Wiener index in iterated line graphs

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Abstract

For a graph G, denote by $L^i(G)$ its i-iterated line graph and denote by $W(G)$ its Wiener index. We prove that the function $W(L^i(G))$ is convex in variable i. Moreover, this function is strictly convex if G is different from a path, a claw $K_{1,3}$ and a cycle. As an application we prove that $W(L^i(T)) \neq W(T)$ for every $i \geq 3$ if T is a tree in which no leaf is adjacent to a vertex of degree 2, $T \neq K_1$ and $T \neq K_2$.

1 Introduction

Let $G = (V(G), E(G))$ be a connected graph. For any two of its vertices, say u and v, we let $d(u, v)$ denote the distance from u to v in G. 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 all unordered pairs of vertices of G, see [22]. Wiener index has many applications in chemistry, see e.g. [9], therefore it is widely studied by chemists. It attracted the attention of mathematicians in 1970's and it was introduced under the name of transmission or the distance of a graph, see [6] and

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[21]. Recently, several special issues of journals were devoted to (mathematical properties of) Wiener index, see [7] and [8]; for surveys see [4] and [5].

The line graph of G, $L(G)$, has vertex set identical with the set of edges of G, i.e. $V(L(G)) = E(G)$. Two vertices of $L(G)$ are adjacent if and only if the corresponding edges are adjacent in G. Iterated line graphs are defined inductively as follows:

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

A connected graph is *trivial* if it contains no edges, i.e., if it has at most one vertex. As shown in [1], for any nontrivial tree T on n vertices we have $W(L(T)) = W(T) - \binom{n}{2}$. Hence, there is no nontrivial tree for which $W(L(T)) = W(T)$. However, there are trees T satisfying $W(L^2(T)) = W(T)$, see e.g. [2, 3]. In [4], the following problem was posed:

Problem 1.1 *Is there any tree T satisfying equality $W(L^i(T)) = W(T)$ for some $i \geq 3$?*

If G is a trivial graph, then clearly $W(L^i(G)) = W(G) = 0$ for all $i \geq 0$. Therefore it is reasonable to consider only nontrivial graphs. However, there are also other graphs, which behave "trivially". If G is a cycle, then $L(G) = G$ and consequently $W(L^i(G)) = W(G)$ for every $i \geq 0$. For a claw $K_{1,3}$ the graph $L(K_{1,3})$ is a triangle, so that $L(K_{1,3}) = L^i(K_{1,3})$ and consequently $W(L(K_{1,3})) = W(L^i(K_{1,3}))$ for every $i \geq 1$. Finally, for a path on n vertices, P_n, we have $L(P_n) = P_{n-1}$ if $n > 1$, while $L(P_1)$ is the empty graph. Hence, $W(L^i(P_n)) = 0$ if $i \geq n$. These three classes of graphs are exceptional. If G is distinct from a path, a cycle and the claw $K_{1,3}$, then $\lim_{i\to\infty} |V(L^i(G))| = \infty$, see [16]. Therefore graphs, different from a path, a cycle and the claw $K_{1,3}$, are called *prolific*.

Define a function $f_G(i) = W(L^i(G))$. What is the behaviour of f_G? If G is a connected non-prolific graph then f_G is a constant function for $i \geq i_G$, where i_G is a constant depending on G. But, we do not know, for instance, if it can happen for some i that $f_G(i) > f_G(0)$ and $f_G(i+1) < f_G(0)$. Therefore it is important to study the general behaviour of f_G. Recall that a function $h(i)$ convex if $h(i) + h(i+2) \geq 2h(i+1)$ for every $i \geq 0$, and $h(i)$ is strictly convex if $h(i) + h(i+2) > 2h(i+1)$. We prove here the following basic statement:

Theorem 1.2 *Let G be a connected graph. Then $f_G(i)$ is a convex function. Moreover, $f_G(i)$ is strictly convex if G is a prolific graph.*

By the analysis above, the first part of Theorem 1.2 is a straightforward consequence of the second.

Analogous functions $f_G(i) = p(L^i(G))$ were already studied for p being the maximum degree, the minimum degree, the diameter and the radius, see [10, 11, 16].

For connectivity, Hamiltonicity and related notions in iterated line graphs see [14, 23, 12, 13, 15].

Theorem 1.2 has following consequences for Problem 1.1.

Corollary 1.3 *Let T be a tree such that $W(L^k(T)) > W(T)$ for some k. Then $W(L^i(T)) > W(T)$ for every $i \geq k$.*

Computer experiments showed us that there is a big proportion of trees for which already $W(L^3(T)) > W(T)$. Although we have no formula for counting $W(L^3(G))$ using distances in G, we can use the following corollary of Theorem 1.2.

Corollary 1.4 *Let T be a nontrivial tree such that $2W(L^2(T)) \geq W(T)+W(L(T))$. Then $W(L^3(T)) > W(T)$.*

By a 2^+-*tree* we mean a tree which is different from K_1 and K_2, and in which no leaf is adjacent to a vertex of degree 2. Using Corollary 1.4 we prove the following statement:

Theorem 1.5 *Let T be a 2^+-tree different from $K_{1,3}$. Then $W(L^3(T)) > W(T)$.*

Hence, if T is a 2^+-tree different from $K_{1,3}$, then $W(L^i(T)) > W(T)$ for every $i \geq 3$, by Corollary 1.3. As $W(K_{1,3}) = 9$ and $W(L^j(K_{1,3})) = 3$ for every $j \geq 1$, we infer that $W(L^i(T)) \neq W(T)$ for every 2^+-tree T and every $i \geq 3$.

We remark that in [17] we use Theorems 1.2 and 1.5 to prove that $W(L^i(T)) > W(T)$ for all $i \geq 3$ and all trees T which are not homeomorphic to a path, claw $K_{1,3}$ and H, where H is a tree on 6 vertices, two of which have degree 3 and four of which have degree 1. Further, in [18] and [19] we consider trees homeomorphic to $K_{1,3}$ and H, respectively, and $i \geq 4$. Finally, in [20] we consider trees homeomorphic to $K_{1,3}$ and H and $i = 3$. Hence, in series of five papers we solve Problem 1.1 completely.

The outline of this paper is as follows. In the next section we give formulae for $W(G)$ and $W(L^2(G))$ involving the degrees and distances in G. In the third section we prove:

Theorem 1.6 *Let G be a connected graph distinct from an isolated vertex and a cycle. Then $W(L^2(G)) - 2W(L(G)) + W(G) > 0$.*

which implies Theorem 1.2. Finally, in the last section we prove Theorem 1.5.

2 Preliminaries

In our proofs, we do not find $W(L(G))$ and $W(L^2(G))$ by first constructing $L(G)$ and $L^2(G)$ and afterwards counting the distances in $L(G)$ and $L^2(G)$. Instead, we compute distances included in $W(L(G))$ and $W(L^2(G))$ already in G. For this, we use the representation of vertices of $L(G)$ and $L^2(G)$ in G.

By the definition of the line graph, every vertex $w \in V(L(G))$ corresponds to an edge of G. Let us denote by $B_1(w)$ this edge of G. Analogously, every vertex $x \in V(L^2(G))$ corresponds to a path of length two in G, denote this path by $B_2(x)$. In fact, vertices of $L(G)$ are in one-to-one correspondence with edges of G, and vertices of $L^2(G)$ are in one-to-one correspondence with paths of length two in G.

Let S_1 and S_2 be two edge-disjoint subgraphs of G. We define the distance $d(S_1, S_2)$ to be the length of a shortest path in G joining a vertex of S_1 to a vertex of S_2. Further, if S_1 and S_2 share $s \geq 1$ edges, then we set $d(S_1, S_2) = -s$. With the thus defined function d, the following holds for any $w, z \in V(L(G))$ and any $x, y \in V(L^2(G))$:

$$d_{L(G)}(w,z) = d(B_1(w), B_1(z)) + 1, \qquad (1)$$

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

We remark that although there is no one-to-one correspondence between the vertices of $L^i(G)$, $i \geq 3$, and subgraphs of G, there are tools for counting distances between vertices of $L^i(G)$ already in G, see [16].

Lemma 2.1 *Let $u, v \in V(G)$ and let $w, z \in V(L(G))$ such that $u \in V(B_1(w))$ and $v \in V(B_1(z))$. Then for some $i \in \{-1, 0, 1\}$ the following holds:*

$$d_{L(G)}(w,z) = d(B_1(w), B_1(z)) + 1 = d(u,v) + i.$$

Proof. The first equality follows from (1). Since $B_1(w)$ contains u and one neighbour of u, while $B_1(z)$ contains v and one neighbour of v, we have

$$d(u,v) - 2 \leq d(B_1(w), B_1(z)) \leq d(u,v).$$

Therefore, $d(B_1(w), B_1(z)) + 1 = d(u,v) + i$, where $-1 \leq i \leq 1$. □

Let u and v be two distinct vertices of G. For $i \in \{-1, 0, 1\}$, let $\alpha_i(u,v)$ denote the number of pairs w, z for which $u \in V(B_1(w))$, $v \in V(B_1(z))$ and $d(B_1(w), B_1(z)) = d(u,v) - 1 + i$.

In the sequel, denote by d_u and d_v the degrees of u and v, respectively.

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

$$W(L(G)) = \frac{1}{4}\sum_{u \neq v}\Big[d_u\, d_v\, d(u,v) - \alpha_{-1}(u,v) + \alpha_1(u,v)\Big] + \frac{1}{4}\sum_{u \in V(G)}\binom{d_u}{2},$$

where the first sum runs through all unordered pairs $u, v \in V(G)$.

Proof. By definition we have

$$W(L(G)) = \sum_{\{uu', vv'\}} d_{L(G)}(uu', vv'),$$

where the sum runs through all pairs of edges uu', vv' of G. By considering the ordered choices for the vertices u, v, u', v', one gets

$$W(L(G)) = \frac{1}{8}\sum_{u \in V(G)}\sum_{v \in V(G)}\sum_{u' \in N(u)}\sum_{v' \in N(v)} d_{L(G)}(uu', vv').$$

Let us first consider the contribution of ordered pairs $u, v \in V(G)$ with $u \neq v$. Then in view of Lemma 2.1, we see that $d_{L(G)}(uu', vv') = d(u,v) + i$ for some $i \in \{-1, 0, 1\}$. By summing over all ordered pairs (u,v), $u \neq v$, one thus gets the contribution of $d_u d_v d(u,v)$ minus the number of choices for $u' \in N(u)$ and $v' \in N(v)$ such that $d_{L(G)}(uu', vv') = d(u,v) - 1$ plus the number of choices for u' and v' such that $d_{L(G)}(uu', vv') = d(u,v) + 1$. This contribution is thus

$$\frac{1}{8}\sum_{u \in V(G)}\sum_{v \in V(G)\setminus\{u\}}\Big[d_u\, d_v\, d(u,v) - \alpha_{-1}(u,v) + \alpha_1(u,v)\Big],$$

which clearly equals the first sum in the statement of the proposition.

On the other hand, if $u = v$, then $d_{L(G)}(uu', vv') = 1$ if $u' \neq v'$ (and 0 otherwise). The contribution of such a pair $\{u, v\}$ to $W(L(G))$ thus equals to

$$\frac{1}{8}\sum_{u' \in N(u)}\sum_{v' \in N(u)} 1 = \frac{1}{8}d_u(d_u - 1) = \frac{1}{4}\sum_{u \in V(G)}\binom{d_u}{2}.$$

The result now follows by adding up the two contributions. □

In a tree, every pair of vertices is joined by a unique path, so that $\alpha_{-1}(u,v) = 1$ and $\alpha_1(u,v) = (d_u - 1)(d_v - 1)$. Hence, we obtain the following consequence of Proposition 2.2.

Corollary 2.3 *Let T be a tree. Then*

$$W(L(T)) = \frac{1}{4}\sum_{u\neq v}\Big[d_u\,d_v\,d(u,v) - 1 + (d_u - 1)(d_v - 1)\Big] + \frac{1}{4}\sum_{u}\binom{d_u}{2},$$

where the first sum runs through all unordered pairs $u, v \in V(G)$ and the second one runs through all $u \in V(G)$.

Now we turn our attention to $L^2(G)$.

Lemma 2.4 *Let $u, v \in V(G)$ and let $x, y \in V(L^2(G))$ such that u is the center of the path $B_2(x)$ and v is the center of $B_2(y)$. Then for some $i \in \{0, 1, 2\}$, the following holds:*

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

Proof. The first equality is simply a restatement of formula (2). Since $B_2(x)$ contains u and two neighbours of u, while $B_2(y)$ contains v and two neighbours of v, analogously as in the proof of Lemma 2.1 we have $d(u, v) - 2 \leq d(B_2(x), B_2(y)) \leq d(u, v)$. Therefore, $d(B_2(x), B_2(y)) + 2 = d(u, v) + i$, where $0 \leq i \leq 2$. □

Let u and v be two distinct vertices of G. For $i \in \{0, 1, 2\}$, denote by $\beta_i(u, v)$ the number of pairs $x, y \in V(L^2(G))$, for which u is the center of $B_2(x)$, the vertex v is the center of $B_2(y)$, and $d(B_2(x), B_2(y)) = d(u, v) - 2 + i$.

Proposition 2.5 *Let G be a connected graph. Then*

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

where the first sum runs through all unordered pairs $u, v \in V(G)$.

Proof. For a pair $\{u, v\}$ of vertices of G, let $C(u, v)$ be the set of all pairs $\{x, y\}$ of distinct vertices of $L^2(G)$ with the centre of one of $\{B_2(x), B_2(y)\}$ being u and the centre of the other being v. Then

$$W(L^2(G)) = \sum_{x\neq y} d_{L^2(G)}(x, y) = \sum_{\{u,v\}}\ \sum_{\{x,y\}\in C(u,v)} d_{L^2(G)}(x, y),$$

where $\{u, v\}$ runs through the set of all unordered pairs of vertices of G. Let us now determine the contribution of a fixed such pair $\{u, v\}$ to the above sum.

If $u \neq v$, then by Lemma 2.4, for every $i \in \{0, 1, 2\}$ we have precisely $\beta_i(u, v)$ pairs x, y such that $d_{L^2(G)}(x, y) = d(u, v) + i$. Moreover, note that $|C(u, v)| = \binom{d_u}{2}\binom{d_v}{2}$. Therefore, the contribution of the pair $\{u, v\}$ is $\binom{d_u}{2}\binom{d_v}{2}d(u, v) + \beta_1(u, v) + 2\beta_2(u, v)$.

If $u = v$, then for a pair $\{x, y\} \in C(u, v)$ we see that $d_{L^2(G)}(x, y)$ equals 0 (when $B_2(x) = B_2(y)$) or 1 (when $B_2(x)$ and $B_2(y)$ share exactly one edge) or 2 (when $B_2(x)$ and $B_2(y)$ are edge-disjoint). The number of pairs $\{x, y\} \in C(u, v)$ for which $B_2(x)$ and $B_2(y)$ share exactly one edge is $3\binom{d_u}{3}$ and the number of pairs $\{x, y\} \in C(u, v)$ for which $B_2(x)$ and $B_2(y)$ are edge-disjoint is $3\binom{d_u}{4}$. Hence, all these pairs contribute $3\binom{d_u}{3} + 6\binom{d_u}{4}$ to $W(L^2(G))$. □

As already mentioned above, in a tree every pair of vertices is joined by a unique path. Therefore $\beta_0(u, v) = (d_u - 1)(d_v - 1)$, $\beta_1(u, v) = (d_u - 1)\binom{d_v - 1}{2} + \binom{d_u - 1}{2}(d_v - 1)$ and $\beta_2(u, v) = \binom{d_u - 1}{2}\binom{d_v - 1}{2}$. Observe that $\beta_0(u, v) + \beta_1(u, v) + \beta_2(u, v) = \binom{d_u}{2}\binom{d_v}{2}$. Hence, we have the following consequence of Proposition 2.5.

Corollary 2.6 *Let T be a tree. Then*

$$\begin{aligned} W(L^2(T)) &= \sum_{u \neq v} \left[\binom{d_u}{2}\binom{d_v}{2} d(u, v) + (d_u - 1)\binom{d_v - 1}{2} \right. \\ &\qquad \left. + \binom{d_u - 1}{2}(d_v - 1) + 2\binom{d_u - 1}{2}\binom{d_v - 1}{2} \right] \\ &\quad + \sum_{u \in V(T)} \left[3\binom{d_u}{3} + 6\binom{d_u}{4} \right], \end{aligned}$$

where the first sum runs through all unordered pairs $u, v \in V(G)$.

3 Convexity of Wiener index

Define

$$\begin{aligned} A(G) &= \sum_{u \neq v} \left(\binom{d_u}{2}\binom{d_v}{2} - \frac{d_u\, d_v}{2} + 1 \right) d(u, v), \\ B(G) &= \sum_{u \neq v} \left[\beta_1(u, v) + 2\beta_2(u, v) + \frac{\alpha_{-1}(u, v)}{2} - \frac{\alpha_1(u, v)}{2} \right], \\ C(G) &= \sum_{u} \left[3\binom{d_u}{3} + 6\binom{d_u}{4} - \frac{1}{2}\binom{d_u}{2} \right], \end{aligned}$$

where the first two sums run through all unordered pairs $u, v \in V(G)$ and the third one runs through all $u \in V(G)$. By Propositions 2.2 and 2.5 we have

Proposition 3.1 *Let G be a connected graph. Then*

$$W(L^2(G)) - 2W(L(G)) + W(G) = A(G) + B(G) + C(G).$$

We will now prove the inequality $A(G) + B(G) + C(G) > 0$ in two steps. First we prove the following:

Lemma 3.2 *Let G be a connected graph other than an isolated vertex or a cycle. Then $A(G) + C(G) > 0$.*

PROOF. Denote by $a_G(u, v)$ the summand of $A(G)$ corresponding to u and v. Since

$$\begin{aligned}\binom{d_u}{2}\binom{d_v}{2} - \frac{d_u\, d_v}{2} + 1 &= \frac{(d_u^2 - d_u)(d_v^2 - d_v) - 2d_u\, d_v + 4}{4} \\ &= \frac{d_u\, d_v(d_u\, d_v - d_u - d_v - 1) + 4}{4},\end{aligned}$$

we have

$$A(G) = \sum_{u \neq v} a_G(u, v) = \sum_{u \neq v} \frac{d_u\, d_v(d_u\, d_v - d_u - d_v - 1) + 4}{4} d(u, v). \tag{3}$$

Further, denote by $c_G(u)$ the summand of $C(G)$ corresponding to u. Then

$$\begin{aligned} C(G) &= \sum_u c_G(u) = \sum_u \left[3\binom{d_u}{3} + 6\binom{d_u}{4} - \frac{1}{2}\binom{d_u}{2}\right] \\ &= \sum_u \left[\frac{d_u(d_u-1)(2d_u-4)}{4} + \frac{d_u(d_u-1)(d_u^2 - 5d_u + 6)}{4} + \frac{d_u(d_u-1)(-1)}{4}\right] \\ &= \sum_u \left[\frac{d_u(d_u - 1)(d_u^2 - 3d_u + 1)}{4}\right]. \end{aligned} \tag{4}$$

Let us first focus on $C(G)$. Since x^2-3x+1 is a quadratic function with minimum at $x = \frac{3}{2}$, and since its values at $x = 2$ and $x = 3$ are -1 and 1, respectively, we have $c_G(u) = 0$ for $d_u = 1$; $c_G(u) = -\frac{1}{2}$ for $d_u = 2$ and $c_G(u) > 0$ for $d_u \geq 3$. Hence, $C(G) \geq -n_2/2$, where n_2 is the number of vertices of degree 2 in G.

Suppose now that the statement of the lemma is wrong, and let G be a minimal (with respect to $|V(G)|$) counterexample. We will now split the proof into two cases, depending on whether G has a vertex of degree 1 or not.

Let us first consider the case where G is a graph with minimum degree $\delta(G) \geq 2$, not isomorphic to a cycle. Let $\{u, v\}$ be an unordered pair of vertices of G and assume that u is the one with smaller degree, that is, $d_u \leq d_v$. If $d_u \geq 3$, then

$$a_G(u, v) \geq \frac{d_u\, d_v(d_u\, d_v - d_u - d_v - 1) + 4}{4} \geq \frac{3d_v(3d_v - d_v - d_v - 1) + 4}{4} > 1.$$

On the other hand, if $d_u = 2$, then

$$\begin{aligned} a_G(u,v) &\geq \frac{d_u\, d_v(d_u\, d_v - d_u - d_v - 1) + 4}{4} = \frac{2d_v(2d_v - 2 - d_v - 1) + 4}{4} \\ &= \frac{d_v^2 - 3d_v + 2}{2} = \frac{(d_v - 1)(d_v - 2)}{2} \geq 0. \end{aligned}$$

Denote by n the number of vertices of G and let v be a vertex of maximum degree in G. If $d_v \geq 4$, then by the above we have that $a_G(u,v) > 1$ for every $u \in V(G)$, $u \neq v$, and therefore $A(G) > n - 1 \geq n_2$. If $d_v = 3$, then $a_G(u,v) \geq 1$ for every $u \in V(G)$, $u \neq v$. In this case there is at least one more vertex of degree 3 in G, so we have $A(G) \geq n - 1 > n_2$. Therefore in both cases we see that $A(G) > n_2$, and thus $A(G) + C(G) > n_2 - \frac{n_2}{2} \geq 0$, as claimed.

Suppose now that G has a vertex of degree 1. Then remove from G this vertex and the incident edge, and denote the resulting graph by G'. Then one of the following occurs:

(i) $G' \cong K_1$ is an isolated vertex;

(ii) $G' \cong C_n$ is a cycle;

(iii) G' is neither an isolated vertex nor a cycle.

If (i) occurs, then $G \cong K_2$, and so $A(G) = \frac{1}{2}$ by (3) and $C(G) = 0$ by (4). Hence, $A(G) + C(G) > 0$ in this case, as claimed.

If (ii) occurs, then G is isomorphic to a cycle C_n with a pending edge attached to it. Let x and y be the vertices in G of degree 3 and 1, respectively (note that $d_u = 2$ for any $u \notin \{x,y\}$). Then we have

$$a_G(u,v) = \begin{cases} 0 & \text{if } \{u,v\} \cap \{x,y\} = \emptyset, \\ -\frac{1}{2} & \text{if } \{u,v\} = \{x,y\}, \\ 0 & \text{if } \{u,v\} = \{y,z\} \text{ for } z \neq x, \\ d(u,v) & \text{if } \{u,v\} = \{z,x\} \text{ for } z \neq y. \end{cases}$$

Since G has $n-1$ vertices of degree 2, one vertex of degree 1 and one vertex of degree 3, the last two vertices being adjacent, we infer $A(G) \geq -\frac{1}{2} + n - 1$. As $C(G) \geq -\frac{n_2}{2} = -\frac{n-1}{2}$ and $n \geq 3$, we conclude $A(G) + C(G) \geq \frac{n-2}{2} > 0$. Hence the statement of the lemma holds in this case.

If (iii) occurs, then by minimality of G we know that $A(G') + C(G') > 0$. To conclude the proof of the lemma it remains to show that introducing a pendant edge to G' cannot decrease the value of $A(G') + C(G')$.

Let u be a vertex of degree d_u in G' and let G be obtained from G' by adding a single edge ua, where a is a new vertex. We show that $A(G) - A(G') \geq \frac{1}{2}$.

Observe that $C(G) = C(G') - c_{G'}(u) + c_G(u) + c_G(a)$. We have $c_G(a) = 0$. Moreover, $c_G(u) - c_{G'}(u) > 0$ if $d_u \geq 2$, while $c_G(u) - c_{G'}(u) = -\frac{1}{2}$ if $d_u = 1$, see

(4). Thus, $C(G) - C(G') \geq -\frac{1}{2}$, so that if we prove $A(G) - A(G') \geq \frac{1}{2}$, we obtain $A(G) + C(G) \geq A(G') + C(G')$, as desired.

To avoid fractions, we investigate the difference $4A(G) - 4A(G')$ and we prove that $4A(G)-4A(G') \geq 2$. In $4A(G)-4A(G')$ the terms which do not contain neither u nor a cancel out. Hence, we need to consider only the terms corresponding to u in both $A(G')$ and $A(G)$ and we have to add the terms corresponding to a, together with the term corresponding to the pair (a, u), see (3). We obtain:

$$\begin{aligned} 4A(G) - 4A(G') &= \sum_{v \in V(G') \setminus \{u\}} \Big[\Big((d_u{+}1)d_v((d_u{+}1)d_v - d_u - d_v - 2) + 4 \Big) d(u,v) \\ &\qquad - \Big(d_u\, d_v (d_u\, d_v - d_u - d_v - 1) + 4 \Big) d(u,v) \\ &\qquad + \Big(1 d_v (1 d_v - d_v - 2) + 4 \Big) \Big(d(u,v) + 1 \Big) \Big] \\ &\quad + \Big(1(d_u{+}1)(1(d_u{+}1) - d_u - 3) + 4 \Big) 1 \\ &= \sum_{v \in V(G') \setminus \{u\}} \Big[2(d_u\, d_v - 2)(d_v - 1) d(u,v) - 2d_v + 4 \Big] - 2d_u + 2. \end{aligned}$$

Let $g(u,v) = (d_u\, d_v - 2)(d_v - 1)d(u,v) - d_v + 2$. Then

$$4A(G) - 4A(G') = 2\Big(\sum_{v \in V(G') \setminus \{u\}} g(u,v) - d_u + 1 \Big).$$

Now, if always $g(u,v) \geq 1$, then $4A(G) - 4A(G') \geq 2(\sum_v 1 - d_u + 1) \geq 2$. If $d_v = 1$, then $g(u,v) = 1$. On the other hand, if $d_v \geq 2$, then $g(u,v) = (d_u\, d_v - 2)(d_v - 1)d(u,v) - d_v + 2 \geq (d_v - 2) - d_v + 2 = 0$, with equality holding only if $d_u = 1$ (and also $d_v = 2$ and $d(u,v) = 1$). Hence, if $d_u > 1$ then $g(u,v) \geq 1$ for every v and $4A(G) - 4A(G') \geq 2$. Suppose therefore that $d_u = 1$. Then $4A(G) - 4A(G') = 2\sum_v g(u,v)$. We already know that $g(u,v) \geq 0$ for every v and that $g(u,v) = 0$ only if $d_v = 2$ (and $d(u,v) = 1$). Hence, $2\sum_v g(u,v) = 0$ only if all the vertices $v \in V(G')$, $v \neq u$, have degrees 2. Since $d_u = 1$, we cannot have $d_v = 2$ for every $v \in V(G') \setminus \{u\}$, so that $4A(G)-4A(G') = 2\sum_v g(u,v) > 0$. Since $g(u,v)$ is integer, we have $4A(G) - 4A(G') \geq 2$ also in this case.

Thus, in any case $A(G) - A(G') \geq \frac{1}{2}$, so that $A(G) + C(G) \geq A(G') + C(G')$, and the lemma is proved. □

Lemma 3.3 *Let G be a connected graph distinct from an isolated vertex and a cycle. Then $B(G) \geq 0$.*

Proof. Consider distinct vertices $u, v \in V(G)$. Partition the neighbours of u into three sets S_1, S_2 and S_3:

$$S_1 = \{a;\, d(a,v) = d(u,v) - 1\},$$

$$\begin{aligned} S_2 &= \{a;\, d(a,v) = d(u,v)\}, \\ S_3 &= \{a;\, d(a,v) = d(u,v)+1\}. \end{aligned}$$

Analogously partition the neighbours of v into three sets T_1, T_2 and T_3:

$$\begin{aligned} T_1 &= \{b;\, d(b,u) = d(u,v)-1\}, \\ T_2 &= \{b;\, d(b,u) = d(u,v)\}, \\ T_3 &= \{b;\, d(b,u) = d(u,v)+1\}. \end{aligned}$$

Denote by $b(u,v)$ the summand of $B(G)$ corresponding to u and v. Further, denote by $b_2(u,v)$ the part of $b(u,v)$ corresponding to $W(L^2(G))$ (i.e., $b_2(u,v) = \beta_1(u,v) + 2\beta_2(u,v)$) and denote by $b_1(u,v)$ the part of $b(u,v)$ corresponding to $2W(L(G))$ (i.e., $b_1(u,v) = (-\alpha_{-1}(u,v) + \alpha_1(u,v))/2$). Then $b(u,v) = b_2(u,v) - b_1(u,v)$. We find a lower bound for $b_2(u,v)$ and an upper bound for $b_1(u,v)$, and we show that $b_2(u,v) - b_1(u,v) \geq 0$, which establishes the lemma.

Consider vertices x and y of $L^2(G)$ such that u is the center of $B_2(x)$ and v is the center of $B_2(y)$. Moreover, denote by u_1 and u_2 the other vertices of $B_2(x)$ and denote by v_1 and v_2 the other vertices of $B_2(v)$. Then $B_2(x) = (u_1, u, u_2)$ and $B_2(y) = (v_1, v, v_2)$. There are several possibilities.

- $\{u_1,u_2\} \cap S_1 \neq \emptyset$ and $\{v_1,v_2\} \cap T_1 \neq \emptyset$: Then $d_{L^2(G)}(x,y) = d(B_2(x), B_2(y)) + 2 \geq d(u,v) + 0$. Hence, the pair x, y contributes at least 0 to $b_2(u,v)$ in this case.

- $\{u_1,u_2\} \cap S_1 \neq \emptyset$ and $\{v_1,v_2\} \cap T_1 = \emptyset$: Then $d_{L^2(G)}(x,y) \geq d(u,v)+1$. Hence, the pair x, y contributes at least 1 to $b_2(u,v)$ in this case.

- $\{u_1,u_2\} \cap S_1 = \emptyset$, $\{u_1,u_2\} \cap S_2 \neq \emptyset$ and $\{v_1,v_2\} \cap (T_1 \cup T_2) \neq \emptyset$: Then $d_{L^2(G)}(x,y) \geq d(u,v)+1$. Hence, the pair x, y contributes at least 1 to $b_2(u,v)$ in this case.

- $\{u_1,u_2\} \cap S_1 = \emptyset$, $\{u_1,u_2\} \cap S_2 \neq \emptyset$ and $\{v_1,v_2\} \cap (T_1 \cup T_2) = \emptyset$: Then $d_{L^2(G)}(x,y) \geq d(u,v)+2$. Hence, the pair x, y contributes at least 2 to $b_2(u,v)$ in this case.

- $\{u_1,u_2\} \cap (S_1 \cup S_2) = \emptyset$ and $\{v_1,v_2\} \cap T_1 \neq \emptyset$: Then $d_{L^2(G)}(x,y) \geq d(u,v)+1$. Hence, the pair x, y contributes at least 1 to $b_2(u,v)$ in this case.

- $\{u_1,u_2\} \cap (S_1 \cup S_2) = \emptyset$ and $\{v_1,v_2\} \cap T_1 = \emptyset$: Then $d_{L^2(G)}(x,y) \geq d(u,v)+2$. Hence, the pair x, y contributes at least 2 to $b_2(u,v)$ in this case.

For $i = 1,2,3$, denote by s_i and t_i the size of S_i and T_i, respectively. Then the above bounds force that

$$b_2(u,v) \;\geq\; 0 + \left[\binom{s_1+s_2+s_3}{2} - \binom{s_2+s_3}{2}\right]\binom{t_2+t_3}{2}$$

$$
\begin{aligned}
&+\left[\binom{s_2+s_3}{2}-\binom{s_3}{2}\right]\left[\binom{t_1+t_2+t_3}{2}-\binom{t_3}{2}\right]\\
&+2\left[\binom{s_2+s_3}{2}-\binom{s_3}{2}\right]\binom{t_3}{2}\\
&+\binom{s_3}{2}\left[\binom{t_1+t_2+t_3}{2}-\binom{t_2+t_3}{2}\right]+2\binom{s_3}{2}\binom{t_2+t_3}{2}\\
= &\left[\binom{s_1+s_2+s_3}{2}-\binom{s_2+s_3}{2}\right]\binom{t_2+t_3}{2}\\
&+\left[\binom{s_2+s_3}{2}-\binom{s_3}{2}\right]\left[\binom{t_1+t_2+t_3}{2}+\binom{t_3}{2}\right]\\
&+\binom{s_3}{2}\left[\binom{t_1+t_2+t_3}{2}+\binom{t_2+t_3}{2}\right]. \qquad (5)
\end{aligned}
$$

Now consider vertices w and z of $L(G)$ such that $u \in B_1(w)$ and $v \in B_1(z)$. Denote by u_1 the other vertex of $B_1(w)$ and denote by v_1 the other vertex of $B_1(z)$. Then $B_1(w) = (u, u_1)$ and $B_1(z) = (v, v_1)$. There are two possibilities.

- $u_1 \in S_1$: Then there is at least one $v_1 \in T_1$ such that $d(B_1(w), B_1(z)) = d(u, v) - 2$. In this case $d_{L(G)}(w, z) = d(B_1(w), B_1(z)) + 1 = d(u, v) - 1$. For other $v_1 \in N(v)$ we have $d_{L(G)}(w, z) \le d(u, v)$.
- $u_1 \in S_2 \cup S_3$: Then for every $v_1 \in T_1$ we have $d_{L(G)}(w, z) \le d(u, v)$. For $v_1 \in T_2 \cup T_3$ we have $d_{L(G)}(w, z) \le d(u, v) + 1$.

This means that (recall that $b_1(u, v) = (-\alpha_{-1}(u, v) + \alpha_1(u, v))/2$)

$$b_1(u,v) \le -\frac{s_1}{2} + \frac{(s_2+s_3)(t_2+t_3)}{2}.$$

Analogously one can derive

$$b_1(u,v) \le -\frac{t_1}{2} + \frac{(s_2+s_3)(t_2+t_3)}{2},$$

so that

$$b_1(u,v) \le \frac{(s_2+s_3)(t_2+t_3)}{2} - \frac{s_1}{4} - \frac{t_1}{4}.$$

In the following we prove that $b(u, v) = b_2(u, v) - b_1(u, v) \ge 0$. Observe that the unique negative term in $b_2(u, v) - b_1(u, v)$ is $(s_2 + s_3)(t_2 + t_3)/2$. If we show that one of the three terms of (5) is not smaller than $(s_2 + s_3)(t_2 + t_3)/2$, then we are done.

Observe that $s_1 \ge 1$. This means that

$$\binom{s_1+s_2+s_3}{2}-\binom{s_2+s_3}{2} \ge \binom{s_2+s_3+1}{2}-\binom{s_2+s_3}{2} = s_2+s_3.$$

If $t_2+t_3 \geq 2$ then $\binom{t_2+t_3}{2} \geq \frac{t_2+t_3}{2}$. This means that if $t_2+t_3 \geq 2$ then for the first term of (5) we have

$$\left[\binom{s_1+s_2+s_3}{2} - \binom{s_2+s_3}{2}\right]\binom{t_2+t_3}{2} \geq \frac{(s_2+s_3)(t_2+t_3)}{2},$$

so that $b(u,v) = b_2(u,v) - b_1(u,v) \geq 0$ in this case.

Obviously, if $t_2+t_3 = 0$, then $(s_2+s_3)(t_2+t_3)/2 = 0$ and we have $b(u,v) = b_2(u,v) - b_1(u,v) \geq 0$ again.

Thus, consider the remaining case $t_2+t_3 = 1$. In this case (5) reduces to

$$\begin{aligned} b_2(u,v) &\geq \left[\binom{s_2+s_3}{2} - \binom{s_3}{2}\right]\binom{t_1+1}{2} + \binom{s_3}{2}\binom{t_1+1}{2} \\ &= \binom{s_2+s_3}{2}\binom{t_1+1}{2} \geq \binom{s_2+s_3}{2} \end{aligned}$$

as $t_1 \geq 1$. Now if $s_2+s_3 \geq 2$ then $\binom{s_2+s_3}{2} \geq \frac{s_2+s_3}{2}$ and consequently $b_2(u,v) \geq (s_2+s_3)(t_2+t_3)/2$. Thus, suppose that $s_2+s_3 = 1$, as in the case $s_2+s_3 = 0$ we have $b(u,v) \geq 0$ trivially. Then

$$-b_1(u,v) \geq \frac{s_1}{4} + \frac{t_1}{4} - \frac{(s_2+s_3)(t_2+t_3)}{2} \geq \frac{1}{4} + \frac{1}{4} - \frac{1}{2} = 0,$$

as both s_1 and t_1 are at least 1. Therefore $b(u,v) = b_2(u,v) - b_1(u,v) \geq 0$ also in this case.

Since we proved $b(u,v) \geq 0$ in all cases, we have $B(G) \geq 0$ and the lemma is proved. □

Proof of Theorem 1.6. By Proposition 3.1 we have $W(L^2(G)) - 2W(L(G)) + W(G) = A(G) + B(G) + C(G)$. By Lemma 3.2 we have $A(G) + C(G) > 0$ and by Lemma 3.3 we have $B(G) \geq 0$ for every graph G distinct from an isolated vertex and a cycle. Hence $A(G) + B(G) + C(G) > 0$ for such a graph. □

4 Wiener index of 2^+-trees

Here we prove Theorem 1.5 using Corollary 1.4. For any tree T, different from an isolated vertex, define

$$D(T) = 8W(L^2(T)) - 4W(L(T)) - 4W(T).$$

If $D(T) \geq 0$ then also $\frac{1}{4}D(T) \geq 0$ and by Corollary 1.4 we obtain $W(L^3(T)) > W(T)$.

Proposition 4.1 *Let T be a tree different from an isolated vertex. Then*

$$\begin{aligned} D(T) &= \sum_{u\neq v}\Big(d_u\,d_v\Big[2(d_u-1)(d_v-1)-1\Big]-4\Big)d(u,v) \\ &\quad+\sum_{u\neq v}\Big((d_u-1)(d_v-1)\Big[4(d_u-1)(d_v-1)-5\Big]+1\Big) \\ &\quad+\sum_{u}\frac{1}{2}d_u(d_u-1)\Big[4(d_u-1)(d_u-2)-1\Big], \end{aligned}$$

where the first two sums run through all unordered pairs $u,v\in V(G)$ and the third one goes through all $u\in V(G)$.

PROOF. By Corolaries 2.3 and 2.6 we have

$$\begin{aligned} D(T) &= 8\Bigg(\sum_{u\neq v}\Bigg[\binom{d_u}{2}\binom{d_v}{2}d(u,v)+(d_u-1)\binom{d_v-1}{2}+\binom{d_u-1}{2}(d_v-1) \\ &\qquad+2\binom{d_u-1}{2}\binom{d_v-1}{2}\Bigg]+\sum\Bigg[3\binom{du}{3}+6\binom{d_u}{4}\Bigg]\Bigg) \\ &\quad-\frac{4}{4}\Bigg(\sum_{u\neq v}\Big[d_u\,d_v\,d(u,v)-1+(d_u-1)(d_v-1)\Big]+\sum_{u}\binom{d_u}{2}\Bigg) \\ &\quad-4\sum_{u\neq v}d(u,v) \end{aligned}$$

and by reordering the terms we obtain the statement of the proposition. □

We start with stars.

Lemma 4.2 *If $G=K_{1,k}$ is a star with $k\geq 4$, then $D(G)\geq 0$.*

PROOF. In $K_{1,k}$ there are k vertices of degree 1 and one vertex of degree k. Moreover, there are $\binom{k}{2}$ pairs of vertices at distance 2 where both vertices are of degree 1, and there are k pairs of vertices at distance 1 where one of these vertices has degree 1 and the other one has degree k. Substituting these pairs and singletons into Proposition 4.1, we obtain

$$\begin{aligned} D(K_{1,k}) &= \binom{k}{2}\Big[(-1-4)2+1\Big]+k\Big[(-k-4)1+1\Big] \\ &\quad+k\cdot 0+\frac{1}{2}k(k-1)\Big[4(k-1)(k-2)-1\Big] \\ &= \frac{k^2-k}{2}(-9)+(-k^2-3k)+\Big(2k^4-8k^3+\frac{19}{2}k^2-\frac{7}{2}k\Big) \\ &= 2\Big[(k-4)k^3+(2k-1)k\Big]. \end{aligned}$$

Since $k \geq 4$, we have $D(K_{1,k}) \geq 0$. $\square$

Lemma 4.2 will serve as the induction anchor for the proof of Theorem 1.5. However, since the statement of Lemma 4.2 is not true for $k = 3$, we need to extend the result slightly; denote by H the tree having six vertices, out of which two have degree 3 and the remaining four have degree 1. (Then H is a graph which "looks" like the letter H.)

Lemma 4.3 *$D(H) = -4$ and $W(L^3(H)) > W(H)$.*

Proof. Observe that $L(H)$ consists of two triangles sharing a common vertex, while $L^2(H)$ consists of a clique K_4, two vertices of which are adjacent to one extra vertex of degree 2, while the other two vertices of this clique are adjacent to another extra vertex of degree 2. It is easy to calculate that $W(H) = 29$, $W(L(H)) = 14$, $W(L^2(H)) = 21$ and $W(L^3(H)) = 64$, where $W(L^3(H))$ can be evaluated using distances between edges of $L^2(H)$. Hence $W(L^3(H)) > W(H)$ and $D(H) = 8 \cdot 21 - 4 \cdot 14 - 4 \cdot 29 = -4$. $\square$

Observe that every vertex of degree 1 in a 2^+-tree is adjacent to a vertex whose degree is at least 3.

Lemma 4.4 *Let T be a 2^+-tree and let a be a leaf of T. Let T' be the tree obtained from T by attaching k leaves at a, $k \geq 2$. Then $D(T') \geq D(T) + 20$.*

Proof. Many pairs of vertices have in T the same degrees and distance as in T'. These pairs we do not need to consider, as the corresponding terms will cancel out. We need to consider only the pairs involving a in both $D(T')$ and $D(T)$, and the pairs involving pendant vertices adjacent to a. Of course, we have to keep in mind that the degree of a is 1 in T and $k+1$ in T'. Hence, using Proposition 4.1 we obtain (the sum is over all $u \in V(T) \setminus \{a\}$)

$$\begin{aligned} D(T') - D(T) \;=\; & \sum_u \Big(d_u(k+1)\Big[2(d_u-1)k-1\Big] - 4\Big) d(u,a) \\ & + \sum_u \Big((d_u-1)k\Big[4(d_u-1)k-5\Big] + 1 \Big) \\ & - \sum_u \Big(d_u[-1] - 4 \Big) d(u,a) - \sum_u 1 \\ & + k\sum_u \Big(d_u[-1] - 4 \Big)\Big(d(u,a)+1 \Big) + k\sum_u 1 \end{aligned}$$

$$
\begin{aligned}
&+k\Big((k+1)[-1]-4\Big)\cdot 1+k\cdot 1+\binom{k}{2}\Big(1[-1]-4\Big)\cdot 2\\
&+\binom{k}{2}\cdot 1+\frac{1}{2}(k+1)k\Big[4k(k-1)-1\Big]-0\\
=\ &\sum_u\bigg(2k^2d_u\,(d_u-1)+2k\,d_u\,(d_u-1)\\
&\quad -d_u\,k-d_u-4+d_u+4-k\,d_u-4k\bigg)d(u,a)\\
&+\sum_u\bigg(4k^2(d_u-1)^2-5k(d_u-1)+1-1-k\,d_u-4k+k\bigg)\\
&-k^2-5k+k-5k^2+5k+\frac{k^2}{2}-\frac{k}{2}+2k^4-2k^2-\frac{k^2}{2}-\frac{k}{2}\\
=\ &k\sum_u\bigg(\Big(2k\,d_u\,(d_u-1)+2(d_u-1)^2-6\Big)d(u,a)\\
&\quad +4k(d_u-1)^2-6(d_u-1)-4\bigg)\\
&+2k^2(k^2-4).
\end{aligned}
$$

Let $g(u)=[2k\,d_u\,(d_u-1)+2(d_u-1)^2-6]d(u,a)+4k(d_u-1)^2-6(d_u-1)-4$. Then

$$D(T')-D(T)=k\sum_{u\in V(T)\setminus\{a\}}g(u)+2k^2(k^2-4).$$

If $d_u\geq 2$, then $2kd_u(d_u-1)+2(d_u-1)^2-6\geq 4$ and $(d_u-1)(4k(d_u-1)-6)-4\geq -2$, so that $g(u)\geq 4-2>0$. On the other hand, $g(u)=-6d(u,a)-4<0$ if $d_u=1$. Nevertheless, we show that $\sum_u g(u)\geq 10$.

Let S be the set of vertices of degree at least 3 in T. For every $u\in S$ denote by $S(u)$ the set consisting of u and all pendant vertices of T adjacent to u. Then $S(u)\cap S(u')=\emptyset$ for every $u,u'\in S$, $u\neq u'$. Since $\cup_{u\in S}S(u)$ contains all vertices of $V(T)\setminus\{a\}$, whose degree is different from 2, and since $g(v)>0$ if $d_v=2$, we have

$$\sum_v g(v)\geq\sum_{u\in S}\sum_{v\in S(u)}g(v).$$

Let $u\in S$. We find a lower bound for $\sum_{v\in S(u)}g(v)$. Suppose that u is adjacent to l leaves in T, where $l\leq d_u-1$. Then

$$
\begin{aligned}
\sum_{v\in S(u)}g(v)\ =\ &\Big(2k\,d_u\,(d_u-1)+2(d_u-1)^2-6\Big)d(u,a)+4k(d_u-1)^2\\
&-6(d_u-1)-4-6l\Big(d(u,a)+1\Big)-4l.
\end{aligned}
$$

Note that for every vertex v of degree 1 we have $g(v) < 0$. Since $l \le d_u - 1$, we obtain

$$\begin{aligned}\sum_{v \in S(u)} g(v) &\ge \Big(2k\, d_u\,(d_u - 1) + 2(d_u - 1)^2 - 6\Big) d(u,a) + 4k(d_u - 1)^2 \\ &\quad - 6(d_u - 1) - 4 - 6(d_u - 1)\Big(d(u,a) + 1\Big) - 4(d_u - 1) \\ &= \Big((2k\, d_u - 6)(d_u - 1) + 2(d_u - 1)^2 - 6\Big) d(u,a) \\ &\quad + \Big(4k(d_u - 1) - 16\Big)(d_u - 1) - 4.\end{aligned}$$

Since $k \ge 2$, $d_u \ge 3$ and $d(u,a) \ge 1$, we have

$$\sum_{v \in S(u)} g(v) \ge 14 d(u,a) - 4 \ge 10.$$

Notice that $2k^2(k^2 - 4) \ge 0$. As T is not a path, we have $|S| \ge 1$, so that

$$k \sum_{v} g(v) + 2k^2(k^2 - 4) \ge k \sum_{u \in S} \sum_{v \in S(u)} g(v) \ge \sum_{u \in S} 10k \ge 10k \ge 20.$$

□

Observe that $W(K_{1,3}) = 9$ while $W(L^i(K_{1,3})) = 3$ for $i \ge 1$, so that $D(K_{1,3}) = 8 \cdot 3 - 4 \cdot 3 - 4 \cdot 9 = -24$. Therefore $D(H) - D(K_{1,3}) = 20$, so that the statement of Lemma 4.4 is sharp.

Lemma 4.5 *Let T be a 2^+-tree, and let a be a vertex of degree $k+1$ in T, $k \ge 2$, such that a is adjacent to exactly k pendant vertices in T. Denote by a' the unique vertex adjacent to a, whose degree is greater than 1. Subdivide once the edge $a'a$ and denote the resulting graph by T'. Then $D(T') \ge D(T) + 8$.*

Proof. Analogously as in the proof of Lemma 4.4, it is enough to consider only those pairs of vertices, whose distance or degrees in T and T', are different. Denote by b the vertex subdividing the edge $a'a$ in T'. In $D(T')$ we need to add pairs containing b, as these pairs do not occure in terms of $D(T)$. Moreover, for all pairs which are connected by a path containing b, we need to increase their distance by 1. Finally, we need to include a single term depending on the degree of b. Hence, using Proposition 4.1 we obtain (the sum is over all $u \in V(T)$ such that $u - b$ path in T' does not contain a, and $d(u,a)$ is considered in T)

$$D(T') - D(T) = \sum_{u} \Big(2d_u \Big[2(d_u - 1) - 1\Big] - 4\Big) d(u,a)$$

$$
\begin{aligned}
& + \sum_u \Big((d_u - 1)\Big[4(d_u-1)-5\Big] + 1 \Big) \\
& + \Big(2(k+1)\Big[2k-1\Big] - 4\Big)\cdot 1 + k\Big[4k-5\Big] + 1 \\
& + k\Big(2[-1]-4\Big)\cdot 2 + k \\
& + \sum_u \Big(d_u\,(k+1)\Big[2(d_u-1)k-1\Big] - 4 \Big) \\
& + k\sum_u \Big(d_u\,[-1]-4\Big) + \frac{1}{2}2[-1] \\
= \; & \sum_u \Big(2d_u\,[2d_u-3]-4\Big) d(u,a) \\
& + \sum_u \Big[(d_u-1)(4d_u-6) - 3d_u + 3 + 1 + 2d_u\,k^2(d_u-1) \\
& \quad + d_u^2\,k + d_u^2\,k - 2d_u\,k - d_u\,k - d_u - 4 - k\,d_u - 4k \Big] \\
& + 4k^2 + 2k - 6 + 4k^2 - 5k + 1 - 12k + k - 1 \\
= \; & \sum_u \Big(\Big(2d_u\,[2d_u-3]-4\Big) d(u,a) + 2d_u\,k\Big(k(d_u-1)-2\Big) \\
& \quad + d_u\,(d_u\,k-4) + k(d_u^2-4) + (d_u-1)2(2d_u-3) \Big) \\
& + 2k(4k-7) - 6 \\
= \; & \sum_u h(u) + 2k(4k-7) - 6.
\end{aligned}
$$

Recall that $k \geq 2$. If $d_u \geq 2$ then $2d_u[2d_u-3]-4 \geq 0$, $k(d_u-1)-2 \geq 0$, $d_u k - 4 \geq 0$, $d_u^2 - 4 \geq 0$ and also $(d_u-1)2(2d_u-3) \geq 0$. Hence, $h(u) \geq 0$ in this case. On the other hand, $h(u) = -6d(u,a) - 6k - 4 < 0$ if $d_u = 1$. Nevertheless, we show that $\sum_u h(u) \geq 10$.

Analogously as in the proof of Lemma 4.4, let S be the set of vertices of degree at least 3 of $V(T) \setminus \{a\}$. For every $u \in S$ denote by $S(u)$ the set consisting of u and all pendant vertices of T adjacent to u. Then $S(u) \cap S(u') = \emptyset$ for every $u, u' \in S$, $u \neq u'$. Observe that $\cup_{u\in S} S(u)$ contains all vertices v of $V(T)$, for which $v-b$ path in T' does not contain a and which degree is different from 2. Since $h(v) \geq 0$ if $d_v = 2$, we have

$$
\sum_v h(v) \geq \sum_{u\in S} \sum_{v\in S(u)} h(v).
$$

Let $u \in S$. We find a lower bound for $\sum_{v\in S(u)} h(v)$. Suppose that u is adjacent to l leaves in T, where $l \le d_u - 1$. Then

$$\begin{aligned}\sum_{v\in S(u)} h(v) &= \Big(2d_u\,(2d_u-3)-4\Big)d(u,a) + 2d_u\,k\Big(k(d_u-1)-2\Big)\\ &\quad + d_u\,(d_u\,k-4) + k(d_u^2-4) + (d_u-1)2(2d_u-3)\\ &\quad - 6l\Big(d(u,a)+1\Big) - 6kl - 4l.\end{aligned}$$

Since for every vertex v of degree 1 we have $h(v) < 0$ and since $l \le d_u - 1$, we have

$$\begin{aligned}\sum_{v\in S(u)} h(v) &\ge \Big(2d_u\,(2d_u-3)-4\Big)d(u,a) + 2d_u\,k\Big(k(d_u-1)-2\Big)\\ &\quad + d_u\,(d_u\,k-4) + k(d_u^2-4) + (d_u-1)2(2d_u-3)\\ &\quad - 6(d_u-1)\Big(d(u,a)+1\Big) - 6k(d_u-1) - 4(d_u-1)\\ &= \Big(2d_u\,(2d_u-6)+2\Big)d(u,a) + 2d_u\,k\Big(k(d_u-1)-4\Big)\\ &\quad + d_u\,(2d_u\,k-2k-4) - 4k + (4d_u^2-10d_u+6)\\ &\quad - 6d_u + 6 + 6k - 4d_u + 4.\end{aligned}$$

Since $d_u \ge 3$, we have $2d_u - 6 \ge 0$ and consequently $2d_u(2d_u-6)+2 > 0$. Thus,

$$\begin{aligned}\sum_{v\in S(u)} h(v) &\ge (4d_u^2-12d_u+2) + 2d_u\,k\Big(k(d_u-1)-4\Big)\\ &\quad + d_u\,(2d_u\,k-2k-8) + (4d_u^2-16d_u+10) + 2k + 6\\ &= 2d_u\,k\Big(k(d_u-1)-4\Big) + 2d_u\,\Big(k(d_u-1)-4\Big)\\ &\quad + (8d_u^2-28d_u+12) + 2(k+3)\\ &= 2d_u\,(k+1)\Big(k(d_u-1)-4\Big) + 4(2d_u-1)(d_u-3) + 2(k+3).\end{aligned}$$

Since $d_u \ge 3$ and $k \ge 2$, we have $k(d_u-1)-4 \ge 0$ and $d_u - 3 \ge 0$, so that

$$\sum_{v\in S(u)} h(v) \ge 2(k+3) \ge 10.$$

Since $k \ge 2$, we have $2k(4k-7)-6 \ge -2$. As T is not a path, we have $|S| \ge 1$, so that

$$\sum_{v} h(v) + 2k(k-7) - 6 \ge \sum_{u\in S}\sum_{v\in S(u)} h(v) - 2 \ge \sum_{u\in S} 10 - 2 \ge 10 - 2 \ge 8.$$

$\square$

Denote by H^s the tree obtained by subdividing the central edge of H. Since $W(H^s) = 48$, $W(L(H^s)) = 27$ and $W(L^2(H^s)) = 38$, we have $D(H^s) = 4$. By Lemma 4.3 $D(H) = -4$, so that Lemma 4.5 is sharp for $T = H$.

Proof of Theorem 1.5. By induction we prove that $D(T) \geq 0$ if T is 2^+-tree different from $K_{1,3}$ and H. If T is a star $K_{1,k}$, $k \geq 4$, then $D(T) \geq 0$ by Lemma 4.2, while $D(H) = -4$ by Lemma 4.3. Thus, suppose that T has at least two vertices of degree at least 3 and T is different from H.

Denote by T^* the subgraph of T formed by vertices of degree at least 2. Then T^* is a nontrivial tree, so that it has at least two pendant vertices. Denote by a a pendant vertex of T^*, whose degree in T is the smallest possible. Moreover, denote by v the vertex of T^* which is adjacent to a. Consider the degree of v in T. We distinguish two cases.

- $d_v \geq 3$: Remove from T all pendant vertices adjacent to a, together with the corresponding edges, and denote the resulting graph by T'. In T' the vertex a has degree 1 and is adjacent to v, where $d_v \geq 3$. Thus, T' is a 2^+-tree. Since $T \neq H$, by the choice of a if T' has only one vertex of degree at least 3, then T' is $K_{1,k}$, where $k \geq 4$, so that $D(T') \geq 0$, by Lemma 4.2. If T' has at least two vertices of degree at least 3, then $D(T') = -4$ if T' is H by Lemma 4.3, while otherwise $D(T') \geq 0$ by induction. Since $D(T) \geq D(T') + 20$ by Lemma 4.4, we have $D(T) \geq 0$.

- $d_v = 2$: Denote by a' the vertex of T adjacent to v, $a' \neq a$. Remove from T the vertex v and the edges va and va', insert the edge aa', and denote the resulting graph by T'. Then T' is a 2^+-tree having at least two vertices of degree at least 3. Hence $D(T') = -4$ if $T' = H$ by Lemma 4.3, while otherwise $D(T') \geq 0$ by induction. Since $D(T) \geq D(T') + 8$ by Lemma 4.5, we have $D(T) \geq 0$.

Hence, in both cases we have $D(T) \geq 0$. Since $D(T) = 4[2W(L^2(T)) - W(L(T)) - W(T)]$, by Corollary 1.4, we have $W(L^3(T)) > W(T)$ for every 2^+-tree different from $K_{1,3}$ and H.

By Lemma 4.3 we have also $W(L^3(H)) > W(H)$, so that $W(L^3(T)) > W(T)$ for every 2^+-tree different from $K_{1,3}$. $\square$

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