On the palindromic Hosoya polynomial of trees

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Abstract

A graph $G$ on $n$ vertices of diameter $D$ is called $H$-palindromic if $\alpha(G, k) = \alpha(G, D - k)$ for all $k = 0, 1, \ldots, \lfloor D/2 \rfloor$, where $\alpha(G, k)$ is the number of unordered pairs of vertices at distance $k$. Quantities $\alpha(G, k)$ form coefficients of the Hosoya polynomial. In 1999, Caporossi, Dobrynin, Gutman and Hansen showed that there are exactly five $H$-palindromic trees of even diameter and conjectured that there are no such trees of odd diameter. We prove this conjecture for bipartite graphs. An infinite family of $H$-palindromic trees of diameter 6 is also constructed.

Keywords: Hosoya polynomial, Wiener index, tree

1 Introduction

Let $G = (V, E)$ be an undirected connected graph without loops and multiple edges. The distance $d(x, y)$ between vertices $x, y \in V$ is the number of edges in the shortest path connecting $x$ and $y$ in $G$. The maximal distance between vertices of a graph is called its diameter $D$. The Hosoya polynomial of a graph $G$ of diameter $D$ is defined as

$$H(G, \lambda) = \sum_{k=0}^{D} \alpha(G, k)\lambda^k,$$

where $\alpha(G, k)$ is equal to the number of unordered pairs of vertices at distance $k$ in $G$. Clearly, $\alpha(G, 0) = |V|$ and $\alpha(G, 1) = |E|$. This polynomial was first proposed by Hosoya under the name Wiener polynomial in 1988 \cite{ Hosoya1988}. It was studied for various classes of abstract and molecular graphs. Historical remarks and the bibliography on the Hosoya polynomial can be found in \cite{ Hosoya1998}. The Wiener index $W(G)$ is a distance-based graph invariant defined as the sum of distances over all unordered pairs of vertices of a graph $G$. Therefore, it can be presented through the coefficients of the Hosoya polynomial as follows

$$W(G) = \sum_{k=1}^{D} \alpha(G, k)k,$$

that is the Wiener index can be calculated as the first derivative of $H(G, \lambda)$ at $\lambda = 1$. This index was introduced by Harry Wiener for molecular graphs of alkanes that are trees in 1947 \cite{ Wiener1947}. It has numerous applications in organic chemistry (see, for example, reviews \cite{ Wiener1950, Wiener1956, Wiener1969}).

A graph $G$ is $H$-palindromic if the equality $\alpha(G, k) = \alpha(G, D - k)$ holds for all $k = 0, 1, \ldots, \lfloor D/2 \rfloor$. The quantity

$$Z(G) = \sum_{k=0}^{\lfloor D/2 \rfloor} |\alpha(G, k) - \alpha(G, D - k)|$$

is called the distance to $H$-palindromicity of a graph $G$. Clearly, a graph is $H$-palindromic if and only if its distance to $H$-palindromicity equals 0. It is known that the Wiener index of $H$-palindromic trees $T$ depends only on the number of vertices $n$ and the diameter $D$: $W(T) = D \frac{n(n+1)}{4}$ \cite{ Wiener1947}. 

Some families of $H$-palindromic cyclic graphs have been constructed in [3]. Based on computer experiments, Gutman conjectured that there are no $H$-palindromic trees [6] (see also [7]). Only five palindromic trees were found by exhaustive computer search among all trees with $n \leq 26$ vertices [1]. The following table shows the number of vertices, diameter and coefficients of the palindromic Hosoya polynomial of these trees.

| $T$ | $n$ | $D$ | $(\alpha(T,0), \alpha(T,1), \ldots, \alpha(T,D))$ |
|-----|-----|-----|-----------------------------------------------|
| $T_1$ | 21 | 8   | $(21, 20, 34, 25, 31, 25, 34, 20, 21)$ |
| $T_2$ | 22 | 6   | $(22, 21, 52, 63, 52, 21, 22)$ |
| $T_3$ | 22 | 6   | $(22, 21, 52, 63, 52, 21, 22)$ |
| $T_4$ | 24 | 8   | $(24, 23, 39, 41, 46, 41, 23, 24)$ |
| $T_5$ | 24 | 8   | $(24, 23, 37, 41, 50, 41, 37, 24)$ |

Table 1: $H$-palindromic trees of diameter $D$ with $n$ vertices.

Some necessary conditions for the existence of $H$-palindromic trees of odd diameter were found and the following conjectures were formulated in [1] (see also [4]).

**Conjecture 1.** For all trees with $n > 4$ vertices and odd diameter the distance to $H$-palindromicity is at least $\left\lceil \frac{n}{2} \right\rceil$.

**Conjecture 2.** There are no $H$-palindromic trees of odd diameter.

Evidently, the second conjecture is a consequence of the first one. An intensive computations were done to test Conjecture 1 in [2]. So far no progress has been made on this problem.

In this work, we prove these conjectures for bipartite graphs. We also prove that there are infinitely many $H$-palindromic trees of diameter 6.

# 2 Trees of odd diameter

In this Section, we consider bipartite graphs of odd diameter.

**Theorem 1.** Let $G$ be a bipartite graph on $n$ vertices of odd diameter. Then

$$Z(G) \geq \left\lceil \frac{n}{2} \right\rceil.$$ 

**Proof.** Let $a$ and $b$ be the cardinalities of the bipartite parts of a graph $G$ of diameter $D$. Obviously, the distance between two vertices of $G$ is even if and only if they belong to the same part. Hence, the sum of $\alpha(G,i)$ over odd $i$ equals the number of pairs from different parts:

$$\sum_{\substack{i=0 \\ i \text{ is odd}}}^{D} \alpha(G,i) = ab,$$

and the sum of $\alpha(G,i)$ over even $i$ equals the number of pairs from the first part and pairs from the second part:

$$\sum_{\substack{i=0 \\ i \text{ is even}}}^{D} \alpha(G,i) = \left(\frac{a}{2}\right) + a + \left(\frac{b}{2}\right) + b = \frac{a^2 + a + b^2 + b}{2}.$$ 

Since the diameter $D$ is odd, quantities $i$ and $D - i$ have different parity. Then

$$Z(G) \geq \sum_{\substack{i=0 \\ i \text{ is even}}}^{D} \alpha(G,i) - \sum_{\substack{i=0 \\ i \text{ is odd}}}^{D} \alpha(G,i) = \frac{(a-b)^2 + a + b}{2} \geq \frac{a+b}{2} = \frac{n}{2}.$$

By definition, $Z(G)$ is an integer, so the claim follows.  

Since an arbitrary tree is a bipartite graph, we immediately have the following result.
Corollary 1. There are no $H$-palindromic trees of odd diameter.

The bound of Theorem 1 is sharp. For instance, consider the Hamming graph $H(m, 2)$ of order $2^m$. Its vertex set consists of all binary words of length $m$ with the usual Hamming distance.

Proposition 1. For the Hamming graph $H(m, 2)$, $Z(H(m, 2)) = 2^{m-1}$.

Proof. By definition, the diameter of $H(m, 2)$ is equal to $m$. Every vertex of the graph has $\binom{m}{k}$ neighbors at distance $k$ for $0 \leq k \leq m$. Hence, $\alpha(G, k) = \alpha(G, m - k)$ for $1 \leq k \leq m - 1$, $\alpha(G, 0) = 2^m$, and $\alpha(G, m) = 2^{m-1}$. Then

$$Z(H(m, 2)) = \sum_{k=1}^{m} \left| \binom{m}{k} - \binom{m}{m-k} \right| + \left| 2^m - 2^{m-1} \right| = 2^{m-1},$$

that is a half of the number of vertices of $H(m, 2)$.

3 Trees of diameter 6

As it was discussed in Section 1, only five $H$-palindromic trees of even diameter are known. It is easy to show that there are no such trees of diameter 2 and 4. It is sufficient to consider a general model of such a tree and find coefficients of Hosoya polynomial by direct calculations. However, trees of diameter 6 may be $H$-palindromic.

Theorem 2. There is an infinite number of $H$-palindromic trees of diameter 6.

Proof. For non-negative integers $a$, $b$, $s$ and $t$, construct a tree $T = T(a, b, s, t)$ by the following steps:

1. take a path of length five: $(v_1, v_2, v_3, v_4, v_5, v_6)$,
2. attach one pendent vertex to vertex $v_2$ and one pendent vertex $u$ to vertex $v_5$,
3. attach $t$, $s$, $a$ and $b$ new pendent vertices to vertices $v_4$, $v_5$, $v_6$ and $u$, respectively (see Fig. 1).

![Construction of $H$-palindromic tree $T(a, b, s, t)$](http://example.com/figure1.png)

Figure 1. Construction of $H$-palindromic tree $T(a, b, s, t)$

Counting pairs of vertices at a given distance in the tree of diameter 6 in Fig. 1, one can calculate values of coefficients $\alpha(T, i)$:

$$\begin{cases}
\alpha(T, 0) = a + b + s + t + 8, \\
\alpha(T, 1) = a + b + s + t + 7, \\
\alpha(T, 2) = \binom{a+1}{2} + \binom{b+1}{2} + \binom{s+3}{2} + \binom{t+2}{2} + 4, \\
\alpha(T, 4) = (s + 2) + (a + b + 2)(t + 1) + ab, \\
\alpha(T, 5) = a + b + 2(s + 2), \\
\alpha(T, 6) = 2(a + b).
\end{cases}$$
Equalities \( \alpha(T, 0) = \alpha(T, 6) \) and \( \alpha(T, 1) = \alpha(T, 5) \) are satisfied under condition \( s = t + 3 = \frac{a + b - 5}{2} \). Since \( s \) and \( t \) are non-negative integers, the sum \( a + b \) should be odd and not less than 11. So it remains to satisfy the equation \( \alpha(T, 2) = \alpha(T, 4) \). After all necessary calculations, one can rewrite this equality in the following form:

\[
(a - 3b + 3)^2 - 2(2b - 3)^2 + 94 = 0.
\]

Using substitution \( x = a - 3b + 3 \) and \( y = 2b - 3 \), the last equality can be presented as the Pell equation

\[
x^2 - 2y^2 = -94.
\]

Methods for solving Pell equation can be found in [1]. It has an infinite series of integer solutions starting from \((x, y) = (2, 7)\). All solutions can be represented by the following recurrent relations:

\[
\begin{align*}
x_{n+1} &= 3x_n + 4y_n \\
y_{n+1} &= 3y_n + 2x_n
\end{align*}
\]

with the initial conditions \( x_0 = 2 \) and \( y_0 = 7 \). It easy to see that \( x_n \) is always even and \( y_n \) is odd. Therefore \( a_n = x_n + \frac{3y_n + 3}{2} \) and \( b_n = \frac{y_n + 3}{2} \) are both integers and their sum \( a_n + b_n \) is odd and not less than \( a_0 + b_0 = 19 \geq 11 \). So, every pair \((a_n, b_n)\) corresponds to some \( H \)-palindromic tree. \[\square\]

Table 3 shows solutions of the Pell equation and parameters of the initial part of the constructed series of \( H \)-palindromic vertex trees \( T \) of diameter 6.

| \( n \) | \( x_n \) | \( y_n \) | \( |V| \) | \( a \) | \( b \) | \( s \) | \( t \) | coefficients of \( H(T, \lambda) \) |
|---|---|---|---|---|---|---|---|---|
| 0 | 2 | 7 | 38 | 14 | 5 | 7 | 4 | (38, 37, 184, 223, 184, 37, 38) |
| 1 | 34 | 25 | 174 | 73 | 14 | 41 | 38 | (174, 173, 4536, 5459, 4536, 173, 174) |
| 2 | 202 | 143 | 982 | 418 | 73 | 243 | 240 | (982, 981, 149572, 179583, 149572, 981, 982) |
| 3 | 1178 | 833 | 5694 | 2429 | 418 | 1421 | 1418 | (5694, 5693, 5059476, 6071939, 5059476, 5693, 5694) |

Table 2: First \( H \)-palindromic trees \( T \) of diameter 6.

It will be interesting to answer the following question.

**Problem 1.** Does there exist an infinite family of \( H \)-palindromic trees of even diameter \( D \geq 8 \)?

We suppose that ideas from Section 3 may be successfully applied for small values of \( D \).

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References

[1] G. Caporossi, A.A. Dobrynin, I. Gutman, and P. Hansen. Trees with palindromic Hosoya polynomials. *Graph Theory Notes N. Y.*, 37:10–16, 1999.

[2] G. Caporossi and P. Hansen. Variable neighborhood search for extremal graphs. V: Three ways to automate finding conjectures. *Discrete Math.*, 276(1-3):81–94, 2004.

[3] A. A. Dobrynin. Graphs with palindromic Wiener polynomials. *Graph Theory Notes N. Y.*, 27:50–54, 1994.
[4] A. A. Dobrynin, R. Entringer, and I. Gutman. Wiener index of trees: Theory and applications. *Acta Appl. Math.*, 66(3):211–249, 2001.

[5] A. A. Dobrynin, I. Gutman, S. Klavžar, and P. Žigert. Wiener index of hexagonal systems. *Acta Appl. Math.*, 72(3):247–294, 2002.

[6] I. Gutman. Some properties of the Wiener polynomial. *Graph Theory Notes N. Y.*, 25:13–18, 1993.

[7] I. Gutman, E. Estrada, and O. Ivanciuc. Some properties of the Wiener polynomial of trees. *Graph Theory Notes N. Y.*, 36:7–13, 1999.

[8] I. Gutman, Y. Zhang, M. Dehmer, and A. Ilić. Altenburg, Wiener, and Hosoya polynomials. In I. Gutman and B. Furtula, editors, *Distance in Molecular Graphs — Theory*, pages 49–70. Univ. Kragujevac, Kragujevac, 2012.

[9] H. Hosoya. On some counting polynomials in chemistry. *Discrete Appl. Math.*, 19:239–257, 1988.

[10] M. Knor, R. Škrekovski, and A. Tepeh. Mathematical aspects of Wiener index. *Ars Math. Contemp.*, 11(2):327–352, 2016.

[11] Don Redmond. *Number theory. An introduction*. Basel: Marcel Dekker, 1996.

[12] H. Wiener. Structural Determination of Paraffin Boiling Points. *J. Am. Chem. Soc.*, 69(1):17–20, 1947.