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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 $d(G,k) = d(G,D-k)$ for all $k = 0,1,\dots,\lfloor \frac{D}{2} \rfloor$, where $d(G,k)$ is the number of unordered pairs of vertices at distance k. Quantities $d(G,k)$ form coefficients of the Hosoya polynomial. In 1999, Caporossi, Dobrynin, Gutman and Hansen found 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.

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. By definition,

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the Hosoya polynomial of a graph G of diameter D is

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

where $d(G,k)$ is equal to the number of unordered pairs of vertices at distance k in G. Clearly, $d(G,0) = |V|$ and $d(G,1) = |E|$. This polynomial was first proposed by Hosoya under the name Wiener polynomial in 1988 [10]. It was studied for various classes of abstract and molecular graphs. Historical remarks and the bibliography on the Hosoya polynomial can be found in [9]. 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

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

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 [13]. It has numerous applications in organic chemistry (see, for example, reviews [5, 6, 11]).

A graph G is H-palindromic if $d(G,k) = d(G,D-k)$ for all $k = 0, 1, \ldots, \lfloor \frac{D}{2} \rfloor$. For a graph G, its H-palindromicity is defined as

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

Clearly, a graph is H-palindromic if and only if its 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: $W(T) = D\frac{n(n+1)}{4}$ [2].

Some families of H-palindromic cyclic graphs have been constructed in [4]. After computer search Gutman conjectured that there are no H-palindromic trees [7] (see also [8]). Exactly five palindromic trees were

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

T	n	D	$(d(T,0), d(T,1), \ldots, d(T,D))$
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	$(24, 23, 39, 41, 46, 41, 39, 23, 24)$
T_5	24	8	$(24, 23, 37, 41, 50, 41, 37, 23, 24)$

found by exhaustive computer search among all trees with $n \leq 26$ vertices [2].

Table 1 shows the number of vertices, diameter and coefficients of the palindromic Hosoya polynomial of these trees.

Some necessary conditions for the existence of H-palindromic trees of odd diameter were found and the following conjectures were formulated in [2] (see also [5]).

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

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 [3]. 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. A preliminary version of this article was published on Arxiv.org [1].

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 $d(G,i)$ over odd i equals the number of pairs from different parts:

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

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

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

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

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

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. *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 2. *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, $d(G,k) = d(G,m-k)$ for $1 \leq k \leq m-1$, $d(G,0) = 2^m$, and $d(G,m) = 2^{m-1}$. Then

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

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 3. *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).

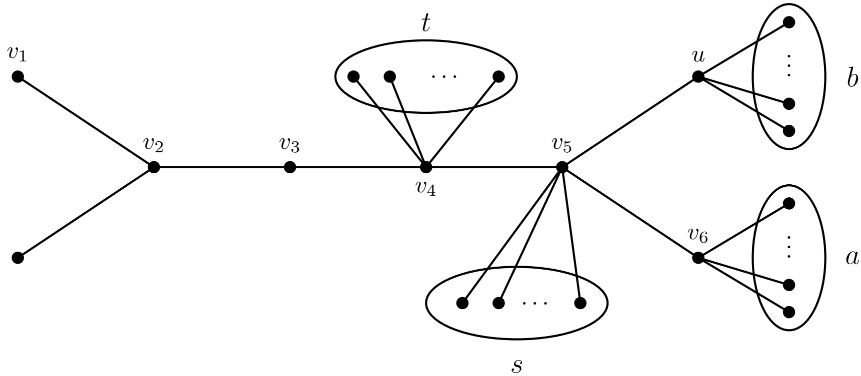

Figure 1. Construction of H-palindromic tree $T(a, b, s, t)$.

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

$$\begin{cases} d(T,0) = a+b+s+t+8, \\ d(T,1) = a+b+s+t+7, \\ d(T,2) = \binom{a+1}{2} + \binom{b+1}{2} + \binom{s+3}{2} + \binom{t+2}{2} + 4, \\ d(T,4) = (s+2) + (a+b+2)(t+1) + ab, \\ d(T,5) = a+b+2(s+2), \\ d(T,6) = 2(a+b). \end{cases}$$

Equalities $d(T,0) = d(T,6)$ and $d(T,1) = d(T,5)$ 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 $d(T,2) = d(T,4)$. 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 [12]. It has an infinite series of integer solutions starting from $(x,y) = (2,7)$. All solutions can be represented by the following recurrent relations:

$$\begin{cases} x_{n+1} = 3x_n + 4y_n \\ y_{n+1} = 3y_n + 2x_n \end{cases}$$

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. ■

Table 2 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.

Table 2. First H-palindromic trees T of diameter 6.

n	x_n	y_n	$\|V\|$	a	b	s	t
0	2	7	38	14	5	7	4
1	34	25	174	73	14	41	38
2	202	143	982	418	73	243	240
3	1178	833	5694	2429	418	1421	1418

n	coefficients of $H(T, \lambda)$
0	(38, 37, 184, 223, 184, 37, 38)
1	(174, 173, 4536, 5459, 4536, 173, 174)
2	(982, 981, 149572, 179583, 149572, 981, 982)
3	(5694, 5693, 5059476, 6071939, 5059476, 5693, 5694)

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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