{\ell-1}\}$ be a set of trees, such that for all j, $1 \leq j \leq \ell - 1$, we have $|V(F_j)| \equiv 2 \pmod{r}$. Third, for every F_j, choose vertices $v_j^1, v_j^2 \in V(F_j)$ (we remark that chosen vertices v_j^1 and v_j^2 are not necessarily distinct). Now, when these three items (namely $\mathcal{H}$, $\mathcal{F}$ and $\{v_j^1, v_j^2\}_{j=1}^{\ell-1}$) are chosen, identify the vertices v_j^i, $1 \leq i \leq 2$ and $1 \leq j \leq \ell$, with some vertices of $H_1 \cup H_2 \cup \cdots \cup H_\ell$ so that each v_j^i will be identified with exactly one vertex of $H_1 \cup H_2 \cup \cdots \cup H_\ell$ (if $v_j^1 = v_j^2$ then this vertex will be identified with two vertices of $H_1 \cup H_2 \cup \cdots \cup H_\ell$). Denote by $\mathcal{G}^T = \mathcal{G}^T(\mathcal{H}, \mathcal{F})$ the class of those graphs obtained by this identification process, which are connected.

We prove that the Wiener index of all graphs in $\mathcal{G}^T$ belongs to the same congruence class modulo $2r$. For this, we improve Lemmas 7 and 9. We start with Lemma 7.

Lemma 15. *Let r be even and $G, G' \in \mathcal{G}^T$, where G' was obtained from G by the operation $[H_a, F_j, H_b]$. Then $W(G) \equiv W(G') \pmod{2r}$.*

Proof. Assume that v_j^k is identified with $u \in V(H_a)$ in G and it is identified with $u' \in V(H_b)$ in G'. Further, denote by G^1 and G^2 the two components which appear after detaching v_j^k from u in G. Assume that $u \in V(G^1)$. Then the notation is identical with that in the proof of Lemma 7. Moreover, $|V(G^1)| = ar$ and $|V(G^2 - v_j^k)| = br$ for some integers a and b such that $(a + b)r = |V(G)|$. Let $u = z_0, z_1, \ldots, z_f = u'$ be a path in G^1. Denote by G_{z_i} a graph obtained from $G^1 \cup G^2$ by identifying z_i with v_j^k. Then $G_{z_0} = G$ and $G_{z_f} = G'$. Now fix i, $0 \leq i \leq f - 1$. We prove that $W(G_{z_{i+1}}) \equiv W(G_{z_i}) \pmod{2r}$.

First, analogously as in the proof of Lemma 7 we have the following analogue of (1):

$$W(G_{z_{i+1}}) - W(G_{z_i}) = \sum \Big(d_{G_{z_{i+1}}}(x,y) - d_{G_{z_i}}(x,y) \Big),$$

where the sum is taken over all $x \in V(G^1)$ and $y \in V(G^2 - v_j^k)$. A shortest path from $x \in V(G^1)$ to $y \in V(G^2 - v_j^k)$ contains $z_i(=v_j^k)$ in G_{z_i} and $z_{i+1}(=v_j^k)$ in $G_{z_{i+1}}$. Since both G_{z_i} and $G_{z_{i+1}}$ are trees, the difference $d_{G_{z_{i+1}}}(x,y) - d_{G_{z_i}}(x,y) = d_{G_{z_{i+1}}}(x, z_{i+1}) - d_{G_{z_i}}(x, z_i)$ is either 1 or -1. Let s be the number of vertices x in $V(G^1)$ for which $d_{G_{z_{i+1}}}(x, z_{i+1}) - d_{G_{z_i}}(x, z_i) = 1$. Then

$$\begin{aligned} W(G_{z_{i+1}}) - W(G_{z_i}) &= \sum_x \sum_y \Big(d_{G_{z_{i+1}}}(x,y) - d_{G_{z_i}}(x,y) \Big) \\ &= br \sum_x \Big(d_{G_{z_{i+1}}}(x, z_{i+1}) - d_{G_{z_i}}(x, z_i) \Big) \\ &= br(s - (ar - s)) = 2brs - abr^2, \end{aligned}$$

where $x \in V(G^1)$ and $y \in V(G^2 - v_j^k)$. Since r is even, we conclude $W(G_{z_{i+1}}) \equiv W(G_{z_i}) \pmod{2r}$.

In this way we get $W(G_{z_0}) \equiv W(G_{z_1}) \equiv W(G_{z_2}) \equiv \cdots \equiv W(G_{z_f}) \pmod{2r}$, and hence $W(G) \equiv W(G') \pmod{2r}$. □

Now we prove an analogue of Lemma 9.

Lemma 16. *Let r be even, $G \in \mathcal{G}^T$ and $1 \leq j \leq \ell - 1$. Let G' be obtained from G by reversing the superedge F_j. Then $W(G) \equiv W(G') \pmod{2r}$.*

Proof. Assume that v_j^1 was identified with $u_a \in V(H_a)$ and v_j^2 was identified with $u_b \in V(H_b)$ in G. Let G^1 and G^2 be the connected components obtained after detaching the vertex v_j^1 from u_a and v_j^2 from u_b, such that $u_a \in V(G^1)$ and $u_b \in V(G^2)$. Then analogously as in the proof of Lemma 9 we obtain

$$W(G) - W(G') = \Big(|V(G^1)| - |V(G^2)| \Big) \sum \Big(d_{F_j}(v_j^1, y) - d_{F_j}(y, v_j^2) \Big), \tag{2}$$

where the sum is taken over all $y \in V(F_j - \{v_j^1, v_j^2\})$.

Let $y \in V(F_j - \{v_j^1, v_j^2\})$. Recall that F_j is a tree. Thus, if $d_{F_j}(v_j^1, v_j^2)$ is even, then $d_{F_j}(v_j^1, y) - d_{F_j}(y, v_j^2)$ is also even. On the other hand if $d_{F_j}(v_j^1, v_j^2)$ is odd, then $d_{F_j}(v_j^1, y) - d_{F_j}(y, v_j^2)$ is also odd. Since $|V(F_j)| \equiv 2 \pmod{r}$, there is even number of vertices in $V(F_j - \{v_j^1, v_j^2\})$, and so the sum in (2) is even. Finally, from $|V(G^1)| \equiv |V(G^2)| \equiv 0 \pmod{r}$, we conclude $W(G) \equiv W(G') \pmod{2r}$. $\square$

By Lemmas 8, 15 and 16, for every $G \in \mathcal{G}^T$ it holds $W(G) \equiv W(\Gamma_{\mathcal{G}^T}) \pmod{2r}$. Hence, we obtain the main result of this section:

Theorem 17. *Let r be even and $G_1, G_2 \in \mathcal{G}^T$. Then $W(G_1) \equiv W(G_2) \pmod{2r}$.*

Analogously as in the previous section, we present some corollaries of Theorem 17. If all the superedges are paths, we obtain:

Corollary 18. *Let r be even and let $H_1, H_2, \ldots, H_\ell$ be a collection of trees which numbers of vertices are congruent to $0 \pmod{r}$. Further, let $F_1, F_2, \ldots, F_{\ell-1}$ be a collection of paths of lengths congruent to $1 \pmod{r}$. Finally, let $\mathcal{G}$ be a class of connected graphs obtained by identifying each end vertex of F_j's with exactly one vertex of $H_1 \cup H_2 \cup \cdots \cup H_\ell$ so that the resulting graph is connected. Then for every $G_1, G_2 \in \mathcal{G}$ we have $W(G_1) \equiv W(G_2) \pmod{2r}$.*

Another interesting case appears when all the superedges are simple edges.

Corollary 19. *Let r be even and let $H_1, H_2, \ldots, H_\ell$ be a collection of trees which numbers of vertices are congruent to $0 \pmod{r}$. Let $\mathcal{G}$ be a class of connected graphs obtained by adding $\ell - 1$ edges to $H_1 \cup H_2 \cup \cdots \cup H_\ell$. Then for every $G_1, G_2 \in \mathcal{G}$ we have $W(G_1) \equiv W(G_2) \pmod{2r}$.*

For graphs having T-factors we have the following corollary.

Corollary 20. *Let r be even and let T be a tree with r vertices. Further, let G_1 and G_2 be trees with the same number of vertices, both having a T-factor. Then $W(G_1) \equiv W(G_2) \pmod{2r}$.*

We remark that an instance of Corollary 20 when T is a path on r vertices, r being even, is exactly the second part of Theorem 5.

Acknowledgement. The first two authors acknowledge partial support by Slovak research grants VEGA 1/0065/13, APVV-0223-10, the APVV support as part of the EUROCORES Programme EUROGIGA, project GREGAS, financed by the European Science Foundation. The second, third and fourth author acknowledge partial support by

Slovenian research agency ARRS, program no. P1-00383, project no. L1-4292, and Creative Core FISNM 3330-13-500033. The authors would like to thank also the anonymous referees for useful comments.

References

[1] V. K. Agrawal, S. Bano, K. C. Mathur, P. V. Khadikar, Novel application of Wiener vis-à-vis Szeged indices: Antitubercular activities of quinolones, *Proc. Indian Acad. Sci. (Chem. Sci.)* **112** (2000) 137–146.

[2] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.

[3] J. K. Doyle, J. E. Graver, Mean distance in a graph, *Discrete Math.* **17** (1977) 147–154.

[4] R. C. Entringer, Distance in graphs: Trees, *J. Comb. Math. Comb. Comput.* **24** (1997) 65–84.

[5] I. Gutman, A new method for the calculation of the Wiener number of acyclic molecules, *J. Mol. Struct. (Theochem)* **285** (1993) 137–142.

[6] I. Gutman, K. Xu, M. Liu, A Congruence Relation for Wiener and Szeged Indices, *Filomat*, in press.

[7] I. Gutman, O. E. Polansky, Mathematical Concepts in Organic Chemistry, *Springer, Berlin* (1986) p. 127.

[8] I. Gutman, D. H. Rouvray, A new theorem for the Wiener molecular branching index of trees with perfect matchings, *Comput. Chem.* **14** (1990) 29–32.

[9] I. Gutman, R. Škrekovski, Vertex version of the Wiener theorem, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 295–300.

[10] I. Gutman, Y. N. Yeh, S. L. Lee, J. C. Chen, Wiener numbers of dendrimers, *MATCH Commun. Math. Comput. Chem.* **30** (1994) 103–115.

[11] I. Gutman, Y. N. Yeh, S. L. Lee, Y. L. Luo, Some recent results in the theory of the Wiener number, *Indian J. Chem.* **32A** (1993) 651–661.

[12] H. Lin, A congruence relation for the Wiener index of trees with path factors, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 575–582.

[13] N. Trinajstić, *Chemical Graph Theory, Second Edition,* CRC Press, Boca Raton, Florida, February 1992.

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

[15] K. Xu, M. Liu, K. C. Das, I. Gutman, B. Furtula A survey on graphs extremal with respect to distance-based topolgical indices, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 461–508.