

## ON THE INDEPENDENCE POLYNOMIALS OF CERTAIN MOLECULAR GRAPHS

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The independence polynomial of a molecular graph  $G$  is the polynomial  $I(G, x) = \sum i_k x^k$ , where  $i_k$  denote the number of independent sets of cardinality  $k$  in  $G$ . In this paper, we consider specific graphs denoted by  $G(m)$  and  $G_1(m)G_2$  and obtain formulas for their independence polynomials which are in terms of Jacobsthal polynomial. Also we compute the independence polynomial of another kind of graphs.

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### 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.

An *independent set* of a graph  $G$  is a set of vertices where no two vertices are adjacent. The *independence number* is the size of a maximum independent set in the graph. For a graph  $G$  with independence  $\beta$ , let  $i_k$  denote the number of independent sets of cardinality  $k$  in  $G$  ( $k=0, 1, \dots, \beta$ ). The *independence polynomial* of  $G$ ,  $I(G, x) = \sum_{k=0}^{\beta} i_k x^k$ , is the generating polynomial for the independent sequence  $(i_0, i_1, i_2, \dots, i_{\beta})$  ([3]). The path  $P_4$  on 4 vertices, for example, has one independent set of cardinality 0 (the empty set), four independent sets of cardinality 1, and three independent sets of cardinality 2; its independence polynomial is then  $I(P_4, x) = 1 + 4x + 3x^2$ .

Hoede and Li [5] obtained the following recursive formula for the independence polynomial of a graph.

**Theorem 1.** *For any vertex  $v$  of a graph  $G$ ,  $I(G, x) = I(G - v, x) + xI(G - [v], x)$  where  $[v]$  is the closed neighborhood of  $v$ , contains of  $v$ , together with all vertices incident with  $v$ .*

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Let us observe that if  $G$  and  $H$  are isomorphic, then  $I(G, x) = I(H, x)$ . The converse is not generally true. For Two graphs  $G$  and  $H$  are independent equivalent, written  $G \sim H$ , if  $I(G, x) = I(H, x)$ . A graph  $G$  is independent unique, if  $I(H, x) = I(G, x)$  implies that  $H \cong G$ . Let  $[G]$  denote the independent equivalence class determined by the graph  $G$  under the equivalence relation  $\sim$ . Clearly,  $G$  is independent unique if and only if  $[G] = \{G\}$ . A zero of  $I(G, x)$  is called a *independence zero* of  $G$ .

The corona of two graphs  $G_1$  and  $G_2$ , as defined by Frucht and Harary in [4], is the graph  $G_1 \circ G_2$  formed from one copy of  $G_1$  and  $|V(G_1)|$  copies of  $G_2$ , where the  $i$ th vertex of  $G_1$  is adjacent to every vertex in the  $i$ th copy of  $G_2$ . The corona  $G \circ K_1$ , in particular, is the graph constructed from a copy of  $G$ , where for each vertex  $v \in V(G)$ , a new vertex  $v'$  and a pendant edge  $vv'$  are added.

In Section 2, we study Jacobsthal polynomial and introduce two graphs with specific structures denoted by  $G(m)$  and  $G_1(m)G_2$ . Using the results related to Jacobsthal polynomial, we compute the independence polynomials of  $G(m)$  and  $G_1(m)G_2$  in Section 3.

## 2. Jacobsthal polynomial

Jacobsthal polynomials,  $J_n(x)$ , named after the German mathematician E. Jacobsthal are related to Fibonacci polynomials. They are defined by

$$J_n(x) = J_{n-1}(x) + xJ_{n-2}(x)$$

where  $J_1(x) = J_2(x) = 1$  (see [6], p.469).

In this section, we shall find the zeros of  $J_n(x)$ . First, we need the following two lemmas to obtain a solution of Jacobsthal polynomials.

**Lemma 1.** For any real number  $u$ ,  $J_n(u^2 + u) = \sum_{i=0}^{n-1} (1+u)^i (-u)^{n-1-i}$ .

**Proof.** It is clear that the result holds when  $n=2$ . Now let  $n \geq 3$ . By induction, we have

$$\begin{aligned} J_n(u^2 + u) &= J_{n-1}(u^2 + u) + (u^2 + u)J_{n-2}(u^2 + u) \\ &= \sum_{i=0}^{n-2} (1+u)^i (-u)^{n-2-i} + (u^2 + u) \sum_{i=0}^{n-3} (1+u)^i (-u)^{n-3-i} \\ &= \sum_{i=0}^{n-2} (1+u)^i (-u)^{n-2-i} - \sum_{i=0}^{n-3} (1+u)^{i+1} (-u)^{n-2-i} \\ &= (1+u)^{n-2} + \sum_{i=0}^{n-3} (1+u)^i (-u)^{n-2-i} - \\ &\quad \sum_{i=0}^{n-3} (1+u)^{i+1} (-u)^{n-2-i} \\ &= (1+u)^{n-2} + \sum_{i=0}^{n-3} (1+u)^i (-u)^{n-1-i} \\ &= \sum_{i=0}^{n-1} (1+u)^i (-u)^{n-1-i}. \quad \blacksquare \end{aligned}$$

**Corollary 1 .** For any real number  $u$ ,  $(2u + 1)J_n(u^2 + u) = (1 + u)^n - (-u)^n$ .

**Proof.** The result follows from Lemma 1 by using the identity

$$a^n - b^n = (a - b) \left( \sum_{i=0}^{n-1} a^i b^{n-1-i} \right),$$

for  $a = 1 + u$ ,  $b = -u$ . ■

**Lemma 2 .** ([2], p.64) For real numbers  $a$ ,  $b$  and positive integer  $n$ ,

$$a^n - b^n = \begin{cases} (a - b) \prod_{s=1}^{\frac{n-1}{2}} \left( a^2 + b^2 - 2ab \cos \frac{2s\pi}{n} \right); & n \text{ is odd,} \\ (a - b)(a + b) \prod_{s=1}^{\frac{n-2}{2}} \left( a^2 + b^2 - 2ab \cos \frac{2s\pi}{n} \right); & n \text{ is even.} \end{cases}$$

**Theorem 2 .** For any positive integer  $n$ ,  $J_n(x) = \prod_{s=1}^{\lfloor \frac{n-1}{2} \rfloor} \left( 2x + 1 + 2x \cos \frac{2s\pi}{n} \right)$ .

**Proof.** If put  $a = 1 + u$ ,  $b = -u$ , we have  $a - b = a^2 - b^2 = 1 + 2u$ , therefore by using Lemma 2 and Corollary 1, for any real number  $u \neq -\frac{1}{2}$ ,

$$J_n(u^2 + u) = \prod_{s=1}^{\lfloor \frac{n-1}{2} \rfloor} \left( 2u^2 + 2u + 1 + 2(u^2 + u) \cos \frac{2s\pi}{n} \right).$$

Observe that for any real number  $x$  with  $x > -\frac{1}{4}$ , there is a real number  $u \neq -\frac{1}{2}$  such that

$$u^2 + u = x. \text{ Thus for each real number with } x > -\frac{1}{4}, J_n(x) = \prod_{s=1}^{\lfloor \frac{n-1}{2} \rfloor} \left( 2x + 1 + 2x \cos \frac{2s\pi}{n} \right).$$

Since  $J_n(x)$  is a polynomial with degree less than  $n$ , the above equality also holds for any real number  $x \leq -\frac{1}{4}$ . Thus the result is obtained. ■

### 3. Independence polynomial of certain graphs

In this section we consider some specific graphs and compute their independence polynomial (see [1]). Let  $P_{m+1}$  be a path with vertices labeled by  $y_0, y_1, \dots, y_m$ , for  $m \geq 0$  and let  $G$  be any graph. Denote by  $G_{v_0}(m)$  (or simply  $G(m)$ , if there is no likelihood of confusion) a graph obtained from  $G$  by identifying the vertex  $v_0$  of  $G$  with an end vertex  $y_0$  of  $P_{m+1}$  (see Figure 1). For example, if  $G$  is a path  $P_2$ , then  $G(m) = P_2(m)$  is the path  $P_{m+2}$ . Also, we denote the graph obtained from graphs  $G_1$  and  $G_2$  by adding a path  $P_m$  from a vertex in  $G_1$  to a vertex

of  $G_2$ , by  $G_1(m)G_2$ . (Figure 1).

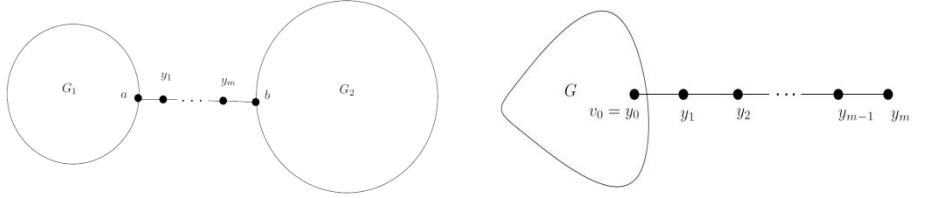


Fig.1. Graphs  $G(m)$  and  $G_1(m)G_2$ , respectively.

**Theorem 3 .** Let  $n \geq 2$  be integer. Then, the independence polynomial of  $G(n)$  is  $I(G(n), x) = J_n(x)I(G(1), x) + xJ_{n-1}(x)I(G, x)$ .

**Proof.** Proof by induction on  $n$ . Since  $J_1(x) = J_2(x) = 1$ , the result is true for  $n = 2$  by Theorem 1. Now suppose that the result is true for all natural numbers less than  $n$  and prove it for  $n$ . By using Theorem 1 for  $v = y_n$ , and induction hypothesis, we have

$$\begin{aligned} I(G(n), x) &= I(G(n-1), x) + xI(G(n-2), x) = \\ &= J_{n-1}(x)I(G(1), x) + xJ_{n-2}(x)I(G, x) \\ &\quad + x(J_{n-2}(x)I(G(1), x) + xJ_{n-3}(x)I(G, x)) \\ &= (J_{n-1}(x) + xJ_{n-2}(x))I(G(1), x) + x(J_{n-2}(x) + xJ_{n-3}(x))I(G, x) \\ &= J_n(x)I(G(1), x) + xJ_{n-1}(x)I(G, x). \quad \blacksquare \end{aligned}$$

The following theorem gives the formula for computing the independence polynomial of graphs  $G_1(m)G_2$  as shown in Figure 1 :

**Theorem 4 .** Let  $n \geq 5$  be integer. The independence polynomial of  $G_1(n)G_2$  is

$$\begin{aligned} I(G_1(n)G_2, x) &= \\ &= I(G_1(1), x)I(G_2(1), x)J_{n-2}(x) + x(I(G_1(1), x)I(G_2, x) \\ &\quad + I(G_1, x)I(G_2(1), x))J_{n-3}(x) + x^2I(G_1, x)I(G_2, x)J_{n-4}(x). \end{aligned}$$

**Proof.** Proof by induction on  $n$ . If  $n = 5$ , then by Theorems 1 and 3, and induction hypothesis, we have

$$\begin{aligned} I(G_1(5)G_2, x) &= I(G_1(1), x)I(G_2(3), x) + xI(G_1, x)I(G_2(2), x) = \\ &= (1+x)I(G_1(1), x)I(G_2(1), x) + x(I(G_1(1), x)I(G_2, x) \\ &\quad + I(G_1, x)I(G_2(1), x)) + x^2I(G_1, x)I(G_2, x). \end{aligned}$$

So the theorem is true for  $n = 5$ . Now suppose that the result is true for less than  $n$  and we prove it for  $n$ . By Theorems 1 and 3, and induction hypothesis, we have

$$\begin{aligned} I(G_1(n)G_2, x) &= \\ &= I(G_1(1), x)I(G_2(n-2), x) + x(I(G_1, x)I(G_2(n-3), x) = \\ &\quad I(G_1(1), x)I(G_2(1), x)J_{n-2}(x) + x(I(G_1(1), x)I(G_2, x) \end{aligned}$$

$$+ I(G_1, x)I(G_2(1), x)J_{n-3}(x) + x^2I(G_1, x)I(G_2, x)J_{n-4}(x). \quad \blacksquare$$

Theorem 3 implies that all forms of  $G_1(m)G_2$  have the same independence polynomials. As application of Theorem 3, we obtain the following formula:

**Corollary 2 .**

1. The independence polynomial of path  $P_n$  is

$$I(P_n, x) = J_{n+2}(x) = \prod_{s=1}^{\lfloor \frac{n+1}{2} \rfloor} \left( 2x + 1 + 2x \cos \frac{2s\pi}{n+2} \right).$$

2. The independence polynomial of cycle  $C_n$  ( $n \geq 2$ ) is

$$I(C_n, x) = J_{n+1}(x) + xJ_{n-1}(x).$$

**Proof.**

1. By using Theorem 1, for  $G = K_1$ , we have

$$\begin{aligned} I(P_{n+1}, x) &= I(K_1(n), x) = J_n(x)I(K_1(1), x) + xJ_{n-1}(x)I(K_1, x) \\ &= (1+2x)J_n(x) + xJ_{n-1}(x) + x^2J_{n-1}(x) \\ &= J_{n+2}(x) + xJ_{n+1}(x) \\ &= J_{n+3}(x). \end{aligned}$$

So we have the result.

2. It follows from Theorems 1 and Part 1.  $\blacksquare$

**References**

- [1] S. Alikhani, M.A. Iranmanesh, Digest Journal of Nanomaterials and Biostructures **5**, (1), 1 (2010).  
 [2] S. Barnard, J.F. Child, Higher-Algebra, Macmillan, London, (1955).  
 [3] I. Gutman, F. Harary, Utilitas Mathematica **24** (1983)97-106.  
 [4] R. Frucht, F. Harary, Aequationes Math, (1970); **4**, 322-324.  
 [5] C. Hoede, X. Li, Discrete Math. **25** (1994), 219-228.  
 [6] T. Koshy, Fibonacci, Lucas Numbers with Applications, A Wiley-Interscience Series of Texts, (2001).