CHROMATIC POLYNOMIALS OF SOME NANOTUBES

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In this paper we consider two types of graphs with specific structures denoted by $G(m)$ and $G'(m)$ and obtain formulas for their chromatic polynomials. Using the chromatic polynomials of $G(m)$ and $G'(m)$, we compute the chromatic polynomials of $TUHC[r,s]$ and $TUC_4C_8(S)$.

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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.

Let $\chi(G,\lambda)$ denotes the number of proper vertex colourings of G with at most λ colours. G. Birkhoff [3], observed in 1912 that $\chi(G,\lambda)$ is, for a fixed graph G, a polynomial in λ, which is now called the chromatic polynomial of G. More precisely, let G be a simple graph and $\lambda \in \mathbb{N}$. A mapping $f: V(G) \to \{1,2,\ldots,\lambda\}$ is called a λ-*colouring* of G if $f(u) \neq f(v)$ whenever the vertices u and v are adjacent in G. The number of distinct λ-colourings of G, denoted by $P(G,\lambda)$ is called the *chromatic polynomial* of G. A zero of $P(G,\lambda)$ is called a *chromatic zero* of G. The book by F.M. Dong, K.M. Koh and K.L. Teo[4] gives an excellent and extensive survey of this polynomial and its root.

A *topological index* is a real number related to a graph. It must be a structural invariant, i.e., it is fixed by any automorphism of the graph. There are several topological indices have been defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of molecules. The Wiener index W and diameter are two examples of topological indices of graphs (or chemical model). For a detailed treatment of these indices, the reader is referred to [6,7].

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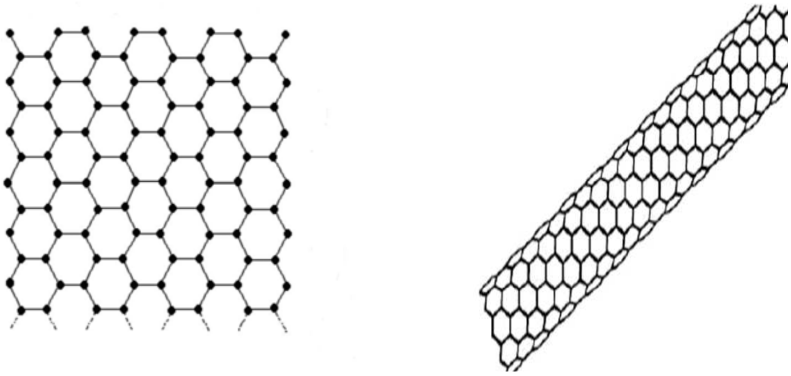

Fig. 1. The zigzag polyhex torus and nanotube, respectively.

There are also some papers which compute some polynomials of some nanotubes [2,8]. As we know one of the important graph polynomial is chromatic polynomial. It is easy to see that the chromatic polynomial is structural invariant, i.e., if $G \cong H$, then $P(G,\lambda) = P(H,\lambda)$. This is a natural question: What are the chromatic polynomials of some nanotubes as $TUHC[r,s]$ and $TUC_4C_8(S)$?(Figs. 1 and 2). To answer this question, we consider two specific graphs $G(m)$ and $G'(m)$ which has considered in[1].

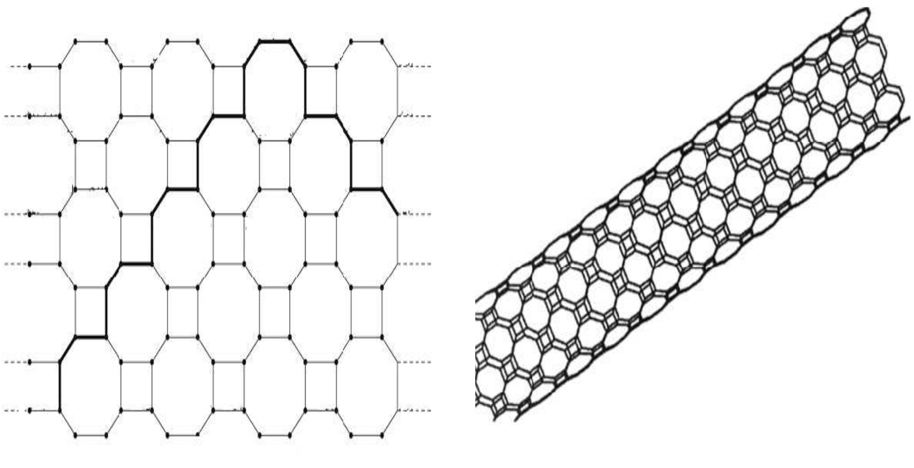

Fig. 2. A $TUC_4C_8(S)$ lattice and nanotube, respectively.

Let P_{m+1} be a path with vertices labeled by $y_0, y_1, \ldots, y_m$, 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 3). For example, if G is a path P_2, then $G(m) = P_2(m)$ is the path P_{m+2}.

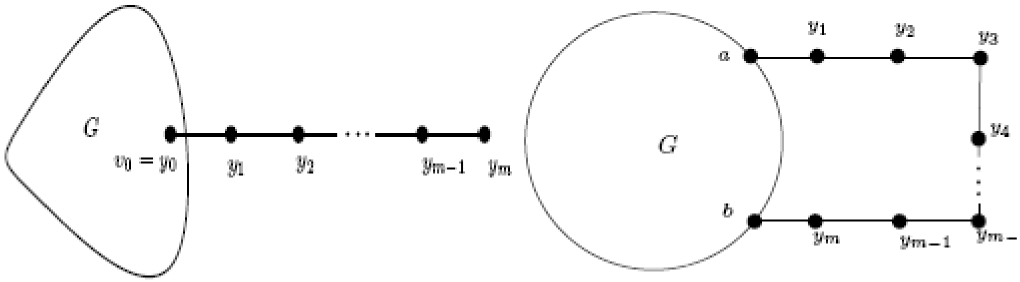

Fig. 3. The graphs $G(m)$ and $G'(m)$, respectively.

Let P_m be a path with vertices labeled $y_1,\ldots,y_m$ and let a,b be two specific vertices of a graph G (note that may be $a=b$). Denote by $G'_{a,b}(m)$ (or simply $G'(m)$, if there is no likelihood of confusion) a graph obtained from graph G and path P_m with vertices $\{y_1,\ldots,y_m\}$, by adding edges ay_1 and by_m. See Figure 2. Through our discussion these two vertices a and b are fixed.

2. Results and discussion

2.1 Outline

In the next section we compute the chromatic polynomials of graphs $G(m)$ and $G'(m)$. Using Theorem 1 we obtain the chromatic polynomial of nanotubes $TUHC_6[2p,q]$ and $TUC_4C_8(S)$ in Section 3.

3. Chromatic polynomials of $G(m)$ and $G'(m)$

In this section we compute the chromatic polynomials of graphs $G(m)$ and $G'(m)$. As an application, we obtain the chromatic polynomial of path P_n and C_n easily. We need the following lemma:

Lemma 1 . (Fundamental Reduction Theorem (Whitney[9])). *Let G be a graph and e be an edge of G. Then $P(G,\lambda)=P(G-e,\lambda)-P(G*e,\lambda)$; where $G-e$ is the graph obtained from G by deleting e, and $G*e$ is the graph obtained from G by identifying the end vertices of e.*

The following theorem gives formula for chromatic polynomial of $G(m)$ and $G'(m)$:

Theorem 1 . *Let $m\in \mathbb{N}$. Then,*

1. the chromatic polynomial of $G(m)$ is

$$P(G(m),\lambda)=(\lambda-1)^m P(G,\lambda).$$

2. Suppose that the vertices a,b are in adjacent in G. The chromatic polynomial of graph $G'_{a,b}(m)$ is

$$P(G'_{a,b}(m),\lambda)=(\sum_{i=0}^{m}(-1)^i(\lambda-1)^{m-i})P(G,\lambda).$$

Proof.

1. By using Lemma 1 for $e=y_{m-1}y_m$, we have

$$\begin{aligned}P(G(m),\lambda)&=\lambda P(G(m-1),\lambda)-P(G(m-1),\lambda)=(\lambda-1)P(G(m-1),\lambda)\\&=(\lambda-1)^2P(G(m-2),\lambda)=\ldots=(\lambda-1)^mP(G(0),\lambda)\\&=(\lambda-1)^mP(G,\lambda).\end{aligned}$$

2. By using Lemma 1 for $e=y_mb$, we have

$$P(G'(m),\lambda)=P(G(m),\lambda)-P(G'(m-1),\lambda).$$

Now by Theorem 1 and the above equation, we conclude that,

$$\begin{aligned}&P(G'(m),\lambda)=P(G(m),\lambda)-(P(G(m-1),\lambda)-P(G'(m-2),\lambda))\\&=(\lambda-1)^mP(G,\lambda)-(\lambda-1)^{m-1}P(G,\lambda)+\ldots+\\&(-1)^mP(G,\lambda)=(\sum_{i=0}^{m}(-1)^i(\lambda-1)^{m-i})P(G,\lambda).\quad\blacksquare\end{aligned}$$

As application of Theorem 1 for $G=K_2$, we have two following famous formula:

Corollary 1 .

1. The chromatic polynomial of path P_n is

$$P(P_n,\lambda)=\lambda(\lambda-1)^{n-1}.$$

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

$$P(C_n,\lambda)=(\lambda-1)^n+(-1)^n(\lambda-1).$$

4. Main results

In this section we consider Nanotubes $TUHC[r,s]$ and $TUC_4C_8(S)$ as shown in Figures 1 and 2, respectively. It is obvious that these two graphs have form $G'(m)$.

Using the chromatic polynomial of $G'(m)$, we obtain the chromatic polynomial of a zigzag polyhex nanotube $\Gamma=TUHC[2p,q]$ (see Figure 1). Suppose that there are rs cycle C_6 (as array) in an $r\times s$ matrix. Let us denote this graph by $T[r,s]$.

Theorem 2 . *The chromatic polynomial of* $T[r,s]$ *is*

$$P(T[r,s],\lambda)=\lambda(\lambda-1)(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^{r+s-1}(\lambda^2-3\lambda+3)^{rs-r-s+1}.$$

Proof. Let denote $G'(m)$ simply by $G'\circ m$. Obviously we can construct $T[r,s]$, as following: We begin with C_6. It's easy to see that $T[1,s]$ is $C'_6\circ\underbrace{4\circ 4\cdots,\circ 4}_{(s-1)times}$. Now we construct the second row and continue this action for another rows. It's easy to see that $T[r,s]=C_6'\circ\underbrace{4\circ 4\cdots\circ 4}_{(r+s-2)times}\circ\underbrace{2\circ\cdots\circ 2}_{(rs-r-s+1)times}$. By using Theorem 1 and Corollary 1 (ii),

$$P(T[r,s],\lambda)=P(C'_6\circ 4\circ 4\circ\ldots\circ 4\circ 2\circ 2\circ\ldots\circ 2,\lambda)=$$
$$P(C_6,\lambda)\Big(\sum_{i=0}^{4}(-1)^i(\lambda-1)^{4-i}\Big)^{r+s-2}\Big(\sum_{i=0}^{2}(-1)^i(\lambda-1)^{2-i}\Big)^{rs-r-s+1}=$$
$$((\lambda-1)^6+(\lambda-1))\Big(\sum_{i=0}^{4}(-1)^i(\lambda-1)^{4-i}\Big)^{r+s-2}(\lambda^2-3\lambda+3)^{rs-r-s+1}=$$
$$\lambda(\lambda-1)(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^{r+s-1}(\lambda^2-3\lambda+3)^{rs-r-s+1}.\ \blacksquare$$

If we choose $r=s=n$ in Theorem2, we get the following corollary, that is, the chromatic polynomial of $T[n,n]$:

Corollary 2 . *The chromatic polynomial of* $T[n,n]$ *is*

$$P(T[n,n],\lambda)=\lambda(\lambda-1)(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^{2n-1}(\lambda^2-3\lambda+3)^{(n-1)^2}.$$

Now consider the case where $G=TUC_4C_8(S)$ and suppose that there are rs cycle C_8 and C_4 (as array) in a $r\times s$ matrix. Let us denote this graph simply by $T8[r,s]$. Similar to the previous case, we are able to compute $P(T8[r,s],\lambda)$. The following theorem gives us a formula for $P(T8[2k+1,2k'+1],\lambda)$.

Theorem 3 . *The chromatic polynomial of* $T8[2k+1,2k'+1]$ *is*

$$\lambda(\lambda-1)(\lambda-2)^{4kk'}(\lambda^2-\lambda+1)^k(\lambda^2-2\lambda+2)^{k(2k'-1)}(\lambda^2-3\lambda+3)^{2k+k'}$$
$$(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^k(\lambda^6-7\lambda^5+21\lambda^4-35\lambda^3+35\lambda^2-21\lambda+7)^{k'+1}.$$

Proof. Obviously we can construct $T8[2k+1,2k'+1]$, as follows:
We begin with C_8. It is obvious that $T8[1,s]$ is $C_8'\circ\underbrace{2\circ 6\circ 2\circ 6,\cdots,\circ 2\circ 6}_{(2k')times}$. Now we construct the second row and continue this action for other rows. It is easy to see that

$$P(T8[2k+1,2k'+1],\lambda)=P(C'_8\circ(2\circ 6)^{k'}(2\circ(3\circ 1)^{k'})^k\circ(5\circ 4\circ(1\circ 3)^{k'-1}\circ 1)^k,\lambda)=$$
$$P(C'_8\circ 2^{k+k'}\circ 6^{k'}\circ 3^{k(2k'-1)}\circ 1^{2kk'}\circ 4^k\circ 5^k,\lambda)=$$
$$P(C_8,\lambda)\Big(\sum_{i=0}^{2}(-1)^i(\lambda-1)^{2-i}\Big)^{k+k'}\Big(\sum_{i=0}^{6}(-1)^i(\lambda-1)^{6-i}\Big)^{k'}\Big(\sum_{i=0}^{3}(-1)^i(\lambda-1)^{3-i}\Big)^{k(2k'-1)}$$
$$\Big(\sum_{i=0}^{1}(-1)^i(\lambda-1)^{1-i}\Big)^{2kk'}\Big(\sum_{i=0}^{4}(-1)^i(\lambda-1)^{4-i}\Big)^{k}\Big(\sum_{i=0}^{5}(-1)^i(\lambda-1)^{5-i}\Big)^{k}=$$
$$\lambda(\lambda-1)(\lambda-2)^{4kk'}(\lambda^2-\lambda+1)^k(\lambda^2-2\lambda+2)^{k(2k'-1)}(\lambda^2-3\lambda+3)^{2k+k'}$$
$$(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^k(\lambda^6-7\lambda^5+21\lambda^4-35\lambda^3+35\lambda^2-21\lambda+7)^{k'+1}.$$

Therefore we have the result. ■

Now we investigate some properties of the coefficients of chromatic polynomial of $T[r,s]$.

Lemma 2 . *Let* G *be a graph with* n *vertices and* m *edges. Then in the chromatic polynomial* $P(G,\lambda)$,

1. $deg(P(G,\lambda)) = n$,
2. the coefficient of λ^n is 1,
3. the coefficient of λ^{n-1} is $-m$,
4. the coefficient of λ^{n-2} is $\binom{m}{2} - t_1(G)$, where $t_1(G)$ is the number of triangles in G, and
5. the coefficient of λ^{n-3} is $-\binom{m}{3} + (m-2)t_1(G) + t_2(G) - 2t_3(G)$, where $t_2(G)$ is the number of induced C_4 (C_4 without chords) and $t_3(G)$ is the number of the complete subgraphs K_4 in G (see [5]).

By Lemma 2 we have the following corollary:

Corollary 3 .

1. $deg(P(T(r,s),\lambda)) = 2(r+s+rs)$
2. The coefficient of $\lambda^{2r+2s+2rs-3}$ in $P(T(r,s),\lambda)$ is $3rs + 2r + 2s - 2$,
3. The coefficient of $\lambda^{2r+2s+2rs-4}$ in $P(T(r,s),\lambda)$ is $\binom{2r+2s+3rs-2}{2}$,
4. The coefficient of $\lambda^{2r+2s+2rs-5}$ in $P(T(r,s),\lambda)$ is $\binom{2r+2s+3rs-2}{3}$.

The following corollary is the immediate conclusion of Theorems 2 and 3:

Corollary 4 .

1. The chromatic roots set of $T[r,s]$ is

$$\{0,1,\underbrace{0.6909830056 \pm 0.9510565163i}_{(r+s-1)-times}, \underbrace{\frac{3\pm\sqrt{3}i}{2}}_{(rs-r-s+1)-times}\}$$

2. The chromatic roots set of $T8[2k+1,2k'+1]$ is

$$\{0,1,\underbrace{2}_{4kk'-times},\underbrace{\frac{3\pm\sqrt{3}i}{2}}_{2k+k'-times},\underbrace{\frac{1\pm\sqrt{3}i}{2}}_{k-times}\underbrace{1\pm i}_{k(2k'-1)-times},$$

$$\underbrace{0.376510198\pm 0.781831482i, 1.22252093\pm 0.974927912i, 1.90096886\pm 0.433883739i}_{(k'+1)-times},$$

$$\underbrace{0.6909830056\pm 0.9510565163i, 1.809016994\pm .5877852523i}_{k-times}\}.$$

The following corollary is an immediate consequence of Corollary 4:

Corollary 5 . *The real chromatic roots of nanotubes* $TUHC[r,s]$ *and* $TUC_4C_8(S)$ *are integers* $0,1$ *and* 2.

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