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TREES AND THEIR QUADRATIC LINE GRAPHS HAVING THE SAME WIENER INDEX*

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Abstract

The Wiener index is a topological index introduced as a structural descriptor for molecular graphs of alkanes, that are trees with vertex degrees at most four (chemical trees). It is the sum of distances between all pairs of vertices in a graph. The line graph $L(G)$ of a graph G has the vertex set $V(L(G)) = E(G)$ and two distinct vertices of $L(G)$ are adjacent if the corresponding edges of G have a common endvertex. It is known that the Wiener index of a tree and of its line graph are always distinct. Infinite families of chemical trees T with the property $W(T) = W(L(L(T)))$ are presented.

1. Introduction

The Wiener index is a well-known distance-based topological index introduced in 1947 as structural descriptor for acyclic organic molecules [1]. It is the sum of distances between all unordered pairs of vertices of a graph G:

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

where $d(u, v)$ is the number of edges in a shortest path connecting the vertices u and v.

This graph invariant belongs to the molecular structure-descriptors, called topological indices, that are successfully used for the design of molecules with special properties,

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including pharmacologic and biological activity (see books [2–4] and selected reviews [5–8]). Mathematical properties of the Wiener index for some classes of chemical graphs are outlined in recent reviews [9–12].

The line graph $L(G)$ of a graph G has the vertex set $V(L(G)) = E(G)$ and two distinct vertices of the graph $L(G)$ are adjacent if the corresponding edges of G have a common endvertex. The concept of line graph has found various applications in chemical research. Parameters of a line graph have been applied for the evaluation of structural complexity of molecular graphs and for design of novel topological indices [13–15]. It has been shown that the Wiener index of a tree and its line graph are always distinct [16].

The iterated line graph, $L^n(G)$, is defined as $L^n(G) = L^{n-1}(L(G))$, where $L^0(G) = G$. The size of $L^n(G)$ rapidly increases reflecting the branching (and, therefore, complexity) of the initial graph. Invariants of iterated line graphs for acyclic molecular graphs have been used for the characterization of their branching and for establishing a partial order among isomeric structures [17].

A graph $L^2(G)$ is called the *quadratic line graph* of G. In this paper we deal with trees T satisfying the following equality

$$W(T) = W(L^2(T)). \tag{1}$$

The number of trees of order $n \le 17$ having this property has been reported in [11, 18]. In this paper, we shall construct infinite families of such trees.

2. Main result

Buckley established an exact relation between the Wiener index of a tree and of its line graph [16]. For a tree with $n \ge 2$ vertices,

$$W(L(T)) = W(T) - \binom{n}{2}.$$

This result immediately implies that there are no n-vertex trees, $n \ge 2$, having the property $W(T) = W(L(T))$.

Trees with property (1) have been found by inspection all trees of order $n \le 17$ [11, 18]. First, we extend data from [11]. Table 1 shows the number of such trees for $n \le 26$. Here t_n is the number of all n-vertex trees and w_n denotes the number of trees having property (1). Diagrams of all such trees for $n \le 15$ are shown in Figure 1. The Wiener index is indicated near every diagram.

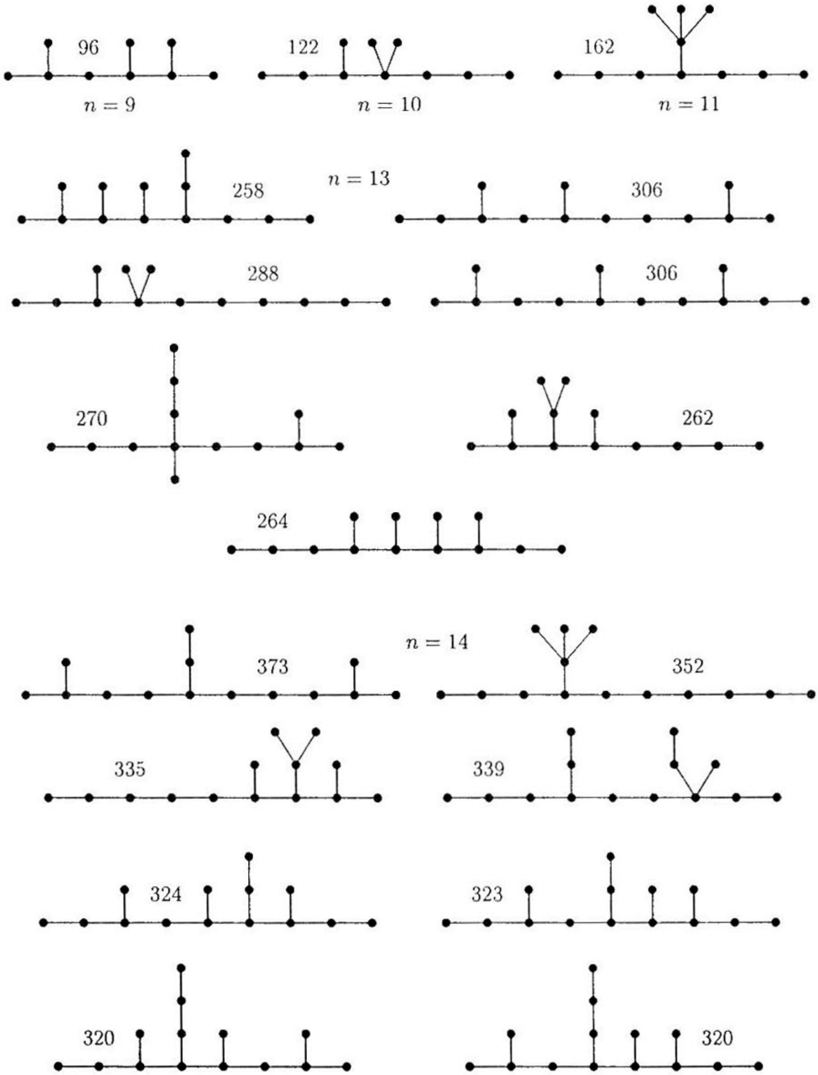

Figure 1. All trees of order $n \leq 15$ having $W(T) = W(L^2(T))$.

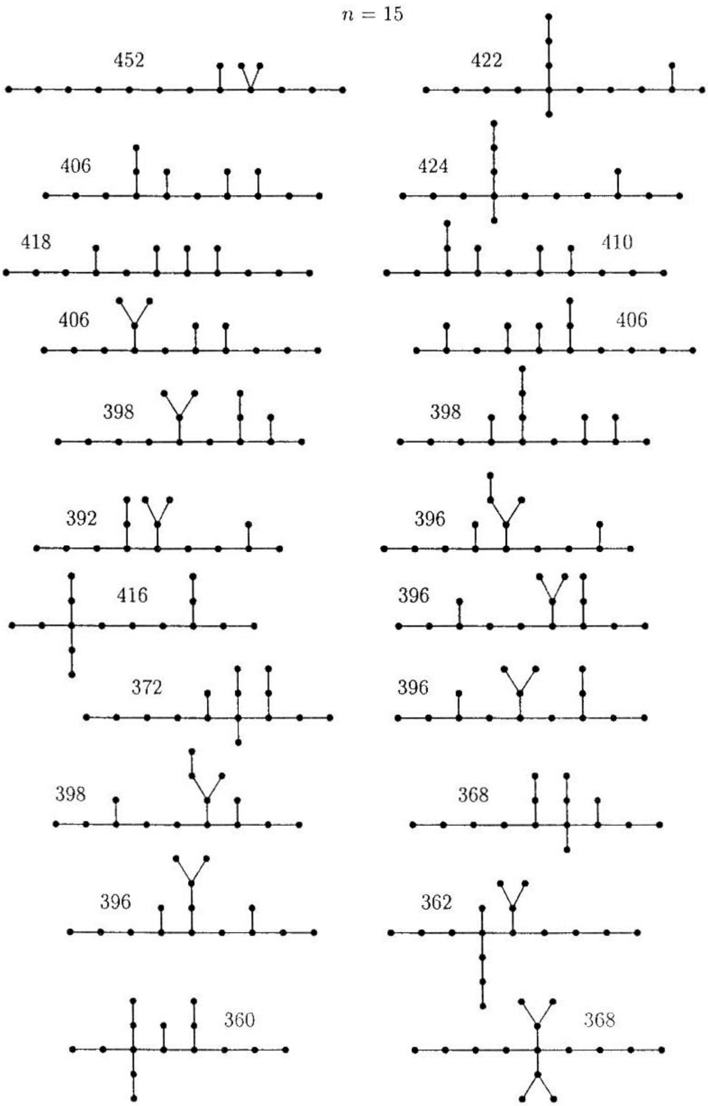

Figure 1. Continue.

Table 1: The number of trees of order n having property(1).

n	t_n	w_n	a_n	l_n	c_n	n	t_n	w_n	a_n	l_n	c_n
9	47	1	0	0	1	18	123867	73	18	23	1
10	106	1	0	0	1	19	317955	204	50	63	4
11	235	1	0	1	0	20	823065	231	36	45	4
12	551	0	0	0	0	21	2144505	513	126	92	7
13	1301	7	1	2	4	22	5623756	576	190	60	7
14	3159	8	2	6	0	23	14828074	1520	469	145	12
15	7741	22	3	13	2	24	39299897	1715	450	99	8
16	19320	25	6	12	3	25	104636890	3763	1188	187	14
17	48629	66	13	27	5	26	279793450	4085	1514	121	4

It should be noted that almost all trees of order $n \leq 26$ with property (1) are chemical trees, *i.e.* their vertex degrees are at most four. For the first time, vertices of degree 5 appear in 19-vertex trees and the total number of non-chemical trees on $n \leq 26$ vertices is equal to 41. The above data leads to the following natural question: does there exist an infinite family of trees having property (1)? We answer this question in affirmative.

Theorem. *There exist infinite families of trees T satisfying equality $W(T) = W(L^2(T))$.*

In order to prove this result, we construct several families of trees in question. They are chemical trees and belong to specific classes of trees known in graph theory as lobsters and caterpillars. A tree is a *caterpillar* if the removal of all its endvertices results in a path. A tree is a *lobster* if the removal of all its endvertices results in a caterpillar. Asymmetric trees have the identity group of automorphisms. Table 1 shows the numbers of asymmetric trees (a_n), caterpillars (c_n) and lobsters (l_n) that are not caterpillars with property (1).

3. Auxiliary results

The distance of a vertex v, $d_T(v)$, is the sum of distances between v and all other vertices of T, *i.e.* $d_T(v) = \sum_{u \in V(T)} d_T(v, u)$. Then the Wiener index can be rewritten as

$$W(T) = \frac{1}{2} \sum_{v \in V(T)} d_T(v).$$

The n-vertex path P_n has maximal Wiener index among all trees on n vertices [3, 19]

$$W(P_n) = \binom{n+1}{3}$$

and the distance of its endvertex is equal to $d_{P_n}(v) = n(n-1)/2$.

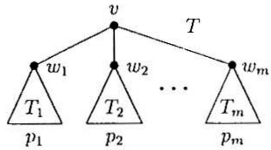

Figure 2. Branching vertex v of a tree T.

In order to calculate the Wiener index for trees and their line graphs, we use two well-known formulas.

A vertex v is said to be a branching vertex of a tree T if $\deg(v) \geq 3$. Denote by $B(T)$ the set of all branching vertices of T. Let $T_1, T_2, \ldots, T_m$ be trees with disjoint vertex sets and orders $p_1, p_2, \ldots, p_m$, $m \geq 2$, and $w_i \in V(T_i)$ for $i = 1, 2, \ldots, m$. In general, any tree T with more than two vertices can be represented as shown in Figure 2. Then the Wiener index of T can be calculated by Doyle–Graver formula [20, 21]

$$W(T) = \binom{n+1}{3} - \sum_{v \in B(T)} \sum_{1 \leq i < j < k \leq m} p_i \, p_j \, p_k \, . \tag{2}$$

The Wiener index of a graph can be expressed through the Wiener index of its subgraphs under some operations [22]. We need a simplest graph operation. Let a graph G be obtained from arbitrary graphs G_1 and G_2 of orders n_1 and n_2 by identifying vertices $v_1 \in V(G_1)$ and $v_2 \in V(G_2)$. Then

$$W(G) = W(G_1) + W(G_2) + (n_1 - 1)\, d_{G_2}(v_2) + (n_2 - 1)\, d_{G_1}(v_1). \tag{3}$$

Formulas (2) and (3) will be used for trees and their line graphs, respectively.

3. Lobsters

Consider the lobster T_k, $k \geq 0$, shown in Figure 3. It has $n_{T_k} = 3k^2 + 11$ vertices including two branching and five pendant vertices. Assume that the numbers of edges of the left and right paths attached to the vertex of degree 3 are equal to

$$x_k = 3(k^2 - k + 2)/2 \quad \text{and} \quad y_k = 3(k^2 + k + 2)/2.$$

Note that $x_{k+1} = y_k$ and $y_{k+1} = x_k + 6k + 3$ or $x_{k+1} = x_k + 3$ and $y_{k+1} = y_k + 3k + 3$. Obviously, a lobster has diameter $diam(T_k) = x_k + y_k = 3k^2 + 6$.

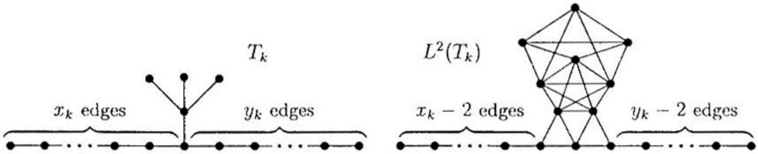

Figure 3. Lobster T_k and its quadratic line graph.

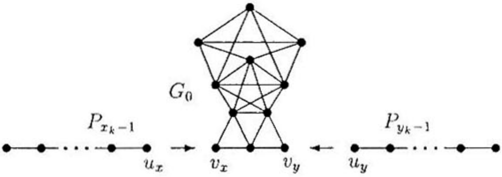

Figure 4. Graphs for constructing $L^2(T_k)$.

Since trees T_k have two branching points, it is convenient to apply formula (2) for calculating the Wiener index. Then

$$W(T_k) = \binom{3k^2+12}{3} - \big(4x_ky_k + 3(x_k+y_k+1)+1\big) = \frac{1}{2}\left(9k^6 + 81k^4 + 290k^2 + 324\right).$$

The quadratic line graph of T_k is depicted in Figure 3. To compute its Wiener index, we consequently join the paths P_{y_k-1} and P_{x_k-1} to the graph G_0 as shown in Figure 4. For the graph G_0, we have $d(v_y) = 21$ and $W(G_0) = 94$. Let the graph G_1 be obtained by identifying the vertices v_y of G_0 and u_y of P_{y_k-1}. By formula (3), we can write

$$\begin{aligned} W(G_1) &= W(G_0) + W(P_{y_k-1}) + \big(n_{P_{y_k-1}} - 1\big)d(v_y) + (n_{G_0} - 1)d(u_y) \\ &= 94 + \binom{y_k}{3} + 21(y_k-2) + 10(y_k-1)(y_k-2)/2 \\ &= \frac{1}{16}\left(9k^6 + 27k^5 + 243k^4 + 441k^3 + 1124k^2 + 908k + 2016\right). \end{aligned}$$

The quadratic line graph $L^2(T_k)$ can be constructed by identifying the vertices v_x of G_1 and u_x of P_{x_k-1}. It easy to see that $d_{G_1}(v_x) = y_k(y_k+1)/2 + 18$. Then

$$\begin{aligned} W(L^2(T_k)) &= W(G_1) + W(P_{x_k-1}) + (n_{P_{x_k-1}} - 1)d_{G_1}(v_x) + (n_{G_1} - 1)d(u_x) \\ &= W(G_1) + \binom{x_k}{3} + (x_k-2)\big(y_k(y_k+1)/2 + 18\big) \\ &\quad + (y_k+8)(x_k-1)(x_k-2)/2 \\ &= \frac{1}{2}\left(9k^6 + 81k^4 + 290k^2 + 324\right). \end{aligned}$$

Table 2: Lobsters T_k having property (1).

k	n_{T_k}	x_k	y_k	$diam$	W	k	n_{T_k}	x_k	y_k	$diam$	W
0	11	3	3	6	162	10	311	138	168	306	4919662
1	14	3	6	9	352	11	374	168	201	369	8582692
2	23	6	12	18	1678	12	443	201	237	438	14297778
3	38	12	21	33	8028	13	518	237	276	513	22902028
4	59	21	33	54	31282	14	599	276	318	594	35467342
5	86	33	48	81	99412	15	686	318	363	681	53340912
6	119	48	66	114	267822	16	779	363	411	774	78188962
7	158	66	87	153	633928	17	878	411	462	873	112043728
8	203	87	111	198	1354978	18	983	462	516	978	157353678
9	254	111	138	249	2669112	19	1094	516	573	1089	217036972

This proves that the constructed lobsters have property (1). Parameters for the first twenty lobsters are presented in Table 2.

By construction, a lobster with property (1), except the initial tree, has three symmetrical vertices from its brush. The initial lobster of order 11 has additionally two symmetrical paths of equal length $x_0 = y_0 = 3$ (see Figure 1).

4. Combs

Consider trees T_k, $k \geq 0$, shown in Figure 5. Such caterpillars are called *combs*. Every comb has four branching and six pendant vertices. We construct two families of combs of order $6k^2 \pm 2k + 13$ which start from the same initial tree of order 13 (see Figure 1).

Let combs T_k have $n_{T_k} = 6k^2 + 2k + 13$ vertices. Assume that the number of edges of long paths attached to the vertices of degree 3 is equal to

$$x_k = 3k^2 - 2k + 2 \quad \text{and} \quad y_k = 3k^2 + 4k + 3.$$

In this case, $x_{k+1} = y_k$ and $y_{k+1} = x_k + 12k + 8$. The diameter of T_k is equal to $diam(T_k) = 6k^2 + 2k + 8$. Applying Doyle–Graver formula (2), we can write

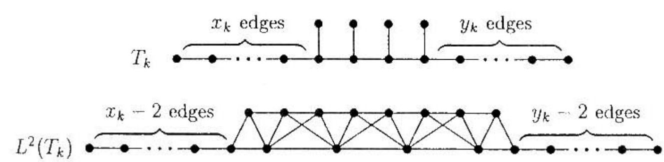

Figure 5. Comb T_k and its quadratic line graph.

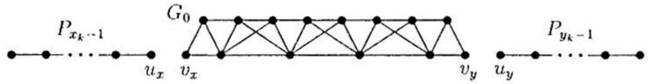

Figure 6. Graphs for constructing $L^2(T_k)$.

$$\begin{aligned}
W(T_k) &= \binom{6k^2+2k+14}{3} - \\
&\quad - \big(x_k(y_k+6)+(x_k+2)(y_k+4)+(x_k+4)(y_k+2)+(x_k+6)y_k\big) \\
&= \frac{1}{3}\left(108k^6+108k^5+630k^4+400k^3+1296k^2+410k+792\right). \qquad (4)
\end{aligned}$$

The quadratic line graph of T_k is depicted in Figure 5. It can be constructed from the graph G_0 and paths P_{x_k-1} and P_{y_k-1} (see Figure 6). For the graph G_0, we have $d(v_y) = 39$ and $W(G_0) = 211$.

Let the graph G_1 be obtained by identifying the vertices v_y of G_0 and u_y of P_{y_k-1}. By formula (3), we can write

$$\begin{aligned}
W(G_1) &= W(G_0) + W(P_{y_k-1}) + \big(n_{P_{y_k-1}}-1\big)d(v_y) + (n_{G_0}-1)d(u_y) \\
&= 211 + \binom{y_k}{3} + 39(y_k-2) + 13(y_k-1)(y_k-2)/2 \\
&= \frac{1}{6}\left(27k^6+108k^5+549k^4+1144k^3+1806k^2+1448k+1584\right).
\end{aligned}$$

To construct the quadratic line graph of T_k, one can identify the vertices v_x of G_1 and u_x of P_{x_k-1}. Since $d_{G_1}(v_x) = (y_k+3)(y_k+4)/2+24$, we have

$$\begin{aligned}
W(L^2(T_k)) &= W(G_1) + W(P_{x_k-1}) + (n_{P_{x_k-1}}-1)d_{G_1}(v_x) + (n_{G_1}-1)d(u_x) \\
&= W(G_1) + \binom{x_k}{3} + (x_k-2)\big((y_k+3)(y_k+4)/2+24\big) \\
&\quad + (y_k+11)(x_k-1)(x_k-2)/2 \\
&= \frac{1}{3}\left(108k^6+108k^5+630k^4+400k^3+1296k^2+410k+792\right). \qquad (5)
\end{aligned}$$

The obtained expressions (4) and (5) immediately imply property (1) for combs of the first family.

A tree T_k of the second comb family has the order $n_{T_k} = 6k^2-2k+13$ and

$$x_k = 3k^2-4k+3 \ \text{ and } \ y_k = 3k^2+2k+2.$$

Table 3: Combs T_k having property (1).

Family 1: $n_{T_k} = 6k^2 + 2k + 13$						Family 2: $n_{T_k} = 6k^2 - 2k + 13$					
k	n_{T_k}	x_k	y_k	$diam$	W	k	n_{T_k}	x_k	y_k	$diam$	W
0	13	2	3	8	264	0	13	3	2	8	264
1	21	3	10	16	1248	1	17	2	7	12	636
2	41	10	23	36	10148	2	33	7	18	28	5164
3	73	23	42	68	60164	3	61	18	35	56	34648
4	117	42	67	112	254336	4	101	35	58	96	162448
5	173	67	98	168	834664	5	153	58	87	148	574964
6	241	98	135	236	2277148	6	217	87	122	212	1658036
7	321	135	178	316	5412748	7	293	122	163	288	4109264
8	413	178	227	408	11574264	8	381	163	210	376	9076248
9	517	227	282	512	22769136	9	481	210	263	476	18320748
10	633	282	343	628	41878164	10	593	263	322	588	34408764

Notice that $x_{k+1} = y_k$ and $y_{k+1} = x_k + 12k + 4$. Applying formulas (2) and (3) to this tree, we obtain the Wiener index for combs of the second family:

$$W(T_k) = W(L^2(T_k)) = \frac{1}{3}\left(108k^6 - 108k^5 + 630k^4 - 400k^3 + 1296k^2 - 410k + 792\right).$$

One can see that the coefficients of the Wiener index for the both families differ only in sign. Indeed, let n_k^*, x_k^*, y_k^* and W_k^* be parameters of a comb from the first family. They are functions of k. It is easy to see that the corresponding comb of the second family has $n_k = n_{-k}^*$, $x_k = x_{-k}^*$ and $y_k = y_{-k}^*$. Since W_k is a symmetrical function with respect to x_k and y_k (see equality (4)), we have $W_k = W_{-k}^*$.

Parameters for the smallest combs of the obtained families are shown in Table 3. By construction, the presented combs with the property (1) are always asymmetrical trees.

4. Forks

The general structure of a *fork* is shown in Figure 7. Such a caterpillar has two branching and five pendant vertices. A fork is almost asymmetric tree; it has a unique two-element orbit of the automorphism group. Forks generate several infinite families of trees having property (1). We deal with two smallest families of forks for odd $m = 1, 3$ and for even $m = 4, 12$.

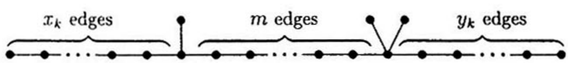

Figure 7. Structure of a fork T_k.

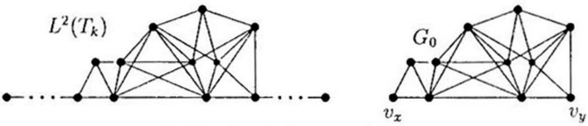

Figure 8. Quadratic line graph of fork T_k.

1. Let $m = 1$. Forks T_k of this class have $n_{T_k} = 4k^2 \pm k + 10$ vertices.

1a. Consider forks on $n_{T_k} = 4k^2 + k + 10$ vertices. First assume that k is even, $k \geq 0$. The number of edges of long terminal paths of the fork is equal to

$$x_k = (4k^2 - 3k + 4)/2 \quad \text{and} \quad y_k = (4k^2 + 5k + 6)/2.$$

For the next tree, $x_{k+2} = y_k + 4k + 4$ and $y_{k+2} = x_k + 12k + 14$. The diameter of T_k is equal to $diam(T_k) = x_k + y_k + 1 = 4k^2 + k + 6$.

By (2), we can write

$$\begin{aligned} W(T_k) &= \binom{4k^2+k+11}{3} - \big(x_k(y_k+3) + (x_k+2) + y_k + (x_k+2)y_k + (x_k+2)y_k\big) \\ &= \frac{1}{12}\left(128k^6 + 96k^5 + 840k^4 + 410k^3 + 2011k^2 + 502k + 1464\right). \end{aligned}$$

The quadratic line graph of T_k is depicted in Figure 8. It can be constructed from the graph G_0 by joining paths P_{x_k-1} and P_{y_k-1}. For the graph G_0, we have $d(v_y) = 19$ and $W(G_0) = 92$. Let the graph G_1 be obtained by identifying the vertices v_y of G_0 and u_y of P_{y_k-1}. By (3), we can write

$$\begin{aligned} W(G_1) &= W(G_0) + W(P_{y_k-1}) + \big(n_{P_{y_k-1}} - 1\big)d(v_y) + (n_{G_0} - 1)d(u_y) \\ &= 92 + \binom{y_k}{3} + 19(y_k - 2) + 10(y_k - 1)(y_k - 2)/2 \\ &= \frac{1}{48}\left(64k^6 + 240k^5 + 1452k^4 + 3005k^3 + 5240k^2 + 4300k + 5856\right). \end{aligned}$$

To construct the quadratic line graph $L^2(T_k)$, one can identify the vertices v_x of G_1 and u_x of P_{x_k-1}. It is easy to see that $d_{G_1}(v_x) = (y_k + 1)(y_k + 2)/2 + 16$. Then

$$\begin{aligned} W(L^2(T_k)) &= W(G_1) + W(P_{x_k-1}) + (n_{P_{x_k-1}} - 1)d_{G_1}(v_x) + (n_{G_1} - 1)d(u_x) \\ &= W(G_1) + \binom{x_k}{3} + (x_k - 2)\big((y_k + 1)(y_k + 2)/2 + 16\big) \\ &\quad + (y_k + 8)(x_k - 1)(x_k - 2)/2 \\ &= \frac{1}{12}\left(128k^6 + 96k^5 + 840k^4 + 410k^3 + 2011k^2 + 502k + 1464\right). \end{aligned}$$

Table 4: Forks T_k of order $4k^2 + k + 10$ having property (1) ($m = 1$).

k	n_{T_k}	x_k	y_k	$diam$	W	k	n_{T_k}	x_k	y_k	$diam$	W
0	10	2	3	6	122	1	15	7	3	11	452
2	28	7	16	24	3208	3	49	28	16	45	18062
4	78	28	45	74	74960	5	115	65	45	111	244198
6	160	65	90	156	664378	7	213	118	90	209	1577780
8	274	118	151	270	3373742	9	343	187	151	339	6639328
10	420	187	228	416	12218132	11	505	272	228	501	21276242
12	598	272	321	594	35376468	13	699	373	321	695	56559602
14	808	373	430	804	87434070	15	925	490	430	921	131272488
16	1050	490	555	1046	192116738	17	1183	623	555	1179	274889820

One can see that the Wiener indices of T_k and $L^2(T_k)$ coincide.

If $k \geq 1$ is odd, then forks T_k have

$$x_k = (4k^2 + 5k + 5)/2 \quad\text{and}\quad y_k = (4k^2 - 3k + 5)/2.$$

In this case, $y_{k+2} = x_k + 4k + 5$ and $x_{k+2} = y_k + 12k + 13$. For forks with branches of length x_k and y_k, one can compute the Wiener index for T_k and $L^2(T_k)$:

$$W(T_k) = W(L^2(T_k)) = \frac{1}{12}\left(128k^6 + 96k^5 + 840k^4 + 410k^3 + 2011k^2 + 478k + 1461\right).$$

Parameters for the smallest forks are presented in Table 4. Diagrams of the first trees are depicted in Figure 1.

1b. Let forks T_k have $n_{T_k} = 4k^2 - k + 10$ vertices ($m = 1$).

Let k be even, $k \geq 0$. The number of edges of long paths of the fork is equal to

$$x_k = (4k^2 + 3k + 4)/2 \quad\text{and}\quad y_k = (4k^2 - 5k + 6)/2.$$

In this case, $x_{k+2} = y_k + 12k + 10$ and $y_{k+2} = x_k + 4k + 4$. By analogy with the previous cases, one can calculate that

$$W(T_k) = W(L^2(T_k)) = \frac{1}{12}\left(128k^6 - 96k^5 + 840k^4 - 410k^3 + 2011k^2 - 502k + 1464\right).$$

Let k be odd, $k \geq 1$, and

$$x_k = (4k^2 - 5k + 5)/2 \quad\text{and}\quad y_k = (4k^2 + 3k + 5)/2.$$

We have $x_{k+2} = y_k + 4k + 3$ and $y_{k+2} = x_k + 12k + 11$. After calculations, we obtain

$$W(T_k) = W(L^2(T_k)) = \frac{1}{12}\left(128k^6 - 96k^5 + 840k^4 - 410k^3 + 2011k^2 - 478k + 1461\right).$$

Table 5: Forks T_k of order $4k^2 - k + 10$ having property (1) ($m = 1$).

k	n_{T_k}	x_k	y_k	$diam$	W	k	n_{T_k}	x_k	y_k	$diam$	W
0	10	2	3	6	122	1	13	2	6	9	288
2	24	13	6	20	1982	3	43	13	25	39	12090
4	70	40	25	66	53868	5	105	40	60	101	185258
6	148	83	60	144	524700	7	199	83	111	195	1284872
8	258	142	111	254	2813798	9	325	142	178	321	5644012
10	400	217	178	396	10548962	11	483	217	261	479	18607598
12	574	308	261	570	31276072	13	673	308	360	669	50467750
14	780	415	360	776	78640208	15	895	415	475	891	118890668
16	1018	538	475	1014	175058290	17	1149	538	606	1145	251835032

There is a relation between parameters of forks of order $4k^2 + k + 10$ and $4k^2 - k + 10$ as in the case of combs. Therefore, the Wiener indices of the corresponding forks have the same coefficients. Parameters for the smallest forks are presented in Table 5.

2. Let $m = 3$. Forks T_k of this class have $n_{T_k} = 4k^2 \pm 3k + 16$ vertices.

2a. Consider forks on $n_{T_k} = 4k^2 + 3k + 16$ vertices. Assume that k is even, $k \geq 0$. The number of edges of long terminal paths of the fork is equal to

$$x_k = (4k^2 - k + 6)/2 \ \text{ and } \ y_k = (4k^2 + 7k + 12)/2.$$

In this case, $x_{k+2} = y_k + 4k + 4$ and $y_{k+2} = x_k + 12k + 18$. The diameter of T_k is equal to $diam(T_k) = x_k + y_k + 3 = 4k^2 + 3k + 12$. By (2), we get

$$\begin{aligned} W(T_k) &= \binom{4k^2 + 3k + 16}{3} - \left(x_k(y_k + 5) + (x_k + 4) + y_k + (x_k + 4)y_k + (x_k + 4)y_k\right) \\ &= \frac{1}{12}\left(128k^6 + 288k^5 + 1608k^4 + 2142k^3 + 6055k^2 + 3990k + 6600\right). \end{aligned}$$

The quadratic line graph of T_k is depicted in Figure 9. It can be constructed from the graph G_0 by joining paths P_{x_k-1} and P_{y_k-1}. For the graph G_0, we have $d(v_y) = 32$ and $W(G_0) = 194$. Let the graph G_1 be obtained by identify the vertices v_y of G_0 and u_y of P_{y_k-1}.

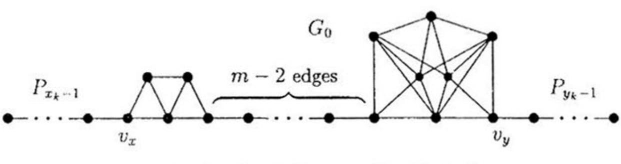

Figure 9. Quadratic line graph of fork T_k.

Table 6: Forks T_k of order $4k^2 + 3k + 16$ having property (1) ($m = 3$).

k	n_{T_k}	x_k	y_k	*diam*	W	k	n_{T_k}	x_k	y_k	*diam*	W
0	16	3	6	12	550	1	23	10	6	19	1726
2	38	10	21	34	8256	3	61	33	21	57	35350
4	92	33	52	88	123948	5	131	72	52	127	362524
6	178	72	99	174	917218	7	233	127	99	229	2068808
8	296	127	162	292	4258394	9	367	198	162	363	8139538
10	446	198	241	442	14639500	11	533	285	241	529	25026546
12	628	285	336	624	40986736	13	731	388	336	727	64706400
14	842	388	447	838	98964478	15	961	507	447	957	147230164
16	1088	507	574	1084	213770798	17	1223	642	574	1219	303764678

Then

$$\begin{aligned} W(G_1) &= W(G_0) + W(P_{y_k-1}) + \left(n_{P_{y_k-1}} - 1\right)d(v_y) + (n_{G_0} - 1)d(u_y) \\ &= 194 + \binom{y_k}{3} + 32(y_k - 2) + 12(y_k - 1)(y_k - 2)/2 \\ &= \frac{1}{48}\left(64k^6 + 336k^5 + 2220k^4 + 6055k^3 + 14438k^2 + 16520k + 22176\right). \end{aligned}$$

To construct the quadratic line graph $L^2(T_k)$, one can identify the vertices v_x of G_1 and u_x of P_{x_k-1}. It easy to see that $d_{G_1}(v_x) = (y_k + 3)(y_k + 4)/2 + 26$. By (3), we have

$$\begin{aligned} W(L^2(T_k)) &= W(G_1) + W(P_{x_k-1}) + (n_{P_{x_k-1}} - 1)d_{G_1}(v_x) + (n_{G_1} - 1)d(u_x) \\ &= W(G_1) + \binom{x_k}{3} + (x_k - 2)\left((y_k + 3)(y_k + 4)/2 + 26\right) \\ &\quad + (y_k + 10)(x_k - 1)(x_k - 2)/2 \\ &= \frac{1}{12}\left(128k^6 + 288k^5 + 1608k^4 + 2142k^3 + 6055k^2 + 3990k + 6600\right). \end{aligned}$$

The Wiener indices for T_k and its quadratic line graph coincide.

If $k \geq 1$ is odd, then forks T_k have

$$x_k = (4k^2 + 7k + 9)/2 \quad \text{and} \quad y_k = (4k^2 - k + 9)/2.$$

Here $x_{k+2} = y_k + 12k + 15$ and $y_{k+2} = x_k + 4k + 7$. Applying formulas (2) and (3), we obtain the Wiener index for forks for odd k:

$$W(T_k) = W(L^2(T_k)) = \frac{1}{12}\left(128k^6 + 288k^5 + 1608k^4 + 2142k^3 + 6055k^2 + 3918k + 6573\right).$$

Parameters of the smallest forks from the both families are presented in Table 6. Two initial trees are depicted in Figure 8.

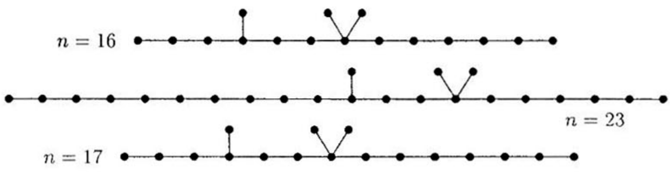

Figure 8. First forks for $m = 3$ (cases 2a and 2b).

2b. Let forks T_k have $n_{T_k} = 4k^2 - 3k + 16$ vertices ($m = 3$).

Let k be even, $k \geq 0$. The number of edges of long paths of the fork is equal to

$$x_k = (4k^2 + k + 6)/2 \quad \text{and} \quad y_k = (4k^2 - 7k + 12)/2.$$

In this case, $x_{k+2} = y_k + 12k + 6$ and $y_{k+2} = x_k + 4k + 4$. By analogy with the previous cases, one can calculate that

$$W(T_k) = W(L^2(T_k)) = \frac{1}{12}\left(128k^6 - 288k^5 + 1608k^4 - 2142k^3 + 6055k^2 - 3990k + 6600\right).$$

Let k be odd, $k \geq 1$, and

$$x_k = (4k^2 - 7k + 9)/2 \quad \text{and} \quad y_k = (4k^2 + k + 9)/2.$$

We have $x_{k+2} = y_k + 4k + 1$ and $y_{k+2} = x_k + 12k + 9$. After calculations, we have

$$W(T_k) = W(L^2(T_k)) = \frac{1}{12}\left(128k^6 - 288k^5 + 1608k^4 - 2142k^3 + 6055k^2 - 3918k + 6573\right).$$

Coefficients of the Wiener index for the corresponding forks of order $4k^2 \pm 3k + 16$ differ only in sign. Parameters of the first forks for even and odd k are presented in Table 7. Diagrams of the initial trees are depicted in Figure 8.

Table 7: Forks T_k of order $4k^2 - 3k + 16$ having property (1) ($m = 3$).

k	n_{T_k}	x_k	y_k	*diam*	W	k	n_{T_k}	x_k	y_k	*diam*	W
0	16	3	6	12	550	1	17	3	7	13	668
2	26	12	7	22	2534	3	43	12	24	39	12088
4	68	37	24	64	49288	5	101	37	57	97	164634
6	142	78	57	138	462868	7	191	78	106	187	1135050
8	248	135	106	244	2497426	9	313	135	171	309	5039056
10	386	208	171	382	9475850	11	467	208	252	463	16813748
12	556	297	252	552	28417924	13	653	297	349	649	46091518
14	758	402	349	754	72160008	15	871	402	462	867	109565494
16	992	523	462	988	161966238	17	1121	523	591	1117	233846500

$n = 19$

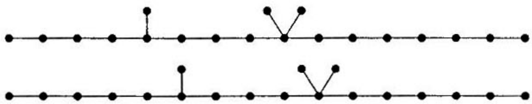

Figure 9. First pair of forks for $m = 4$.

3. Let $m = 4$. Forks T_k of this family have $n_{T_k} = k^2 + k + 19$ vertices. For every k, there are two trees having property (1) and the second tree is defined by the first one.

Consider the first tree. The number of edges of long paths of the fork is equal to

$$x_k = (k^2 - k + 8)/2 \quad \text{and} \quad y_k = (k^2 + 3k + 14)/2.$$

In this case, $x_{k+1} = y_k - 3k - 3$ and $y_{k+1} = x_k + 3k + 5$. The diameter of T_k is equal to $diam(T_k) = x_k + y_k + 4 = k^2 + k + 15$

By (2), we can write

$$\begin{aligned} W(T_k) &= \binom{k^2+k+20}{3} - \big(x_k(y_k+6) + (x_k+5) + y_k + (x_k+5)y_k + (x_k+5)y_k\big) \\ &= \frac{1}{12}\left(2k^6 + 6k^5 + 111k^4 + 212k^3 + 1999k^2 + 1918k + 11352\right). \end{aligned}$$

The quadratic line graph (see Figure 9) can be constructed from the graph G_0 by joining paths P_{x_k-1} and P_{y_k-1}. We have $d_{G_0}(v_y) = 40$ and $W(G_0) = 264$. Let the graph G_1 be obtained by identifying the vertices v_y of G_0 and u_y of P_{y_k-1}. Then

$$\begin{aligned} W(G_1) &= W(G_0) + W(P_{y_k-1}) + (n_{P_{y_k-1}} - 1)d(v_y) + (n_{G_0} - 1)d(u_y) \\ &= 264 + \binom{y_k}{3} + 40(y_k - 2) + 13(y_k - 1)(y_k - 2)/2 \\ &= \frac{1}{48}\left(k^6 + 9k^5 + 141k^4 + 711k^3 + 4130k^2 + 9312k + 33312\right). \end{aligned}$$

To construct the quadratic line graph, one can identify the vertices v_x of G_1 and u_x of P_{x_k-1}. Since $d_{G_1}(v_x) = (y_k + 4)(y_k + 5)/2 + 31$,

$$\begin{aligned} W(L^2(T_k)) &= W(G_1) + W(P_{x_k-1}) + (n_{P_{x_k-1}} - 1)d_{G_1}(v_x) + (n_{G_1} - 1)d(u_x) \\ &= W(G_1) + \binom{x_k}{3} + (x_k - 2)\big((y_k+4)(y_k+5)/2 + 31\big) \\ &\quad + (y_k + 10)(x_k - 1)(x_k - 2)/2 \\ &= \frac{1}{12}\left(2k^6 + 6k^5 + 111k^4 + 212k^3 + 1999k^2 + 1918k + 11352\right). \end{aligned}$$

Table 8: Forks T_k of order k^2+k+19 having property (1) ($m=4$).

k	n_{T_k}	x_k	y_k	$diam$	W	k	n_{T_k}	x_k	y_k	$diam$	W
0	19	4	7	15	946	5	49	14	27	45	18066
–	19	5	6	15	944	–	49	25	16	45	18044
1	21	4	9	17	1300	6	61	19	34	57	35370
–	21	7	6	17	1294	–	61	32	21	57	35344
2	25	5	12	21	2248	7	75	25	42	71	66508
–	25	10	7	21	2238	–	75	40	27	71	66478
3	31	7	16	27	4394	8	91	32	51	87	119894
–	31	14	9	27	4380	–	91	49	34	87	119860
4	39	10	21	35	8944	9	109	40	61	105	207544
–	39	19	12	35	8926	–	109	59	42	105	207506

For the second fork T_k of a pair,

$$x_k = y_k^* - 2 \text{ and } y_k = x_k^* + 2,$$

where x_k^* and y_k^* are the corresponding quantities for the first tree. By analogy with the previous calculations, one can obtain the Wiener index for T_k and its quadratic line graph:

$$W(T_k) = W(L^2(T_k)) = \frac{1}{12}\left(2k^6 + 6k^5 + 111k^4 + 212k^3 + 1999k^2 + 1870k + 11328\right).$$

Parameters of ten pairs of forks T_k for initial values of k are presented in Table 8. Trees of the first pair are shown in Figure 9.

4. Let $m = 12$. Forks T_k of this family have $n_{T_k} = k^2 - k + 59$ vertices. As in the previous case, there are two trees satisfying property (1) for every k.

Consider the first tree T_k in a pair. The number of edges of long paths of the fork is equal to

$$x_k = (k^2 - 3k + 38)/2 \text{ and } y_k = (k^2 + k + 48)/2.$$

We have $x_{k+1} = y_k - k - 6$ and $y_{k+1} = x_k + 3k + 6$. The diameter of T_k is equal to $diam(T_k) = x_k + y_k + 12 = k^2 - k + 55$.

By (2), we can write

$$\begin{aligned} W(T_k) &= \binom{k^2 - k + 60}{3} - \left(x_k(y_k + 14) + (x_k + 13) + y_k + (x_k + 13)y_k + (x_k + 13)y_k\right) \\ &= \frac{1}{12}\left(2k^6 - 6k^5 + 351k^4 - 692k^3 + 20239k^2 - 19822k + 382872\right). \end{aligned}$$

The quadratic line graph can be constructed from the graph G_0 by joining paths P_{x_k-1} and P_{y_k-1}. For the graph G_0, we have $d(v_y) = 140$ and $W(G_0) = 1412$. Let the graph G_1

Table 9: Forks T_k of order $k^2 - k + 59$ having property (1) ($m = 12$).

k	n_{T_k}	x_k	y_k	$diam$	W	k	n_{T_k}	x_k	y_k	$diam$	W
1	59	18	25	55	31912	6	89	28	45	85	112052
-	59	19	24	55	31906	-	89	39	34	85	111986
2	61	18	27	57	35350	7	101	33	52	97	164640
-	61	21	24	57	35332	-	101	46	39	97	164562
3	65	19	30	61	42942	8	115	39	60	111	244222
-	65	24	25	61	42912	-	115	54	45	111	244132
4	71	21	34	67	56252	9	131	46	69	127	362572
-	71	28	27	67	56210	-	131	63	52	127	362470
5	79	24	39	75	77926	10	149	54	79	145	535546
-	79	33	30	75	77872	-	149	73	60	145	535432

be obtained by identify the vertices v_y of G_0 and u_y of P_{y_k-1}. Then by formula (3)

$$\begin{aligned} W(G_1) &= W(G_0) + W(P_{y_k-1}) + (n_{P_{y_k-1}} - 1)d(v_y) + (n_{G_0} - 1)d(u_y) \\ &= 1412 + \binom{y_k}{3} + 140(y_k - 2) + 21(y_k - 1)(y_k - 2)/2 \\ &= \frac{1}{48}\left(k^6 + 3k^5 + 267k^4 + 529k^3 + 21308k^2 + 21044k + 567792\right). \end{aligned}$$

By identifying the vertices v_x of G_1 and u_x of P_{x_k-1}, one can construct the quadratic line graph of the fork. It easy to see that $d_{G_1}(v_x) = (y_k + 12)(y_k + 13)/2 + 71$. Then

$$\begin{aligned} W(L^2(T_k)) &= W(G_1) + W(P_{x_k-1}) + (n_{P_{x_k-1}} - 1)d_{G_1}(v_x) + (n_{G_1} - 1)d(u_x) \\ &= W(G_1) + \binom{x_k}{3} + (x_k - 2)\big((y_k + 12)(y_k + 13)/2 + 71\big) \\ &\quad + (y_k + 19)(x_k - 1)(x_k - 2)/2 \\ &= \frac{1}{12}\left(2k^6 - 6k^5 + 351k^4 - 692k^3 + 20239k^2 - 19822k + 382872\right). \end{aligned}$$

The second fork T_k^* of a pair has

$$x_k^* = y_k - 6 \quad \text{and} \quad y_k^* = x_k + 6,$$

where x_k and y_k are parameters of the first tree. Then the Wiener index is equal to

$$W(T_k) = W(L^2(T_k)) = \frac{1}{12}\left(2k^6 - 6k^5 + 351k^4 - 692k^3 + 20239k^2 - 19966k + 382944\right).$$

Parameters of the smallest forks of this family are presented in Table 9.

Suppose that forks T_k have $n_{T_k} = k^2 + k + 59$ vertices. Note that $n_{T_k} = n'_{T_{k-1}}$, $x_k = x'_{k-1}$ and $y_k = y'_{k-1}$ for $k \geq 2$, where n', x' and y' are the corresponding quantities of the first tree of order $k^2 - k + 59$. Therefore, forks of order $k^2 \pm k + 59$ ($m = 12$) form one family.

In conclusion of this section we remark that there are many other families of forks having property (1).

Conclusion

The Wiener index for trees and their quadratic line graphs are considered. Several infinite families of chemical trees with the property $W(T) = W(L^2(T))$ are presented. All the constructed trees are caterpillars or lobsters. Combs are asymmetric trees. Do there exist other trees having the structure of the considered lobsters, combs or forks and satisfying property (1)? Except two examples (forks with $m = 5$ of order 23 and 24), our families contain all such trees on $n \leq 26$ vertices (see Tables). Based on data of Table 1, we believe that almost all trees having property (1) are chemical trees. We also conjecture that all such trees have vertices of degree 2. Note that trees of the presented infinite families have only two long paths attached to its centers.

Problem. Construct an infinite family of trees satisfying equality $W(T) = W(L^2(T))$ such that they have several paths growing from its centers.

The following question on iterated line graphs of high power was formulated in [18]:

Question. For $n \geq 3$, does there exist a tree satisfying equality $W(T) = W(L^n(T))$? Attempts to find such trees lead to the following conjecture.

Conjecture. There is no tree satisfying equality $W(T) = W(L^n(T))$ for any $n \geq 3$.

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