On the independent sets of some nano-structures

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Let $G=(V,E)$ be a simple graph. A set $S \subseteq V$ is independent set of G, if no two vertices of S are adjacent. The independence number $\alpha(G)$ is the size of a maximum independent set in G. An independent set with cardinality $\alpha(G)$ is called a α-set of G. The problem of finding a α-set is NP-complete. We consider two kind of nanotubes and show that these two nanotubes have the same α-sets. Also we consider independence polynomial and obtain recurrence relations for independence polynomial of some polyphenyl hexagonal chains.

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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 $\alpha(G)$ is the size of a maximum independent set in the graph. An independent set with cardinality $\alpha(G)$ is called a α-set. The problem of finding a α-set is NP-complete even for the class of planar graphs, cubic planar graphs or triangle free graphs [10]. Tang Jian [9] has designed an exponential algorithm for solving maximum independent set problem for general graphs. For more details reader can refer to [3,5,6,12].

For a graph G with independence number α, let i_k denote the number of independent sets of cardinality k in G ($k=0,1,\ldots,\alpha$). The *independence polynomial* of G, $I(G,x)=\sum_{k=0}^{\alpha} i_k x^k$, is the generating polynomial for the independent sequence $(i_0,i_1,i_2,\ldots,i_\alpha)$ ([2,7]). 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 $I(P_4,x)=1+4x+3x^2$. For more information the reader refer to [2,11].

Nanotechnology creates many new materials and devices with a wide range of applications in medicine, electronics, and computer. Nanotechnology is expected to revolutionize the 21st century as space, entertainment and communication technology revolutionized the 20th century. It involves different structures of nanotubes and nanostars. Recently these structures considered by several authors (see [1]).

Spiro compounds are an important class of cycloalkanes in organic chemistry. A spiro union in spiro compounds is a linkage between two rings that consists of a single atom common to both rings and a free spiro union is a linkage that consists of the only direct union between the rings. The common atom is designated as the spiro atom. According to the number of spiro atoms present, compounds are distinguished as monospiro, dispiro, trispiro, etc., ring systems. Two or more benzene rings are linked by cut edges consisting of aromatics called polycyclic aromatic hydrocarbons which is a class of aromatics. A class of compounds in which two and more benzene rings are directly linked by a cut edge known as the biphenyl compounds, and their graphs are called polyphenyl hexagonal chains [4]. Fig. 1 illustrates ortho-terphenyl, meta-terphenyl and para-terphenyl.

In Section 2 we consider two kind of nanotubes and show that these two nanotubes have the same α-sets. In Section 3 we obtain recurrence relations for some polyphenyl hexagonal chains.

2. Maximum independent sets of nanotubes

The most significant nano structures are carbon nanotubes and boron triangular nanotubes. See Fig. 1. Nanotubes are three dimensional cylindrical structures formed out of the two dimensional sheets.

In this section we show that the maximum independent set of these two nanotubes are the same.

A carbon hexagonal nanotube of order $n \times m$ is a tube obtained from a carbon hexagonal sheet of n rows and m columns by merging the vertices of last column with the respective vertices of first column (in other words we have mn hexagon in this structure). A boron triangular nanotube of order $n \times m$ is obtained from a hexagonal nanotube of order $n \times m$ by adding a new vertex at the center of each hexagon of the hexagonal nanotube. See

Fig. 1.

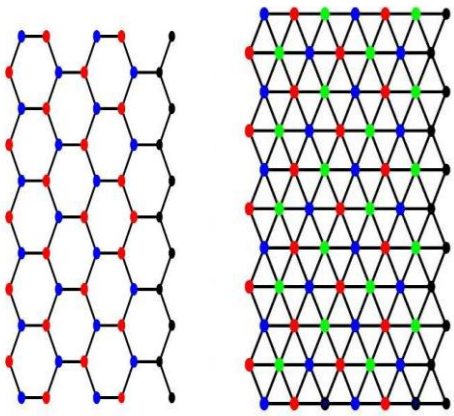

Fig. 1. Carbon hexagonal sheet and Boron triangular sheet, respectively.

Theorem 1 . *The α-sets of carbon hexagonal nanotube and boron triangular nanotube of order $n\times m$ are the same and have size $\frac{nm}{2}$.*

Proof. Let CHNT denote a carbon hexagonal nanotube of order $n\times m$. CHNT is bipartite which is two colorable. Let us color the CHNT by red and blue colors. It is easy to verify that the set of red vertices form an independent set of the CHNT. Let us now show that the cardinality of any independent set of a CHNT of order $n\times m$ does not exceed $\frac{nm}{2}$. There are m columns in a CHNT of order $n\times m$ and each column is a path. Thus a CHNT of order $n\times m$ is partitioned into m paths. The cardinality of any independent set of a path of order n does not exceed $\frac{n}{2}$. Hence the cardinality of any independent set of a CHNT of order $n\times m$ does not exceed $\frac{nm}{2}$. The cardinality of set of red vertices of the CHNT is $\frac{nm}{2}$. Hence the set of red vertices is a maximum independent set of the CHNT. Now we prove that the set of red nodes is a α-set of boron triangular nanotube. A boron triangular nanotube is obtained by adding a new vertex to the center of each hexagon of carbon hexagonal nanotube. These additional vertices are assigned green color. Thus the vertices of the boron triangular nanotube are partitioned by red, blue and green colors (Fig. 1). A green node cannot be a member of any maximum independent set of the boron triangular nanotube because inclusion of one green node into a maximum independent set leads to the exclusion of three red nodes from the maximum independent set. Thus the set of red nodes is a maximum independent set of the boron triangular nanotube. Therefore we have the result.

Here we interested in the number of independent sets of these nano-structures. We need the following theorem:

Theorem 2 . ([13]) *For any d-regular graph G of order N, and any $x\geq 0$*

$$I(G,x)\leq (2(1+x)^{d}-1)^{\frac{N}{2d}}.$$

When $x=1$, we obtain the following corollary.

Corollary 1 . *For any N-vertex, d-regular graph G,*

$$I(G,1)\leq (2^{d+1}-1)^{\frac{N}{2d}}.$$

It is easy to obtain the following result.

Theorem 3 .

1. *A carbon hexagonal nanotube of order $n\times m$ has $2(n+m+nm)$ vertices.*

2. *A boron triangular nanotube of order $n\times m$ has $2(n+m)+3nm$ vertices.*

By Corollary 1 and above theorem we have the following result for carbon nanotubes and boron triangular nanotubes.

Theorem 4 .

1. The number of independent sets of carbon hexagonal nanotube of order $n\times m$ is at most $15^{\frac{n+m+nm}{3}}$.

2. The number of independent sets of boron triangular nanotube of order $n\times m$ is at most $127^{\frac{2(n+m)+3nm}{12}}$.

3. Recurrence relations for independence polynomials of polyphenyl hexagonal chain

Let G be a cactus graph in which block is either an edge or a hexagon. G is called a polyphenyl hexagonal chain if each hexagon of G has at most two cut-vertices, and each cut vertex is shared by exactly one hexagon and one cut-edge. The number of hexagons in G is called the length of G. Obviously, a polyphenyl hexagonal chain of length n has $6n$ vertices and $7n-1$ edges. Furthermore, any polyphenyl hexagonal chain of length greater than one has exactly two hexagons with only one cut-vertex. Such hexagons are called terminal hexagons. Any remaining hexagons are called internal hexagons. The polyphenyl ortho-, meta- and para-chain of length n is denoted by $\overline{O}_n, \overline{M}_n$ and $\overline{P}_n$, respectively. Examples of polyphenyl ortho-, meta-, and para-chains are shown in Fig. 2.

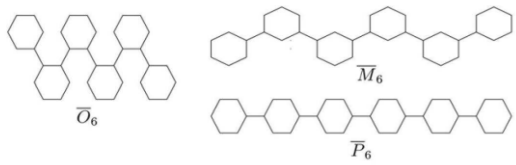

Fig. 2. Example of polyphenyl ortho-, meta-, and para-chains.

In this section we give a recurrence for computing the independence polynomial of polyphenyl hexagonal chains.

Hoede and Li [8] obtained the following recursive formula for the independence polynomial of a graph.

Theorem 5. *For any vertex v of a graph G, $I(G,x) = I(G-v,x) + xI(G-[v],x)$ where $[v]$ is the closed neighberhood of v, contains of v, together with all vertices incident with v.*

Here we obtain recurrence relations for the independence polynomials of $\overline{P}_n, \overline{O}_n$ and $\overline{M}_n$.

Theorem 6 . *If $n \geq 2$, then*

1.
$$I(\overline{O}_n,x) = (1+6x+9x^2+2x^3)I(\overline{O}_{n-1},x) - (x^2+6x^3+11x^4+6x^5+x^6)I(\overline{O}_{n-2},x)$$

2.
$$I(\overline{P}_n,x) = (1+5x+6x^2+2x^3)I(\overline{P}_{n-1},x) + (2x^2+9x^3+9x^4+4x^5-x^6)I(\overline{P}_{n-2},x)$$

3.
$$I(\overline{M}_n,x) = (1+6x+8x^2+x^3)I(\overline{M}_{n-1},x) + (-x-4x^2-x^3-9x^4+6x^5+x^6)I(\overline{M}_{n-2},x).$$

Proof. We prove the Part (i). Another parts prove similarly.

1. To prove this part we apply Theorem 5 for vertex as u which shown in Fig. 2. Therefore we have

$$I(\overline{O}_n,x) = I(P_5,x)I(\overline{O}_{n-1},x) + xI(P_3,x)I(\overline{O'}_{n-1},x), \quad (1)$$

where $\overline{O}_4$ and $\overline{O'}_4$ shown in Fig. 3. Now we obtain recurrence relation for the independence polynomial of $\overline{O'}_n$. By Theorem 5 for vertex v as shown in Fig. 2 we have

$$I(\overline{O'}_n,x) = I(\overline{O'}_n - v,x) + xI(\overline{O'}_n - N[v],x)$$

$$= I(P_4,x)I(\overline{O}_{n-1},x) + xI(P_3,x)I(\overline{O'}_{n-1},x).$$

So we have

$$I(\overline{O'}_n,x) = I(P_4,x)I(\overline{O}_{n-1},x) + I(\overline{O}_n,x) - I(P_5,x)I(\overline{O}_{n-1},x). \quad (2)$$

Now by equations (1) and (2) we have

$$I(\overline{O}_n,x) = I(P_5,x)I(\overline{O}_{n-1},x) + xI(P_3,x)I(P_4,x)I(\overline{O}_{n-2},x) + xI(P_3,x)I(\overline{O}_{n-1},x) - xI(P_3,x)I(P_5,x)I(\overline{O}_{n-2},x)$$

Therefore

$$I(\overline{O}_n,x) = (I(P_5,x)+xI(P_3,x))I(\overline{O}_{n-1},x) + (xI(P_3,x)(I(P_4,x)-I(P_5,x)))I(\overline{O}_{n-2},x)$$

So we have the result.

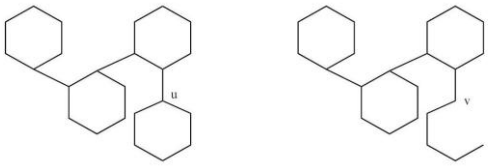

Fig. 3. The graphs $\overline{O}_4$ and $\overline{O}'_4$, respectively.

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