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Chromatic polynomials of some nanostars

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ABSTRACT

Let G be a simple graph and $\chi(G,\lambda)$ denotes the number of proper vertex colourings of G with at most λ colours, which is for a fixed graph G, a polynomial in λ, which is called the chromatic polynomial of G. Using the chromatic polynomial of some specific graphs, we obtain the chromatic polynomials of some nanostars.

Keywords: Chromatic polynomial, nanostar, graph.

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 [4], 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. The book by Dong, Koh and Teo [5] gives an excellent and extensive survey of this polynomial.

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 [8,9].

The nanostar dendrimer is a part of a new group of macromolecules that seem photon funnels just like artificial antennas and also is a great resistant of photo bleaching. Recently some people investigated the mathematical properties of this nanostructures in [2,3, 6,10,11,14]. Also we investigated the chromatic polynomials of some certain dendrimers [1]. In this paper we would like to investigate some further results of this kind.

In Section 2, we introduce two graphs with specific structures and state their chromatic polynomials. Using results in Section 2, we study the chromatic polynomials of some nanostars in Section 3.

2. CHROMATIC POLYNOMIAL OF CERTAIN GRAPHS

In this section we consider some specific graphs and compute their chromatic polynomial. We need the following lemma:

Lemma 1(Fundamental Reduction Theorem (Whitney [12])). *Let G be a graph and e be an edge of G. Then $P(G,\lambda) = P(G-e,\lambda) - P(G\cdot e,\lambda)$; where $G-e$ is the graph obtained from G by deleting e, and $G\cdot e$ is the graph obtained from G by identifying the end vertices of e.*

Let P_{m+1} be a path with vertices labeled by $y_0, y_1, \ldots, y_m$, for $m \geq 1$ 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}.

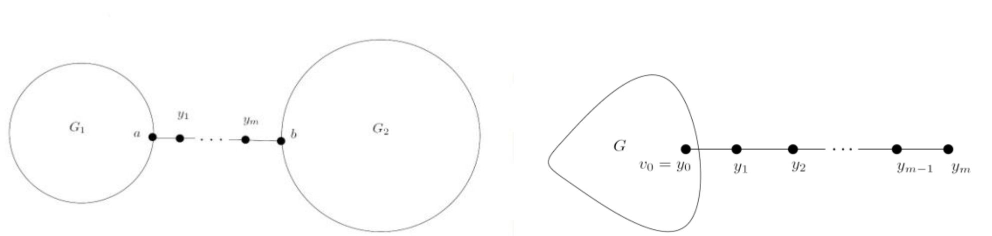

Figure 1. Graphs $G(m)$ and $G_1(m)G_2$, respectively.

Theorem 1([1]). *Let $m \in \mathbb{N}$. Then, the chromatic polynomial of $G(m)$ is*

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

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

Theorem 2 ([1]). *Let* $m \in \mathbb{N}$. *The chromatic polynomial of* $G_1(m)G_2$ *is*

$$P(G_1(m)G_2, \lambda) = \frac{(\lambda - 1)^{m+1}}{\lambda} P(G_1, \lambda) P(G_2, \lambda).$$

Theorem 2 implies that all forms of $G_1(m)G_2$ have the same chromatic polynomials. We need the following Lemma to obtain our results:

Lemma 3([7]). *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* $-m$.

3. Chromatic polynomial of some nanostars

In this section we shall compute the chromatic polynomials of some nanostars. Let us consider the nanostar $NS_1[n]$ ($NS_1[3]$ has shown in Figure 3).

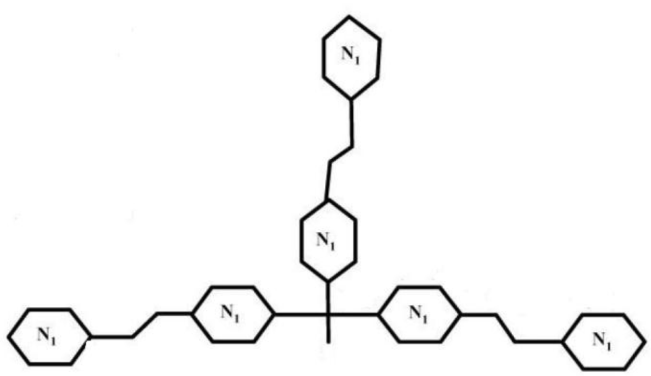

Figure 2. The kernel of $NS_1[3]$.

We shall compute $P(NS_1[n], \lambda)$. We consider the kernel of $NS_1[3]$ which has shown in Figure 2. As usual we denote it by $NS_1[0]$.

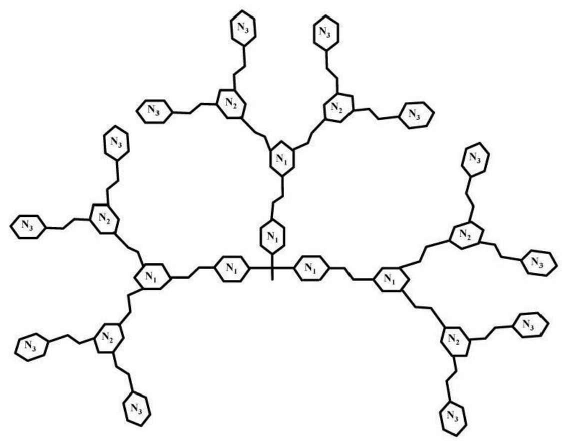

Figure 3. $NS_1[3]$.

Theorem 3. *The chromatic polynomial of* $NS_1[0]$ *is*

$$P(NS_1[0],\lambda)=\lambda(\lambda-1)^7(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^3.$$

Proof. By applying Lemma 1, Theorems 1, 2 and simplifying, we have

$$P(NS_1[0],\lambda)=\frac{(\lambda-1)^4(P(C_6,\lambda))^3}{\lambda^2}$$

which is equal with $\lambda(\lambda-1)^7(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^3$.

The following theorem give us the chromatic polynomial of nanostar $NS_1[n]$.

Theorem 4. *The chromatic polynomial of nanostar* $NS_1[n]$ *is*

$$P(NS_1[n],\lambda)=\lambda(\lambda-1)^{3\times 2^{n+2}-5}\times(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^{3\times 2^n}.$$

Proof. By induction on n. The theorem is true for $n=0$ by Theorem 3. Now suppose that the result is true for less than n and we prove it for n. Since the chromatic polynomial of $NS_1[n]$ is equal with the chromatic polynomial of

$$(NS_1[n-1] \quad \underbrace{(2)C_6 \quad}_{(3\times 2^{n-1})\text{times}}),$$

by Theorem 2, we have

$$P(NS_1[n],\lambda)=P(NS_1[n-1],\lambda)\left(\frac{(\lambda-1)^3P(C_6,\lambda)}{\lambda}\right)^{3\times 2^{n-1}}$$

Now by induction hypothesis

$$P(NS_1[n],\lambda) = \lambda(\lambda-1)^{3\times 2^{n+1}-5}(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^{3\times 2^{n-1}}$$
$$\cdot(\lambda-1)^{3\times 2^{n+1}}(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^{3\times 2^{n-1}}$$
$$= \lambda(\lambda-1)^{3\times 2^{n+2}-5}(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^{3\times 2^{n}}.$$

Corollary 1.

1. *The order of* $NS_1[n]$ *is* $|V(NS_1[n]|= 24\times 2^n-4$.
2. *The size of* $NS_1[n]$ *is* $|E(NS_1[n])|= 27\times 2^n-5$.

Proof.

1. By Lemma $3(i)$, $deg(P(G,\lambda))=|V(G)|$. From Theorem 4, $deg(P(NS_1[n]))=24\times 2^n-4$. Therefore $|V(NS_1[n]|= 24\times 2^n-4$.
2. By Lemma $3(iii)$, the coefficient of $-\lambda^{|V(G)|-1}$ is equal with the number of edges of G. Therefore we have the result by Theorem 4.

Now we shall compute the chromatic polynomial of nanostar $NS_2[n]$. The nanostar $NS_2[3]$ shown in Figure 4.

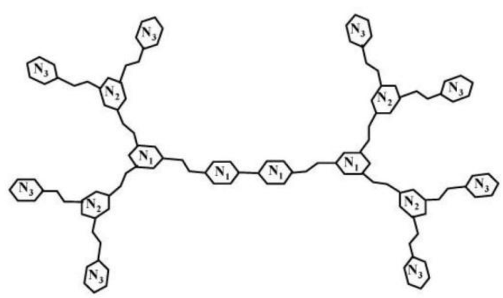

Figure 4. $NS_2[3]$.

Theorem 5. *The chromatic polynomial of nanostar* $NS_2[n]$ *is*

$$P(NS_2[n],\lambda) = \lambda(\lambda-1)^{4\times 2^{n+1}-5}(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^{2^{n+1}}.$$

Proof. By induction on n. Since $P(NS_2[1],\lambda)=P(C_6(2)C_6(0)C_6(2)C_6,\lambda)$, by Theorem 2,

$$P(NS_2[1],\lambda)=\frac{(\lambda-1)^7(P(C_6,\lambda))^4}{\lambda^3}.$$

So the theorem is true for $n=1$. Now suppose that the result is true for less than n and we prove it for n. Since the chromatic polynomial of $NS_2[n]$ is equal with the chromatic polynomial of $(NS_2[n-1]\underbrace{(2)C_6}_{(2^n)times})$, by Theorem 2, we have

$$P(NS_2[n],\lambda)=P(NS_2[n-1],\lambda)\left(\frac{(\lambda-1)^3P(C_6,\lambda)}{\lambda}\right)^{2^n}$$

Now by induction hypothesis

$$\begin{aligned}P(NS_2[n],\lambda) &= \lambda(\lambda-1)^{4\times 2^n-5}(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^{2^n}\\ &\quad\cdot(\lambda-1)^{4\times 2^n}(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^{2^n}\\ &= \lambda(\lambda-1)^{4\times 2^{n+1}-5}(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^{2^{n+1}}.\end{aligned}$$

The following corollary is an consequence of Theorem 5 and Lemma 3.

Corollary 2.

1. *The order of* $NS_2[n]$ *is* $|V(NS_2[n]|=16\times 2^n-4$.
2. *The size of* $NS_2[n]$ *is* $|E(NS_2[n])|=18\times 2^n-5$.

Now, we consider another kind of nanostars. This nanostar denoted by $NS_3[n]$. See $NS_3[2]$ in Figure 5.

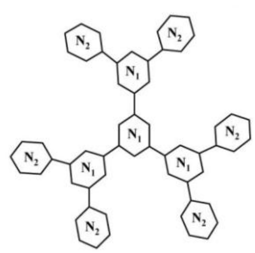

Figure 5. $NS_3[2]$

Theorem 6. *The chromatic polynomial of nanostar* $NS_3[n]$ *is*

$$P(NS_3[n],\lambda)=\lambda(\lambda-1)^{3\times 2^{n+1}-5}(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^{3\times 2^n-2}.$$

Proof. By induction on n. Since

$$P(NS_3[1],\lambda)=P(C_6(0)C_6(0)C_6(0)C_6,\lambda)=\frac{(\lambda-1)^7((\lambda-1)^5+1)^4}{\lambda^3},$$

the result is true for $n=1$. Now suppose that the result is true for less than n and we prove it for n. Since $P(NS_3[n],\lambda)$ is equal with $P((NS_3[n-1]\underbrace{(0)C_6}_{3\times(2^{n-1})times}),\lambda)$, by Theorem 2, we have

$$P(NS_3[n],\lambda) = P(NS_3[n-1],\lambda)(\frac{(\lambda-1)P(C_6,\lambda)}{\lambda})^{3\times 2^{n-1}}$$

Now by induction hypothesis

$$\begin{aligned} P(NS_3[n],\lambda) &= \lambda(\lambda-1)^{3\times 2^{n}-5}(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^{3\times 2^{n-1}-2} \\ &\cdot(\lambda-1)^{3\times 2^{n}}(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^{3\times 2^{n-1}} \\ &= \lambda(\lambda-1)^{3\times 2^{n+1}-5}(\lambda^4-5\lambda^3+10\lambda^2-10\lambda+5)^{3\times 2^{n}-2}. \end{aligned}$$

The following corollary is an consequence of Theorem 6 and Lemma 3.

Corollary 3.

1. *The order of* $NS_3[n]$ *is* $|V(NS_3[n])| = 18\times 2^n - 12$.
2. *The size of* $NS_3[n]$ *is* $|E(NS_3[n])| = 21\times 2^n - 15$.

Theorem 7 ([13]). *For any non-trivial connected graph G, the multiplicity of the root 1 of* $P(G,\lambda)$ *is the number of blocks in G.*

By Theorems 4, 5, 6 and 7 we have the following corollary:

Corollary 4. *The nanostars* $NS_1[n]$, $NS_2[n]$ *and* $NS_3[n]$ *have* $3\times 2^{n+2}-5$, $4\times 2^{n+1}-5$ *and* $3\times 2^{n+1}-5$ *blocks.*

Here we state the following corollary:

Corollary 5. *The real chromatic roots of nanostars are integers* 0 *and* 1.

Whitney have the following theorem:

Theorem ([12]). *Let G be an (n,m)-graph. Then*

$$P(G,\lambda) = \sum_{p=1}^{n}(\sum_{r=0}^{m}(-1)^r N(p,r))\lambda^p .$$

where N(p,r) denotes the number of spanning subgraphs of G with p components and r edges.

The study of the number of spanning subgraphs is important for chemist. We think that the esearchers are able to use our chromatic polynomials and previous theorems to find the number of spanning subgraphs of certain nano-structures.

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