A class of trees and its Wiener index.*

Stephan G. Wagner

Department of Mathematics
Graz University of Technology
Steyrergasse 30, A-8010 Graz, Austria
wagner@finanz.math.tu-graz.ac.at

Abstract

In this paper, we will consider the Wiener index for a class of trees that is connected to partitions of integers. Our main theorem is the fact that every integer ≥ 470 is the Wiener index of a member of this class. As a consequence, this proves a conjecture of Lepović and Gutman. The paper also contains extremal and average results on the Wiener index of the studied class.

Mathematics Subject Classifications (2000): 05C12, 05C05.

Key words: Wiener index, trees, partitions.

1 Introduction

Let G denote a simple, connected tree. Throughout this paper, we will use the graph-theoretical notation from [1]. The Wiener index of G is defined by

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v), \tag{1}$$

where $d_G(u,v)$ denotes the distance of u and v. Obviously, $W(G)/\binom{|V(G)|}{2}$ gives the average distance between the vertices of G. It was first studied by Harold Wiener in 1947 for acyclic molecular graphs G. The Wiener index is one of the most popular topological indices in combinatorial chemistry.

There is a lot of mathematical and chemical literature on the Wiener index, especially on the Wiener index of trees – [2] gives a summary of known results and open problems and conjectures. One major problem for many topological

*This work was supported by Austrian Science Fund project no. S-8307-MAT.

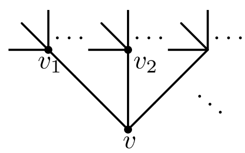
indices is the so-called "inverse" problem, i.e. finding a graph from a certain class given its index.

A conjecture of Lepović and Gutman [6] states that there is some bound M such that for all $w \geq M$ there is a tree T of Wiener index $W(T) = w$. The proof of their conjecture will be the main result of this paper. To prove our result, we investigate a class of trees we will call "star-like". It is the class of all trees with diameter ≤ 4. However, there is another class of trees – the trees with only one vertex of degree > 2 – that is also called "star-like" in some papers, e.g. [3]. The star-like trees of this paper have been studied in [5] for another topological index, and they turned out to be quite useful in that context. Here, we will even be able to give an easy and explicit construction of a tree T, given its Wiener index $W(T)$.

In the second section, we will develop the necessary preliminaries for our theorems. The third section deals with an extremal result – we will characterize the star-like tree of maximal Wiener index. Section 4 will contain the proof of our main result. The last chapter is devoted to the asymptotical analysis of the Wiener index of star-like trees.

2 Preliminaries

Definition 1 Let $(c_1, \ldots, c_d)$ be a partition of n. The star-like tree assigned to this partition is the tree



where $v_1, \ldots, v_d$ have degree $c_1, \ldots, c_d$ respectively. It has exactly n edges. The tree itself is denoted by $S(c_1, \ldots, c_d)$, its Wiener index by $W(c_1, \ldots, c_d)$.

Lemma 1

$$W(c_1, \ldots, c_d) = 2n^2 - (d-1)n - \sum_{i=1}^{d} c_i^2. \tag{2}$$

Proof: For all pairs (x, y) of vertices in $S(c_1, \ldots, c_d)$, we have $d(x, y) \leq 4$. Thus we only have to count the number of pairs (x, y) with $d(x, y) = k$, for $1 \leq k \leq 4$. We divide the vertices into three groups - the center v, the neighbors $v_1, \ldots, v_d$ of the center, and the leaves $w_1, \ldots, w_{n-d}$.

- Obviously, there are n pairs with $d(x, y) = 1$.

- All pairs of the form $(x, y) = (v, w_i)$, $(x, y) = (v_i, v_j)$ or $(x, y) = (w_i, w_j)$ (where w_i, w_j are neighbors of the same v_k) satisfy $d(x, y) = 2$. There are

$$(n-d) + \binom{d}{2} + \sum_{i=1}^{d} \binom{c_i - 1}{2}$$

such pairs.

- For all pairs of the form $(x, y) = (v_i, w_j)$ with $v_i \not\sim w_j$ we have $d(x, y) = 3$. The number of these pairs is

$$\sum_{i=1}^{d} (n - d - c_i + 1).$$

- Finally, $d(w_i, w_j) = 4$ if w_i, w_j are not neighbors of the same v_k. There are

$$\binom{n-d}{2} - \sum_{i=1}^{d} \binom{c_i - 1}{2}$$

such pairs.

Summing up, the Wiener index of $S(c_1, \ldots, c_d)$ is

$$\begin{aligned} W(c_1, \ldots, c_d) = n + 2 \left((n-d) + \binom{d}{2} + \sum_{i=1}^{d} \binom{c_i - 1}{2} \right) + 3 \sum_{i=1}^{d} (n - d - c_i + 1) \\ + 4 \left(\binom{n-d}{2} - \sum_{i=1}^{d} \binom{c_i - 1}{2} \right). \end{aligned}$$

Simple algebraical manipulations yield

$$\begin{aligned} W(c_1, \ldots, c_d) &= n + 2(n-d) + d^2 - d + \sum_{i=1}^{d} (c_i^2 - 3c_i + 2) + 3d(n - d + 1) \\ &\quad - 3 \sum_{i=1}^{d} c_i + 2(n-d)(n-d-1) - 2 \sum_{i=1}^{d} (c_i^2 - 3c_i + 2) \\ &= 2n^2 + n + 2d - dn - \sum_{i=1}^{d} (c_i^2 + 2) \\ &= 2n^2 - (d-1)n - \sum_{i=1}^{d} c_i^2. \end{aligned}$$

$\square$

3 An extremal result

Clearly, as the star is the tree of minimal Wiener index, it is also the star-like tree of minimal Wiener index. Now, this section will be devoted to the characterization of the star-like tree of maximal Wiener index. First, we note the following:

Lemma 2 If a partition contains two parts c_1, c_j such that $c_i \geq c_j + 2$, the corresponding Wiener index increases if they are replaced by $c_i - 1, c_j + 1$.

Proof: Obviously, n and d remain unchanged. The only term that changes is the sum $\sum_i c_i^2$, and the difference is

$$c_i^2 + c_j^2 - (c_i - 1)^2 - (c_j + 1)^2 = 2(c_i - c_j - 1) > 0.$$

□

Therefore, if a partition satisfies the condition of the lemma, its Wiener index cannot be maximal. So we only have to consider partitions consisting of two different parts k and $k + 1$. Let $r < d$ be the number of $k + 1$'s and $d - r$ the number of k's. Then $n = kd + r$ and we have to maximize

$$2n^2 + n - dn - r(k + 1)^2 - (d - r)k^2.$$

We neglect the constant part $2n^2 + n$ and arrive – after some easy manipulations – at the minimization of the expression

$$n(k + d) + r(k + 1)$$

subject to the restrictions that $kd + r = n$ and $r < d$. We assume that $k \leq d$ – otherwise, we may change the roles of k and d, decreasing the term $r(k + 1)$. Next, we note that $k + d$ is an integer and $r(k + 1) = kr + r < kd + r = n$. Therefore, the expression can only be minimal if $k + d$ is. But

$$k + d = \left\lfloor \frac{n}{d} \right\rfloor + d = \left\lfloor \frac{n}{d} + d \right\rfloor,$$

and the function $f(x) = \frac{n}{x} + x$ is convex and attains its minimum at $x = \sqrt{n}$. So $k + d$ is minimal if either $d = \lfloor \sqrt{n} \rfloor$ or $d = \lceil \sqrt{n} \rceil$ (and perhaps, for other values of d, too). If we write $n = Q^2 + R$, where $0 \leq R \leq 2Q$, we see that the minimum of $k + d$ is

$$\begin{cases} 2Q & R < Q \\ 2Q + 1 & Q \leq R \leq 2Q. \end{cases}$$

In the first case, we write $d = Q + S$ and $k = Q - S$. Then we have $r = S^2 + R$ and thus

$$r(k + 1) = (S^2 + R)(Q - S + 1) = -S^3 + (Q + 1)S^2 - RS + (Q + 1)R.$$

For $1 \leq S \leq Q$, we have

$$S^2-(Q+1)S+R = (S-(Q+1)/2)^2-(Q+1)^2/4+R \leq (Q-1)^2/4-(Q+1)^2/4+R = R-Q < 0$$

and thus

$$-S^3+(Q+1)S^2-RS > 0.$$

So the minimum in this case is obtained when $S=0$ or $k=d=Q=\lfloor\sqrt{n}\rfloor$. Analogously, we write $d=Q+1+S$ and $k=Q-S$ in the second case. Again, we obtain the minimum for $S=0$ or $d=Q+1=\lceil\sqrt{n}\rceil$ and $k=Q=\lfloor\sqrt{n}\rfloor$. Summing up, we have the following theorem:

Theorem 3 *The star-like tree with n edges of maximal Wiener index is the tree corresponding to the partition*

$$(k,\dots,k,k+1,\dots,k+1),$$

where $k=\lfloor\sqrt{n}\rfloor$. The part k appears k^2+k-n times if $k^2+k>n$ and $k^2+2k+1-n$ times otherwise. The part $k+1$ appears $n-k^2$ times if $k^2+k>n$ and $n-k^2-k$ times otherwise.

Remark: A short calculation shows that the maximal Wiener index of a star-like tree is asymptotically

$$2n^2-2n\sqrt{n}+n+O(\sqrt{n}).$$

4 Main result

Lepović and Gutman [6] conjectured that there are only finitely many “forbidden values” for the Wiener index of trees. In particular, they claimed that all natural numbers, except 2, 3, 5, 6, 7, 8, 11, 12, 13, 14, 15, 17, 19, 21, 22, 23, 24, 26, 27, 30, 33, 34, 37, 38, 39, 41, 43, 45, 47, 51, 53, 55, 60, 61, 69, 73, 77, 78, 83, 85, 87, 89, 91, 99, 101, 106, 113, 147 and 159, are Wiener indices of trees. By an extensive computer search, they were able to prove that any other “forbidden value” must exceed 1206.

This chapter deals with the proof of their conjecture. We will even show a stronger result: every integer ≥ 470 is the Wiener index of a star-like tree. By Lemma 1, this is equivalent to showing that every integer ≥ 470 is of the form

$$2n^2-(d-1)n-\sum_{i=1}^{d} c_i^2$$

for some partition $(c_1,\dots,c_d)$ of n. First, we consider the special case of partitions of the form

$$p(l,k) = (\underbrace{2,\dots,2}_{l\text{ times}},\underbrace{1,\dots,1}_{k\text{ times}}).$$

By Lemma 1, the Wiener index of the corresponding star-like tree is

$$w(l,k) = 2 \cdot (2l+k)^2 - (l+k-1) \cdot (2l+k) - (4l+k) = 6l^2 + (5k-2)l + k^2.$$

Next, we need a simple lemma similar to Lemma 2.

Lemma 4 If a partition contains the part $c \geq 2$ twice, and if these parts are replaced by $c+1$ and $c-1$, the corresponding Wiener index decreases by 2.

Proof: Obviously, n and d remain unchanged. The only term that changes is the sum $\sum_i c_i^2$, and the difference is $(c+1)^2 + (c-1)^2 - 2c^2 = 2$. □

Definition 2 Replacing a pair (c,c) by $(c+1, c-1)$ is called a "splitting step". By $s(l)$, we denote the number of splitting steps that one can take beginning with a sequence of l 2's.

Applying Lemma 4 $s(l)$ times, beginning with the partition $p(l,k)$, one can construct star-like trees of Wiener index $w(l,k), w(l,k)-2, \ldots, w(l,k)-2s(l)$. Our next goal is to show that there is a $c > 1$ such that $s(l) > cl$ if l is large enough (indeed, one can prove that $s(l)/l$ tends to infinity for $l \to \infty$).

Lemma 5 For all $l \geq 0$, $s(l) \geq \frac{19l-77}{16}$.

Proof: First, $\lfloor \frac{l}{2} \rfloor \geq \frac{l-1}{2}$ splitting steps can be taken using pairs of 2's. Then, $\lfloor \frac{l}{4} \rfloor \geq \frac{l-3}{4}$ splitting steps can be taken using pairs of 3's. Now, we may split the 4's and 2's ($\lfloor \frac{l}{8} \rfloor \geq \frac{l-7}{8}$ pairs each), and finally the 5's and 3's ($\lfloor \frac{l}{16} \rfloor \geq \frac{l-15}{16}$ and $\lfloor \frac{l}{8} \rfloor \geq \frac{l-7}{8}$ pairs respectively). This gives a total of at least $\frac{19l-77}{16}$ splitting steps, all further possible steps are ignored. □

It is not difficult to determine $s(l)$ explicitly for small l. We obtain the following table:

l	2	3	4	5	6	7	8	9	10	11	12	13	14	15
$s(l)$	1	1	3	4	4	7	9	10	10	14	17	19	20	20
l	16	17	18	19	20	21	22	23	24	25	30	50	75	100
$s(l)$	25	29	32	34	35	35	41	46	50	53	69	155	283	445

Trivially, $s(l)$ is a non-decreasing function. Therefore, this table, together with Lemma 5, shows that $s(l) \geq l+5$ for $l \geq 12$ and $s(l) \geq l+9$ for $l \geq 16$.

Now, we are able to prove the following propositions:

Proposition 6 Every even integer $W \geq 1506$ is the Wiener index of a star-like tree.

Proof: It was mentioned that one can construct star-like trees of Wiener index $w(l,k), w(l,k)-2, \ldots, w(l,k)-2s(l)$. For $k = 0, 2, 4, 6, 8, 10$ and $l = x+1-k/2$, we have $w(l,k) = 6x^2+(10-k)x+4$. For $x \geq 16$, $l \geq 12$ and thus $s(l) \geq l+5 \geq l+k/2 = x+1$. Thus, all even numbers in the interval

$$[6x^2+(10-k)x+4-2(x+1), 6x^2+(10-k)x+4] = [6x^2+(8-k)x+2, 6x^2+(10-k)x+4]$$

are Wiener indices of star-like trees. The union of these intervals (over k) is

$$[6x^2-2x+2, 6x^2+10x+4] = [6x^2-2x+2, 6(x+1)^2-2(x+1)]$$

Finally, the union of these intervals (over all $x \geq 16$) is $[1506, \infty)$. Thus, all even integers ≥ 1506 are Wiener indices of star-like trees. $\square$

Proposition 7 Every odd integer $W \geq 2385$ is the Wiener index of a star-like tree.

Proof: First, let x be an even number, and let $k = 15, 1, 11, 21, 7, 17$ and $l = x-6, x, x-4, x-8, x-2, x-6$ respectively. Then we obtain the following table:

k	l	$w(l,k)$
15	$x-6$	$6x^2+x+3$
1	x	$6x^2+3x+1$
11	$x-4$	$6x^2+5x+5$
21	$x-8$	$6x^2+7x+1$
7	$x-2$	$6x^2+9x+7$
17	$x-6$	$6x^2+11x+7$

For $x \geq 20$, we have $l \geq 12$ in all cases and thus $s(l) \geq l+5$. Using the same argument as in the previous proof, all odd numbers (as x is even, the terms $w(l,k)$ are indeed all odd) in the following intervals are Wiener indices of star-like trees:

k	l	Interval
15	$x-6$	$[6x^2-x+5, 6x^2+x+3]$
1	x	$[6x^2+x-9, 6x^2+3x+1]$
11	$x-4$	$[6x^2+3x+3, 6x^2+5x+5]$
21	$x-8$	$[6x^2+5x+7, 6x^2+7x+1]$
7	$x-2$	$[6x^2+7x+1, 6x^2+9x+7]$
17	$x-6$	$[6x^2+9x+9, 6x^2+11x+7]$

The union over all these intervals (considering odd numbers only) is $[6x^2-x+5, 6x^2+11x+7]$.

Now, on the other hand, let x be odd, and take $k = 3, 13, 23, 9, 19, 5$ and

$l = x-1, x-5, x-9, x-3, x-7, x-1$ respectively. Then we obtain the following table:

k	l	$w(l,k)$
3	$x-1$	$6x^2+x+2$
13	$x-5$	$6x^2+3x+4$
23	$x-9$	$6x^2+5x-2$
9	$x-3$	$6x^2+7x+6$
19	$x-7$	$6x^2+9x+4$
5	$x-1$	$6x^2+11x+8$

Now, for $x \geq 21$, we have $l \geq 12$ in all cases and thus $s(l) \geq l+5$; furthermore, $x-3 \geq 18$ and thus $s(x-3) \geq (x-3)+9 = x+6$. Therefore, all odd numbers in the following intervals are Wiener indices of star-like trees:

k	l	Interval
3	$x-1$	$[6x^2-x-6, 6x^2+x+2]$
13	$x-5$	$[6x^2+x+4, 6x^2+3x+4]$
23	$x-9$	$[6x^2+3x+6, 6x^2+5x-2]$
9	$x-3$	$[6x^2+5x-6, 6x^2+7x+6]$
19	$x-7$	$[6x^2+7x+8, 6x^2+9x+4]$
5	$x-1$	$[6x^2+9x, 6x^2+11x+8]$

The union over all these intervals (considering odd numbers only) is $[6x^2-x-6, 6x^2+11x+8]$. Combining the two results, we see that for any $x \geq 20$, all odd integers in the interval

$$[6x^2-x+4, 6x^2+11x+8] = [6x^2-x+4, 6(x+1)^2-(x+1)+3]$$

are Wiener indices of star-like trees. The union of these intervals (over all $x \geq 20$) is $[2384, \infty)$. $\square$

It is not difficult to check (by means of a computer) that all integers $470 \leq W \leq 2384$ can be written as $W = W(S)$ for a star-like tree S with ≤ 40 edges. Therefore, we obtain

Theorem 8 (Main Theorem) *The list of Lepović and Gutman is complete, and all integers not appearing in their list are Wiener indices of trees.*

Remark: There are only 55 further values which are Wiener indices of trees, but not of star-like trees, namely 35, 50, 52, 56, 68, 71, 72, 75, 79, 92, 94, 98, 119, 123, 125, 127, 129, 131, 133, 135, 141, 143, 149, 150, 152, 156, 165, 181, 183, 185, 187, 193, 195, 197, 199, 203, 217, 219, 257, 259, 261, 263, 267, 269, 279, 281, 285, 293, 351, 355, 357, 363, 369, 453 and 469.

EXAMPLE: Suppose we want to construct a star-like tree of Wiener index 9999. This number is odd, and it is contained in the interval

$$[9564 = 6 \cdot 40^2 - 40 + 4, 6 \cdot 40^2 + 11 \cdot 40 + 8 = 10048].$$

40 is even, so we use the first case of proposition 7. 9999 is contained in

$$[9969 = 6 \cdot 40^2 + 9 \cdot 40 + 9, 6 \cdot 40^2 + 11 \cdot 40 + 7 = 10047],$$

so we start with the partition $(2, \ldots, 2, 1, \ldots, 1)$ consisting of $40 - 6 = 34$ 2's and 17 1's. As $10047 - 9999 = 48$, 24 splitting steps are necessary. After 17 splitting steps, we have the partition containing 17 3's and 34 1's. After 7 further steps, we arrive at the partition

$$(\underbrace{4, \ldots, 4}_{7 \text{ times}}, \underbrace{3, \ldots, 3}_{3 \text{ times}}, \underbrace{2, \ldots, 2}_{7 \text{ times}}, \underbrace{1, \ldots, 1}_{34 \text{ times}}).$$

Indeed, the Wiener index of the corresponding star-like tree with 85 edges is

$$2 \cdot 85^2 - (51 - 1) \cdot 85 - 7 \cdot 4^2 - 3 \cdot 3^2 - 7 \cdot 2^2 - 34 \cdot 1^2 = 9999.$$

REMARK: The proof of the theorem generalizes in some way to the modified Wiener index of the form

$$W_\lambda(G) := \sum_{\{u,v\} \subseteq V(G)} d_G(u, v)^\lambda$$

for positive integers λ. Using essentially the same methods together with the fact that $s(l)$ grows faster than any linear polynomial, one can show the following: if there is some star-like tree T such that $W(T) \equiv r \mod 2^\lambda(2^\lambda - 1)$, then all members of the residue class r modulo $2^\lambda(2^\lambda - 1)$ – with only finitely many exceptions – are Wiener indices of trees. For $\lambda = 2, 3, 5, 6, 7, 9, 10$, this implies that all integers, with finitely many exceptions, can be written as $W_\lambda(T)$ for some star-like tree T, as all residue classes modulo $2^\lambda(2^\lambda - 1)$ are covered. Unfortunately, for $\lambda = 4$ and all other multiples of 4, this is not the case any more.

5 The average Wiener index of a star-like tree

Finally, one might ask for the average size of $W(T)$ for a star-like tree with n edges. First we note that the correlation between partitions of n and star-like trees with n edges is almost bijective: given a tree of diameter 4, the center is uniquely defined, being the center of a path of length 4. For trees of diameter 3 (which have the form of "double-stars", there are two possible centers, giving the representations $S(k, 1, \ldots, 1)$ and $S(n + 1 - k, 1, \ldots, 1)$. The star (with diameter 2) has the two representation $S(n)$ and $S(1, \ldots, 1)$. It follows that there are only $\lfloor \frac{n}{2} \rfloor$ exceptional trees belonging to two different partitions. This number, as well as the sum of their Wiener indices, is small compared to $p(n)$, So, we mainly have to determine the asymptotics of

$$\frac{1}{p(n)}\left(\sum_c \left(2n^2-(d-1)n-\sum_{i=1}^d c_i^2\right)\right),$$

where the sum goes over all partitions c of n and d denotes the length of c. For the average length of a partition, an asymptotic formula is known (see [4]):

$$\frac{1}{p(n)}\sum_c d = \frac{\sqrt{n}}{\nu}\Big(\log n + 2\gamma - 2\log(\nu/2)\Big) + O\Big((\log n)^3\Big), \tag{3}$$

where $\nu = \sqrt{2/3}\,\pi$ and γ is Euler's constant. Thus, our main problem is to find the asymptotics of the sum

$$\sum_c \sum_{i=1}^d c_i^2. \tag{4}$$

First, we have the following generating function for this expression:

Lemma 9 The generating function of (4) is given by $S(z)F(z)$, where

$$S(z) = \sum_{i=1}^\infty \frac{i^2 z^i}{1-z^i}$$

is the generating function of $\sigma_2(n) = \sum_{d|n} d^2$ and

$$F(z) = \prod_{i=1}^\infty (1-z^i)^{-1}$$

is the generating function of the partition function $p(n)$.

Proof: This is simply done by some algebraic transformations: the number of k's in all partitions of n is $p(n-k)+p(n-2k)+\ldots$. Therefore,

$$\begin{aligned}\sum_c \sum_{i=1}^d c_i^2 &= \sum_{k\geq 1} k^2 \sum_{i\geq 1} p(n-ik)\\ &= \sum_{m\geq 1}\sum_{d|m} d^2 p(n-m)\\ &= \sum_{m\geq 1} \sigma_2(m)p(n-m).\end{aligned}$$

So the expression (4) is indeed the convolution of σ_2 and p, which proves the lemma. □

Now, we can proceed along the same lines as in [4]. We use the following lemmas:

Lemma 10 (Newman [7]) Let

$$\phi(z) = \sqrt{\frac{1-z}{2\pi}}\ \exp\left(\frac{\pi^2}{12}\Big(-1+\frac{2}{1-z}\Big)\right).$$

Then we have

$$|F(z)| < \exp\Big(\frac{1}{1-|z|}+\frac{1}{|1-z|}\Big) \tag{5}$$

for $|z|<1$ and

$$F(z) = \phi(z)(1+O(1-z)) \tag{6}$$

for $|1-z| \le 2(1-|z|)$ and $|z|<1$.

Lemma 11 Let

$$\psi(z) = \frac{2\zeta(3)}{(1-z)^3},$$

where $\zeta(s)$ denotes the Riemann ζ-function. Then we have

$$|S(z)| \le \frac{4}{(1-|z|)^3} \tag{7}$$

for $|z|<1$ and

$$S(z) = \psi(z) + O(|1-z|^{-2}) \tag{8}$$

for $|1-z| \le 2(1-|z|)$ and $\frac{1}{3} \le |z| < 1$.

Proof: For $|z|<1$, we obtain

$$\begin{aligned}
|S(z)| &\le \frac{1}{1-|z|}\sum_{i=1}^{\infty}\frac{i^2|z|^i}{1+|z|+\ldots+|z|^{i-1}}\\
&= \frac{1}{1-|z|}\sum_{i=1}^{\infty}\frac{i^2|z|^{(i+1)/2}}{|z|^{-(i-1)/2}+|z|^{-(i-1)/2+1}+\ldots+|z|^{(i-1)/2}}\\
&\le \frac{1}{1-|z|}\sum_{i=1}^{\infty}\frac{i^2|z|^{(i+1)/2}}{i} = \frac{1}{1-|z|}\sum_{i=1}^{\infty} i|z|^{(i+1)/2}\\
&= \frac{|z|}{(1-|z|)(1-\sqrt{|z|})^2} \le \frac{4}{(1-|z|)^3}.
\end{aligned}$$

Now, let $z=e^{-u}$. By the Euler-Maclaurin summation formula, we have

$$S(e^{-u}) = \sum_{i=1}^{\infty}\frac{i^2}{e^{iu}-1} = \int_0^{\infty}\frac{t^2}{e^{tu}-1}\,dt - \int_0^{\infty}\Big(\{t\}-\frac{1}{2}\Big)\frac{-2t+e^{ut}(2t-ut^2)}{(e^{ut}-1)^2}\,dt.$$

Now

$$\int_0^{\infty}\frac{t^2}{e^{tu}-1}\,dt = \frac{1}{u^3}\int_0^{\infty}\frac{s^2}{e^s-1}\,ds = \frac{1}{u^3}\int_0^{\infty}\sum_{i=1}^{\infty}s^2e^{-is}\,ds = \frac{1}{u^3}\sum_{i=1}^{\infty}\frac{2}{i^3} = \frac{2\zeta(3)}{u^3}$$

and, for $v = \operatorname{Re} u$,

$$\begin{aligned}
\Big|\int_0^\infty \Big(\{t\} - \frac{1}{2}\Big)\frac{-2t + e^{ut}(2t - ut^2)}{(e^{ut}-1)^2}\,dt\Big| &\le \frac{1}{2}\int_0^\infty \left|\frac{-2t + e^{ut}(2t - ut^2)}{(e^{ut}-1)^2}\right| dt \\
&\le \frac{1}{2}\int_0^\infty \left|\frac{2t}{e^{ut}-1}\right| dt + \frac{1}{2}\int_0^\infty \left|\frac{ut^2e^{ut}}{(e^{ut}-1)^2}\right| dt \\
&\le \int_0^\infty \frac{t}{e^{vt}-1}\,dt + \frac{|u|}{2}\int_0^\infty \frac{t^2e^{vt}}{(e^{vt}-1)^2}\,dt \\
&= \frac{1}{v^2}\int_0^\infty \frac{s}{e^s-1}\,ds + \frac{|u|}{2v^3}\int_0^\infty \frac{s^2e^s}{(e^s-1)^2}\,ds \\
&= O(v^{-2}) + O(|u|v^{-3}) = O(|u|v^{-3}).
\end{aligned}$$

If $|1-z| \le 2(1-|z|)$ and $\frac{1}{3} \le |z| < 1$, $|u|/v$ is bounded by some constant K. Therefore, the latter expression is $O(|u|^2)$. Replacing u by $-\log z = 1 - z + O(|1-z|^2)$ gives us the desired result. $\square$

Proposition 12 If $s(n) = \sum_c \sum_{i=1}^d c_i^2$ and $F(z)\psi(z) = \sum_{n=0}^\infty s'(n)z^n$, then

$$s(n) = s'(n) + O\Big(n^{1/4}\exp(\pi\sqrt{2n/3})\Big). \tag{9}$$

Proof: Let $\mathcal{C} = \{z \in \mathbb{C} \mid |z| = 1 - \pi/\sqrt{6n}\}$. Then, by Cauchy's residue theorem,

$$s(n) - s'(n) = \frac{1}{2\pi i}\int_{\mathcal{C}} \frac{(FS - F\psi)(z)}{z^{n+1}}\,dz.$$

We split $\mathcal{C}$ into two parts: $\mathcal{A} = \{z \in \mathcal{C}\ |1-z| < \pi\sqrt{2/(3n)}\}$ and $\mathcal{B} = \mathcal{C} \setminus \mathcal{A}$. On $\mathcal{A}$, we use the approximations (6) and (8) from Lemmas 10 and 11:

$$\begin{aligned}
I_{\mathcal{A}} &= \Big|\frac{1}{2\pi i}\int_{\mathcal{A}} \frac{(FS - F\psi)(z)}{z^{n+1}}\,dz\Big| \\
&\ll \int_{\mathcal{A}} \frac{|\phi(z)|}{|1-z|^2|z|^{n+1}}\,dz \\
&\ll \int_{\mathcal{A}} |1-z|^{-3/2}\exp\Big(\frac{\pi^2}{6(1-|z|)}\Big)|z|^{-n}\,dz \\
&\ll n^{3/4}\exp(\pi\sqrt{n/6})\exp(\pi\sqrt{n/6})n^{-1/2} \\
&= n^{1/4}\exp(\pi\sqrt{2n/3}).
\end{aligned}$$

Similarly, on $\mathcal{B}$, we use (5) together with the estimate $\psi(z), S(z) \ll (1-|z|)^{-3}$ from Lemma 11:

$$\begin{aligned}
I_{\mathcal{B}} &= \Big|\frac{1}{2\pi i}\int_{\mathcal{B}} \frac{(FS - F\psi)(z)}{z^{n+1}}\,dz\Big| \\
&\ll \int_{\mathcal{B}} \exp\Big(\frac{1}{|1-z|} + \frac{1}{1-|z|}\Big)\cdot\frac{1}{(1-|z|)^3}\cdot |z|^{-n}\,dz \\
&\ll \exp\Big(\sqrt{\frac{3n}{2\pi^2}} + \sqrt{\frac{6n}{\pi^2}}\Big) n^{3/2} \exp\Big(\sqrt{\frac{\pi^2 n}{6}}\Big) \\
&= \exp\Big(\frac{9+\pi^2}{\pi\sqrt{6}}\sqrt{n}\Big) n^{3/2} \\
&\ll \exp\Big(\frac{2\pi^2}{\pi\sqrt{6}}\sqrt{n}\Big) = \exp(\pi\sqrt{2n/3}).
\end{aligned}$$

Thus

$$|s(n) - s'(n)| \le I_{\mathcal{A}} + I_{\mathcal{B}} = O\Big(n^{1/4}\exp(\pi\sqrt{2n/3})\Big).$$

□

Proposition 13

$$s'(n) = \frac{12\sqrt{6}\zeta(3)}{\pi^3} p(n)(n^{3/2} + O(n(\log n)^2)). \tag{10}$$

Proof: From the definition of $s'(n)$, we have

$$s'(n) = 2\zeta(3)\sum_{k=0}^{n}\binom{k+2}{2} p(n-k).$$

We divide the sum into three parts and use the well-known estimate

$$p(n) = \frac{e^{\nu\sqrt{n}}}{4\sqrt{3}n} + O\Big(\frac{e^{\nu\sqrt{n}}}{n^{3/2}}\Big),$$

which follows directly from Rademachers asymptotic formula ([8], cf. also [4]). The first sum is

$$A_1 = \sum_{k>n/2}\binom{k+2}{2} p(n-k) \ll n^3 p(n/2) \ll n^2 e^{\nu\sqrt{n}/2},$$

the second sum is

$$
\begin{aligned}
A_2 &= \sum_{n/2 \ge k > \sqrt{n}\log n/\nu} \binom{k+2}{2} p(n-k) \\
&\ll \sum_{n/2 \ge k > \sqrt{n}\log n/\nu} k^2 \frac{e^{\nu\sqrt{n-k}}}{n-k}\Big(1 + O\Big(\frac{1}{\sqrt{n-k}}\Big)\Big) \\
&\ll \frac{1}{n} e^{\nu\sqrt{n}} \sum_{k > \sqrt{n}\log n/\nu} k^2 e^{\nu(\sqrt{n-k}-\sqrt{n})} \le \frac{1}{n} e^{\nu\sqrt{n}} \sum_{k > \sqrt{n}\log n/\nu} k^2 e^{-(\nu k)/(2\sqrt{n})} \\
&\sim \frac{1}{n} e^{\nu\sqrt{n}} \int_{\sqrt{n}\log n/\nu}^{\infty} t^2 e^{-(\nu t)/(2\sqrt{n})}\, dt = \frac{1}{n} e^{\nu\sqrt{n}} e^{-(\log n)/2} \frac{2 + \log n + (\log n)^2/4}{(\nu/(2\sqrt{n}))^3} \\
&\ll (\log n)^2 e^{\nu\sqrt{n}},
\end{aligned}
$$

and the third sum, which gives the main part,

$$
\begin{aligned}
A_3 &= \sum_{k \le \sqrt{n}\log n/\nu} \binom{k+2}{2} p(n-k) \\
&= \sum_{k \le \sqrt{n}\log n/\nu} \binom{k+2}{2} \frac{e^{\nu\sqrt{n-k}}}{4\sqrt{3}(n-k)}\Big(1 + O\Big(\frac{1}{\sqrt{n-k}}\Big)\Big) \\
&= \frac{e^{\nu\sqrt{n}}}{4\sqrt{3}n} \sum_{k \le \sqrt{n}\log n/\nu} \binom{k+2}{2} e^{\nu(\sqrt{n-k}-\sqrt{n})}\Big(1 + O\Big(\frac{\log n}{\sqrt{n}}\Big)\Big) \\
&= \frac{e^{\nu\sqrt{n}}}{4\sqrt{3}n} \sum_{k \le \sqrt{n}\log n/\nu} \binom{k+2}{2} e^{-(\nu k)/(2\sqrt{n}) + O(k^2 n^{-3/2})}\Big(1 + O\Big(\frac{\log n}{\sqrt{n}}\Big)\Big) \\
&= \frac{e^{\nu\sqrt{n}}}{4\sqrt{3}n} \sum_{k \le \sqrt{n}\log n/\nu} \binom{k+2}{2} e^{-(\nu k)/(2\sqrt{n})}\Big(1 + O\Big(\frac{(\log n)^2}{\sqrt{n}}\Big)\Big).
\end{aligned}
$$

The last sum has the form

$$
\sum_{k=0}^{N} \binom{k+2}{2} q^k = \frac{1}{2(1-q)^3}\Big(2 - q^{N+1}(N^2(1-q)^2 + N(1-q)(5-3q) + 2(q^2-3q+3))\Big)
$$

with $N = \sqrt{n}\log n/\nu + O(1)$, $q = e^{-\nu/(2\sqrt{n})} = 1 - \nu/(2\sqrt{n}) + O(n^{-1})$ and $q^N \sim 1/\sqrt{n}$, which gives us

$$
A_3 = \frac{e^{\nu\sqrt{n}}}{4\sqrt{3}n} \cdot \frac{8n^{3/2}}{\nu^3}\Big(1 + O\Big(\frac{(\log n)^2}{\sqrt{n}}\Big)\Big) = p(n) \cdot \frac{6\sqrt{6}n^{3/2}}{\pi^3}\Big(1 + O\Big(\frac{(\log n)^2}{\sqrt{n}}\Big)\Big).
$$

Summing A_1, A_2 and A_3 yields the desired result. □

Combining Propositions 12 and 13 with the expression (3), we arrive at our final result:

Theorem 14 *The average Wiener index* $\mathrm{av}(n)$ *of a star-like tree with* n *edges is given by*

$$\mathrm{av}(n) = 2n^2 - \frac{\sqrt{6}n^{3/2}}{2\pi}\Big(\log n + 2\gamma - \log\frac{\pi^2}{6} + \frac{24\zeta(3)}{\pi^2}\Big) + O(n(\log n)^3). \quad (11)$$

REMARK: We have noted that the maximal Wiener index of a star-like tree is aymptotically $2n^2 - 2n\sqrt{n} + n + O(\sqrt{n})$. On the other hand, the minimal Wiener index is n^2. This shows that "most" star-like trees have a Wiener index close to the maximum.

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