Trees T satisfying $W(L^3(T)) = W(T)$

M. Knor*, M. Mačaj†, P. Potočnik‡, R. Škrekovski§

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Abstract

Let G be a graph. Denote by $L^i(G)$ its i-iterated line graph and denote by $W(G)$ its Wiener index. We find an infinite class of trees T satisfying $W(L^3(T)) = W(T)$, which disproves a conjecture of Dobrynin and Entringer [Electronic Notes in Discrete Math. **22** (2005) 469–475].

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1 Introduction

Let G be a graph. We denote its vertex set and edge set by $V(G)$ and $E(G)$, respectively. For any two vertices u, v let $d(u, v)$ be the distance from u to v. The *Wiener index* of G, $W(G)$, is defined as

$$W(G) = \sum_{u \neq v} d(u, v),$$

where the sum is taken over unordered pairs of vertices of G. The Wiener index was introduced by Wiener in [23]. Since it is related to several properties of chemical molecules (see [15]), it is widely studied by mathematical chemists. The interest

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

†Department of Algebra and Number Theory, Faculty of Mathematics, Physics and Informatics, Comenius University, Mlynská Dolina, 842 15 Bratislava, Slovakia, `martin.macaj@fmph.uniba.sk`.

‡Faculty of Mathematics and Physics, University of Ljubljana, and Institute of Mathematics, Physics and Mechanics, Jadranska 21, 1000 Ljubljana, Slovenia, `primoz.potocnik@fmf.uni-lj.si`.

§Faculty of Mathematics and Physics, University of Ljubljana, and Institute of Mathematics, Physics and Mechanics, Jadranska 21, 1000 Ljubljana, Slovenia, `skrekovski@gmail.com`.

of pure mathematicians was attracted in 1970's, when it was reintroduced as *the transmission* and *the distance of a graph*; see [22] and [12], respectively. Wiener index (and its variations) has now become a classical topic in mathematical chemistry spurring numerous interesting articles (see for example [4, 16, 17, 18]) surveys [7, 8] and even special issues of journals [13, 14].

An important variation of a Wiener index is that of the Wiener index of the line graph (also called the edge-Wiener index); see for example [2, 3, 11, 19, 24]. The topic of this paper is a natural generalization of the edge-Wiener index, namely the Wiener index of iterated line graphs. This notion has attracted quite a bit of attention (see [5, 6, 7, 9, 10]) and a number of interesting conjectures have been posed. The main result of this paper is a counterexample to a conjecture posed in [6] (see Conjecture 1.2 and Theorem 1.3. Let us explain this in more detail.

The line graph of G, $L(G)$, has vertex set identical to the set of edges of G and two vertices of $L(G)$ are adjacent if and only if the corresponding edges share an endvertex in G. Iterated line graphs are defined inductively as follows:

$$L^i(G) = \begin{cases} G & \text{if } i = 0, \\ L(L^{i-1}(G)) & \text{if } i > 0. \end{cases}$$

The Wiener index of the line graph of a tree T can easily be computed from $W(T)$ by using the following result of Buckley [1]:

Theorem 1.1 *Let T be a tree on n vertices. Then $W(L(T)) = W(T) - \binom{n}{2}$.*

Since $\binom{n}{2} > 0$ if $n \geq 2$, there is no tree for which $W(L(T)) = W(T)$ (with the exception of the tree with a single vertex). However, there are trees T satisfying $W(L^2(T)) = W(T)$, see e.g. [5]. In [6], Dobrynin and Entringer stateded the following conjecture:

Conjecture 1.2 *There is no tree T satisfying equality $W(T) = W(L^i(T))$ for any $i \geq 3$.*

By the definition, if G has a unique vertex, then $W(G) = 0$. In this case, we say that the graph G is *trivial*. We set $W(G) = 0$ also when the set of vertices of G is empty. Of course, if T is a trivial tree, then $W(L^i(T)) = W(T)$ for every $i \geq 1$, although here the graph $L^i(T)$ is empty. Therefore, Conjecture 1.2 should be viewed in the context of nontrivial trees T.

Let $H'_{a,b,c}$ be the tree on $a + b + c + 4$ vertices, out of which two have degree 3, four have degree 1 and the remaining $a + b + c - 2$ have degree 2. The two vertices of degree 3 are connected by a path of length 2. Finally, there are two pendant paths of lengths a and b attached to one vertex of degree 3 and two pendant paths of lengths c and 1 attached to the other vertex of degree 3, see Figure 1 for $H'_{3,2,4}$.

Here we prove the following theorem which disproves Conjecture 1.2:

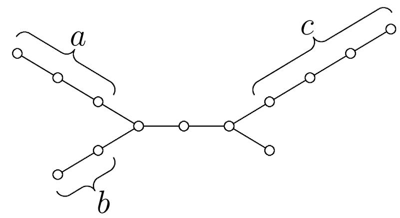

Figure 1: The graph $H'_{a,b,c}$.

Theorem 1.3 *For every $i, j \in \mathbb{Z}$ define*

$$\begin{aligned} a &= 128 + 3i^2 + 3j^2 - 3ij + i, \\ b &= 128 + 3i^2 + 3j^2 - 3ij + j, \\ c &= 128 + 3i^2 + 3j^2 - 3ij + i + j. \end{aligned}$$

Then $W(L^3(H'_{a,b,c})) = W(H'_{a,b,c})$.

Let $k \in \{i, j, i+j\}$. Since for every integer i and j the inequality $3i^2+3j^2-3ij+k \geq 0$ holds, we see that $a, b, c \geq 128$ in Theorem 1.3. Hence, the smallest graph satisfying the assumptions is $H'_{128,128,128}$ on 388 vertices obtained when $i = j = 0$.

We remark that for $i \geq 4$, Conjecture 1.2 is true; see [21]. In fact, in a forthcoming paper we prove that the class of trees described in Theorem 1.3 is the unique class of trees (beside the trivial tree) violating Conjecture 1.2.

In the next section we state a formula which enables us to calculate $W(L^3(T)) - W(T)$ and we prove Theorem 1.3.

2 Proofs

A degree of a vertex, say v, is denoted by d_v. Analogously as a vertex of $L(G)$ corresponds to an edge of G, a vertex of $L^2(G)$ corresponds to a path of length 2 in G. For $x \in V(L^2(G))$ we denote the corresponding path in G by $B_2(x)$. For two subgraphs S_1 and S_2 of G, the shortest distance in G between a vertex of S_1 and a vertex of S_2 is denoted by $d(S_1, S_2)$. If S_1 and S_2 share an edge, then we set $d(S_1, S_2) = -1$.

Let x and y be two vertices of $L^2(G)$, such that u is the center of $B_2(x)$, the vertex v is the center of $B_2(y)$ and $u \neq v$. Then

$$d_{L^2(G)}(x, y) = d(B_2(x), B_2(y)) + 2.$$

Let u and v be distinct vertices of G. Let $\beta_i(u, v)$ denote the number of pairs $x, y \in V(L^2(G))$, with u being the center of $B_2(x)$ and v being the center of $B_2(y)$, such that $d(B_2(x), B_2(y)) = d(u,v) - 2 + i$. Since $d(u,v) - 2 \le d(B_2(x), B_2(y)) \le d(u,v)$, we have $\beta_i(u,v) = 0$ for all $i \notin \{0,1,2\}$. Moreover, $\sum_{i=0}^{2} \beta_i(u,v) = \binom{\mathrm{d}_u}{2}\binom{\mathrm{d}_v}{2}$. In [20, Proposition 2.5] we have the following statement:

Proposition 2.1 *Let G be a connected graph. Then*

$$\begin{aligned} W(L^2(G)) &= \sum_{u \neq v} \left[\binom{\mathrm{d}_u}{2}\binom{\mathrm{d}_v}{2} d(u,v) + \beta_1(u,v) + 2\beta_2(u,v) \right] \\ &+ \sum_{u} \left[3\binom{\mathrm{d}_u}{3} + 6\binom{\mathrm{d}_u}{4} \right], \end{aligned}$$

where the first sum is taken over unordered pairs of vertices $u, v \in V(G)$ and the second one is taken over $u \in V(G)$.

Let

$$h(u,v) = \left(\binom{\mathrm{d}_u}{2}\binom{\mathrm{d}_v}{2} - 1 \right) d(u,v) + \beta_1(u,v) + 2\beta_2(u,v). \tag{1}$$

Then we have:

Lemma 2.2 *Let G be a connected graph. Then*

$$W(L^2(G)) - W(G) = \sum_{u \neq v} h(u,v) + \sum_{u} \left[3\binom{\mathrm{d}_u}{3} + 6\binom{\mathrm{d}_u}{4} \right],$$

where the first sum is taken over unordered pairs of vertices $u, v \in V(G)$ such that either $\mathrm{d}_u \neq 2$ or $\mathrm{d}_v \neq 2$, and the second one is taken over $u \in V(G)$.

Proof. Observe that if $\mathrm{d}_u = \mathrm{d}_v = 2$, then $\beta_0(u,v) = 1$ and $\beta_1(u,v) = \beta_2(u,v) = 0$, and hence $h(u,v) = 0$. Since $W(G) = \sum_{u \neq v} d(u,v)$, the proof follows from Proposition 2.1. □

Now we can state a formula counting the difference $W(L^3(H'_{a,b,c})) - W(H'_{a,b,c})$.

Lemma 2.3 *Let $a, b, c \ge 2$. Then*

$$W(L^3(H'_{a,b,c})) - W(H'_{a,b,c}) = 3(a^2 + b^2 + c^2) - 3(ab + ac + bc) - a - b + c + 128.$$

Proof. Denote $\Delta = W(L^3(H'_{a,b,c})) - W(H'_{a,b,c})$. We prove the lemma by counting the distances in $L(H'_{a,b,c})$ instead of in $H'_{a,b,c}$ and $L^3(H'_{a,b,c})$. Denote $LH' = L(H'_{a,b,c})$. Since $a, b, c \ge 2$, the graph LH' has eight vertices whose degree is different from 2. The three vertices of degree 1 we denote by x_1, x_2 and

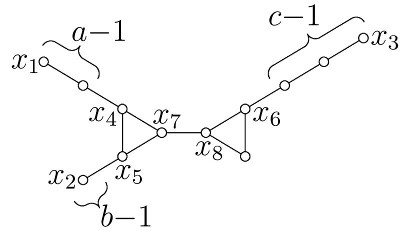

Figure 2: The graph $LH' = L(H'_{a,b,c})$.

x_3, while the five vertices of degree 3 we denote by x_4, x_5, …, x_8, see Figure 2 for $LH' = L(H'_{3,2,4})$.

Define $A_i = \sum_u h(u, x_i)$, where $u \in V(LH') \setminus \{x_1, x_2, \ldots, x_i\}$. Observe that $\sum_{i=1}^{8} A_i$ sums $h(u, v)$ for all pairs $\{u, v\}$ of vertices such that either $\mathrm{d}_u \neq 2$ or $\mathrm{d}_v \neq 2$. Since $H'_{a,b,c}$ has $a+b+c+4$ vertices, we have $W(H'_{a,b,c}) = W(LH') + \binom{a+b+c+4}{2}$, by Theorem 1.1. Thus, by Lemma 2.2, we have

$$\Delta = W(L^2(LH')) - W(LH') - \binom{a+b+c+4}{2} = \sum_{i=1}^{8} A_i + 5 \cdot 3\binom{3}{3} - \binom{a+b+c+4}{2},$$

since there are just five vertices of degree 3 in LH' and all the other vertices have degree at most 2.

Now we evaluate A_i, $1 \leq i \leq 8$. Since $\deg(x_1) = 1$, we have $\beta_j(u, x_1) = 0$, $0 \leq j \leq 2$. Hence, $h(u, x_1) = -d(u, x)$, see (1). The sum of distances from x_1 to all vertices of $x_1 - x_2$ path is $1 + 2 + \cdots + (a{+}b{-}1) = \binom{a+b}{2}$ (see Figure 2). The sum of distances from x_1 to all vertices of $x_1 - x_3$ path, not included in the previous calculation, is $a + (a{+}1) + \cdots + (a{+}c{+}1) = \binom{a+c+2}{2} - \binom{a}{2}$. In this way we get:

$$\begin{aligned}
A_1 &= -\binom{a+b}{2} - \binom{a+c+2}{2} + \binom{a}{2} - (a{+}2),\\
A_2 &= -\binom{a+b-1}{2} - \binom{b+c+2}{2} + \binom{b}{2} - (b{+}2),\\
A_3 &= -\binom{a+c+1}{2} - \binom{b+c+1}{2} + \binom{c+2}{2} - c.
\end{aligned}$$

If $4 \leq i \leq 8$, then in A_i we sum $h(u, x_i)$, where $\mathrm{d}_u = 2$ or $\mathrm{d}_u = 3$. If $\mathrm{d}_u = 2$, then regardless of the choice of u we have $\beta_0(u, x_i) = 2$, $\beta_1(u, x_i) = 1$ and $\beta_2(u, x_i) = 0$. Since $\binom{\mathrm{d}_u}{2}\binom{\mathrm{d}_{x_i}}{2} - 1 = 2$, we have $h(u, x_i) = 2d(u, x_i) + 1$ in this case. Thus, the sum of $h(u, x_4)$ for interior vertices u of $x_4 - x_1$ path is $2(1 + 2 + \ldots + (a{-}2)) + (a{-}2) = 2\binom{a-1}{2} + (a{-}2)$ (see Figure 2). If $\mathrm{d}_u = 3$ then $\binom{\mathrm{d}_u}{2}\binom{\mathrm{d}_{x_i}}{2} - 1 = 8$ and $\beta_0(u, x_i) = 4$. If u and x_i lie in a common triangle, then $d(u, x_i) = 1$, $\beta_1(u, x_i) = 5$ and $\beta_2(u, x_i) = 0$, while if u and x_i do not lie in a common triangle, then $\beta_1(u, x_i) = 4$ and $\beta_2(u, x_i) = 1$. This means that $h(x_4, x_5) = 8d(x_4, x_5) + 5 = 13$, while $h(x_4, x_6) = 8d(x_4, x_6) + 6$.

In this way we get the following formulae, where we first count the contribution of vertices u with degree 2 and then the contribution of vertices of degree 3.

$$
\begin{aligned}
A_4 &= 2\binom{a-1}{2} + (a-2) + 2\binom{b}{2} + (b-4) + 2\binom{c+2}{2} + (c-14) \\
&\quad + (2\cdot 3+1) + 13 + (8\cdot 3+6) + 13 + (8\cdot 2+6), \\
A_5 &= 2\binom{a}{2} + (a-4) + 2\binom{b-1}{2} + (b-2) + 2\binom{c+2}{2} + (c-14) \\
&\quad + (2\cdot 3+1) + (8\cdot 3+6) + 13 + (8\cdot 2+6), \\
A_6 &= 2\binom{a+2}{2} + (a-14) + 2\binom{b+2}{2} + (b-14) + 2\binom{c-1}{2} + (c-2) \\
&\quad + (2\cdot 1+1) + (8\cdot 2+6) + 13, \\
A_7 &= 2\binom{a}{2} + (a-4) + 2\binom{b}{2} + (b-4) + 2\binom{c+1}{2} + (c-8) \\
&\quad + (2\cdot 2+1) + (8\cdot 1+6), \\
A_8 &= 2\binom{a+1}{2} + (a-8) + 2\binom{b+1}{2} + (b-8) + 2\binom{c}{2} + (c-4) \\
&\quad + (2\cdot 1+1).
\end{aligned}
$$

Now expanding the terms (using a computer package, for instance), we get $\Delta = 3(a^2+b^2+c^2) - 3(ab+ac+bc) - a - b + c + 128$ as required. □

Now we are in a position to prove Theorem 1.3.

Proof of Theorem 1.3. Denote $\Delta = W(L^3(H'_{a,b,c})) - W(H'_{a,b,c})$. By Lemma 2.3, we have

$$
\begin{aligned}
\Delta &= 3(a^2+b^2+c^2) - 3(ab+ac+bc) - a - b + c + 128 \\
&= \tfrac{3}{2}\Big[(a-b)^2 + (c-b)^2 + (c-a)^2\Big] - a - b + c + 128 \\
&= \tfrac{3}{2}\Big[(i-j)^2 + i^2 + j^2\Big] - 3i^2 - 3j^2 + 3ij \\
&= 0,
\end{aligned}
$$

which completes the proof. □

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