On the roots of Hosoya polynomial of a graph

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ABSTRACT

Let $G = (V, E)$ be a simple graph. Hosoya polynomial of G is $H(G,x) = \sum_{\{u,v\}\subseteq V(G)} x^{d(u,v)}$, where, $d(u\ ,v)$ denotes the distance between vertices u and v. As is the case with other graph polynomials, such as chromatic, independence and domination polynomial, it is natural to study the roots of Hosoya polynomial of a graph. In this paper we study the roots of Hosoya polynomials of some specific graphs.

Keywords: Hosoya polynomial, root, path, cycle.

1. INTRODUCTION

A simple graph $G = (V, E)$ is a finite nonempty set $V(G)$ of objects called vertices together with a (possibly empty) set $E(G)$ of unordered pairs of distinct vertices of G called edges. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds.

The Hosoya polynomial of a graph is a generating function about distance distributing, introduced by Hosoya [10] in 1988 and for a connected graph G is defined as:

$$H(G,x) = \sum_{\{u,v\}\subseteq V(G)} x^{d(u,v)},$$

Where $d\ (u\ ,v)$ denotes the distance between vertices u and v. This polynomial has computed for some nano-structures, e.g. [3, 16]. The Hosoya polynomial has many chemical applications [7, 8, 9]. Especially, the two well-known topological indices, i.e. Wiener index and hyper-Wiener index, can be directly obtained from the Hosoya polynomial.

The Wiener index of a connected graph G is denoted by $W(G)$, is defined as the sum of distances between all pairs of vertices in G ([11]), i.e.,

$$W(G,x) = \sum_{\{u,v\} \subseteq V(G)} d(u,v).$$

The hyper-Wiener index is denoted by $WW(G)$ and defined as follows:

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} d(u,v) + \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} d^2(u,v).$$

Note that the first derivative of the Hosoya polynomial at $x = 1$ is equal to the Wiener index:

$$W(G) = (H(G,x))'|_{x=1}.$$

Also we have the following relation:

$$WW(G) = \frac{1}{2}(xH(G,x))''|_{x=1}.$$

Graph polynomials are a well-developed area useful for analyzing properties of graphs. For some graph polynomials, their roots have attracted considerable attention, both for their own sake, as well for what the nature and location of the roots imply. Woodal [17] explored the zeros and zero-free regions of chromatic and flow polynomials. Also, the zero distribution of chromatic and flow polynomials of graphs and characteristic polynomials of matroids have been examined by Jackson [12]. Also the zeros of independence polynomials have been studied in [2, 4]. Finally the roots of domination polynomial has considered in some papers, e.g. [1, 5].

In this paper we study the roots of Hosoya polynomial of specific graphs. We denote the roots of Hosoya polynomial of graph G by $Z(H(G,x))$.

2. MAIN RESULTS

In this section we consider some specific graphs and obtain the roots of their Hosoya polynomials. Let S_n, P_n and C_n denote the star, path and cycle with n vertices, respectively. A simple calculation gives the following theorem:

Theorem 1.

1. $H(S_n,x) = \binom{n-1}{2}x^2 + (n-1)x.$

2. $H(P_n,x) = x^{n-1} + 2x^{n-2} + \ldots + (n-1)x.$

3. $H(C_{2n},x) = (2n)(x + x^2 + \ldots + x^{n-1}) + nx^n.$

4. $H(C_{2n+1},x) = (2n+1)(x + x^2 + \ldots + x^n).$

Theorem 2 . *For* $n \geq 3$,

$$Z(H(S_n, x)) = \{0, \frac{2}{2-n}\}.$$

Proof. It follws from Theorem 1(i). ■

Here we state the following theorem:

Theorem 3 . ([14]) *Let* $f(z) = a_n z^n + a_{n-1} z^{n-1} + \ldots + a_0$, $a_i \in \mathbb{R}, i = 1, \ldots, n$ *be a polynomial with real coefficients satisfying* $a_0 \geq a_1 \geq \ldots \geq a_n > 0$. *Then, no zeros of* $f(z)$ *lie in* $\{z \in \mathbb{C}, |z| < 1\}$.

The following theorem is an consequence of Theorem 3, see Figure 1.

Theorem 4 . $H(P_n, x)$ *and* $H(C_{2n}, x)$ *do not possess zeros in* $\{z \in \mathbb{C}, |z| < 1\}$.

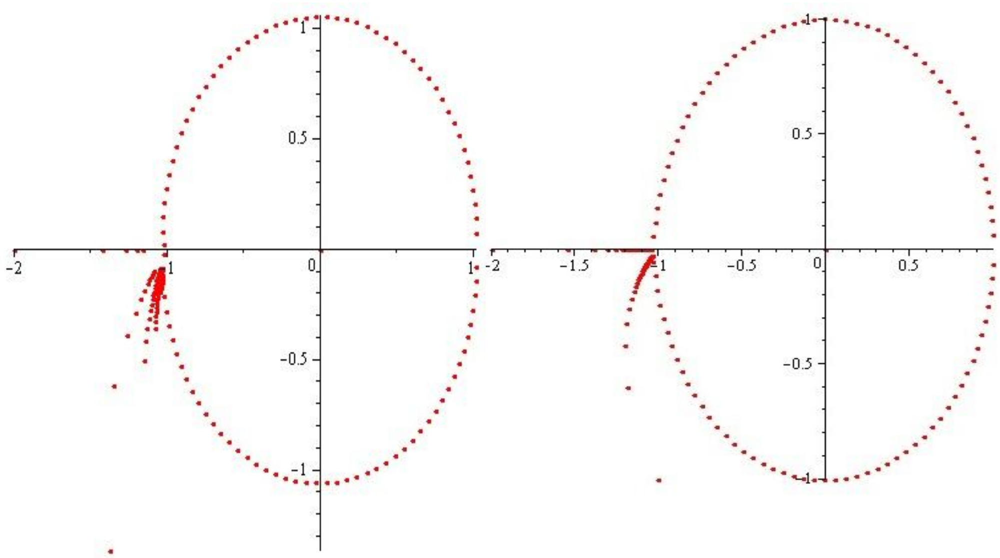

Figure 1. Roots of Hosoya polynomial of P_{100} and C_{200}, respectively.

We recall that the n-th root of unity are roots $e^{\frac{2k\pi i}{n}}$ of equation $x^n = 1$. Now we state and prove the following theorem:

Theorem 5 . *Let* $f(z) = az^n + az^{n-1} + \ldots + az + a$, $a \neq 0$, *be a complex polynomial. All zeros of* $f(z)$ *lie on the unit circle.*

Proof. We have

$$f(z) = \frac{a(z^{n+1}-1)}{z-1} = a\prod_{i=1}^{n}(z-w^i),$$

where w denotes the $(n+1)$-th root of unity. Since all roots of unity lie on the unit circle, so we have the result. ■

Corollary 1: All roots of $H(C_{2n+1}, x)$ lie on the unit circle.

Proof. It follows from Theorems 1 and 5. ■

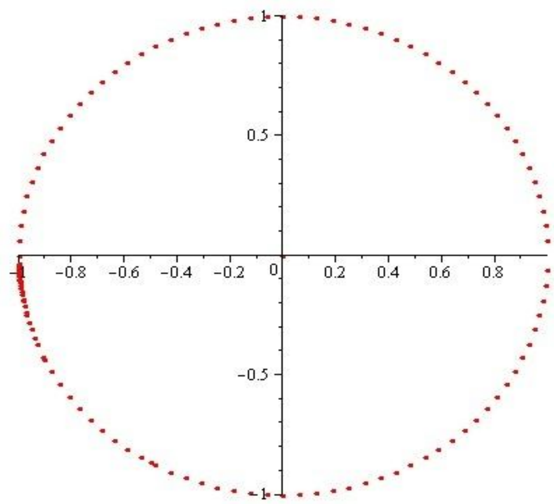

Figure 2. Roots of $H(C_{201}, x)$.

Figure 2 shows roots of $H(C_{201}, x)$. We need the following theorem:

Theorem 6 . ([13]) *Let* $f(z) = a_n z^n + a_{n-1}z^{n-1} + \ldots + a_0$, $a_i \in \mathbb{R}$, *be a polynomial with real coefficients. All zeros of* $f(z)$ *lie in the closed disk* $\{z \in \mathbb{C}, |z| \le r\}$ *where* $r > 1$ *denotes the largest positive root of the equation* $(z^2-1)(|a_n|z - |a_{n-1}|)^2 - 2\theta_2^2 = 0$, *and*

$$\theta_2 = \frac{1}{\sqrt{2}}\left(\sum_{j=1}^{n}(a_{n-j} - a_{n-j-1})^2\right)^{\frac{1}{2}}.$$

Theorem 7. *All zeros of* $H(C_{2n}, x)$ *lie in the closed disk* $\{z \in \mathbb{C}, |z| \le 2.77321\}$.

Proof. By Theorem 6, since we have $a_n = n$ and $a_i = 2n$, $(1 \le i \le n-1)$, so $\theta_2 = \sqrt{2}n$. Now we have $(z^2-1)(nz-2n)^2 - 4n^2 = 0$. The largest positive root of this equation is

2.77321. So, we have the result as desired. ■

The join $G_1 \vee G_2$ of two graph G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph union $G_1 \cup G_2$ together with all the edges joining V_1 and V_2.

Theorem 8 . *Let n_i and m_i be order and size of graphs G_i $(i = 1,2)$, respectively. Then*

$$Z(H(G_1 \vee G_2, x)) = \left\{ 0, -\frac{m_1 + m_2 + n_1 n_2}{\binom{n_1}{2} + \binom{n_2}{2} - (m_1 + m_2)} \right\}.$$

Proof. Since $H(G_1 \vee G_2, x) = (\binom{m}{2} + \binom{n}{2})x^2 - (|E(G_1)| + |E(G_2)|)x(x-1) + mnx$ (see [15]), we have the result. ■

The following corollary is an immediate consequence of Theorem 8:

Corollary 2.

1. The roots of Hosoya polynomial of complete bipartite graph $K_{m,n}$ is

$$Z(H(K_{m,n}, x)) = \left\{ 0, \frac{-mn}{\binom{n}{2} + \binom{m}{2}} \right\}.$$

2. The roots of Hosoya polynomial of wheel graph W_n is

$$Z(H(W_n, x)) = \left\{ 0, \frac{2-2n}{\binom{n-1}{2} - (n-1)} \right\}.$$

Proof.

1. Since $K_{m,n} = \overline{K_m} \vee \overline{K_n}$, we have the result by Theorem 8.
2. Since $W_n = K_1 \vee C_{n-1}$, we have the result by Theorem 8. ■

For two graphs G and H, let G[H] be the graph with vertex set V (G)×V (H) and such that vertex (a, x) is adjacent to vertex (b, y) if and only if a is adjacent to b (in G) or a = b and x is adjacent to y (in H). The graph G[H] is the lexicographic product (or composition) of G and H, and can be thought of as the graph arising from G and H by substituting a copy of H for every vertex of G. We need the following theorem:

Theorem 9. ([15]) *Let* G_1 *and* G_2 *be two graphs of order* m *and* n, *respectively. The Hosoya polynomial of* $G_1[G_2]$ *is*

$$H(G_1[G_2],x) = n^2 H(G_1,x) + m\binom{n}{2}x^2 - m|E(G_2)|x(x-1)$$

Corollary 3. *Let* G_1 *and* G_2 *be two graphs of order* m *and* n, *respectively. The only common root of* $H(G_1,x)$ *and* $H(G_1[G_2],x)$ *is* $\dfrac{|E(G_2)|}{|E(G_2)|-\binom{n}{2}}$.

Proof. Let α be a common root of $H(G_1,x)$ and $H(G_1[G_2],x)$. Therefore by Theorem 9 we have $\left(\binom{n}{2}-|E(G_2)|\right)\alpha = -|E(G_2)|$. So we have the result. ∎

Here we shall consider the roots of Hosoya polynomial of another specific graph. Consider the graph K_m and m copies of K_n. The graph $Q(m,n)$ is obtained by identifying each vertex of K_m with a vertex of a unique K_n (see [6]). We have shown the graph $Q(6,4)$ in Figure 3.

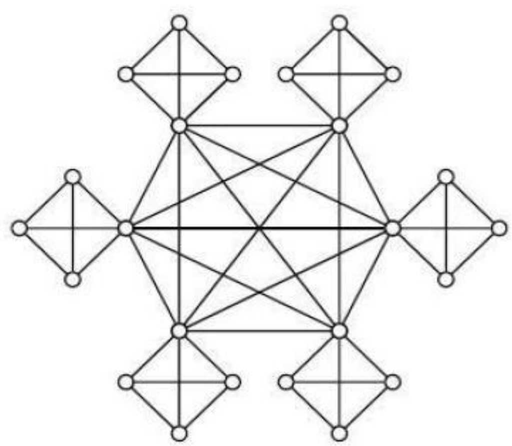

Figure 3. $Q(6,4)$.

Theorem 10 . ([6]) *The Hosoya polynomial of* $Q(m,n)$ *is*

$$\frac{1}{2}m(m+n^2-n-1)x+m(m-1)(n-1)x^2+\frac{1}{2}m(m-1)(n-1)^2x^3$$

The following theorem is about roots of Hosoya polynomial of $Q(m,n)$:

Theorem 11 . *All non-zero roots of* $H(Q(m,n),x)$ *are complex.*

Proof. By Theorem 10 we have the following equation:

$$(m-1)(n-1)^2x^2+2(m-1)(n-1)x+(m+n^2-n-1)=0.$$

It is easy to see that $\Delta=-4n(n-1)^3(m-1)$, where Δ is the discriminant of the quadratic equation. Since $m,n\in\mathbb{N}$, we have $\Delta<0$. Therefore we have the result. ■

We have seen that there are graphs whose their nonzero roots of Hosoya polynomial are complex. We think that the following problem has worth to consider:

Problem. Characterize graphs whose nonzero roots of their Hosoya polynomial have are complex.

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