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The Neighbourhood Polynomial of some Nanostructures

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ABSTRACT. The neighbourhood polynomial $N(G,x)$, is generating function for the number of faces of each cardinality in the neighbourhood complex of a graph. In other word $N(G,x) = \sum_{U \in N(G)} x^{|U|}$, where $N(G)$ is neighbourhood complex of a graph, whose vertices are the vertices of the graph and faces are subsets of vertices that have a common neighbour. In this paper we compute this polynomial for some nanostructures.

Keywords: Neighbourhood polynomial, Dendrimer nanostar.

1. INTRODUCTION

A (*simplicial*) *complex* on a finite set *X* is a collection *C* of subsets of *X*, closed under containment. Each set in *C* is called a *face* of the complex, and the maximal faces (with respect to containment) are called *facets* or *bases*. The *dimension* of a complex *C* is the maximum cardinality of a face.

The *f–vector* (or *face–vector*) of a *d*–dimensional complex *C* is $(f_0, f_1, ..., f_d)$, where f_i is the number of faces of cardinality *i* in *C*. The *f–polynomial* of a *d*–dimensional complex *C* is the generating function $f(C,x) = \sum_i f_i x^i$ for the *f*–vector $(f_0, f_1, ..., f_d)$ of the complex. For each graph polynomials, there is a complex for which the graph polynomial is a simple evaluation of the *f*–polynomial. For instance, the independence complex *I*(*G*) of graph *G* is the complex on the vertex set *V* of *G* whose faces are the independent sets of *G*. The independence polynomial is merely the *f*–polynomial of the independence complex. One of the applications of simplicial complexes to graph theory is undoubtedly Lovasz's proof [4] of the chromatic number of Kneser graphs. His argument centers on the *neighbourhood complex N*(*G*) of a graph, whose vertices are the vertices of the graph and

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whose faces are subsets of vertices that have a common neighbour.
We consider a univariate polynomial, which called the *neighbourhood polynomial* of graph G, $N(G,x)=\Sigma_{U\in N(G)}x^{|U|}$ ([3]) where $N(G)$ is neighbourhood complex of a graph, whose vertices are the vertices of the graph and faces are subsets of vertices that have a common neighbour.

Example 1. For a cycle with four vertices {a,b,c,d} we have $N(C_4,x)=1+4x+2x^2$. Because the empty set trivially has a common neighbour (as the graph has at least one vertex) while each of the single vertices has a neighbour. Each set {a, c} and {b, d} has two common neighbours, but one suffices, and there is no subset of three vertices that have a common neighbour. Thus the neighbourhood complex is

$$\{\emptyset, \{a\}, \{b\}, \{c\}, \{d\}, \{a, b\}, \{b, d\}\}$$

and so we have the result.

Example 2: For a complete graph K_n we have $N(K_n,x)=(1+x)^n-x^n$. Since every subset of the vertices of a complete graph except the entire vertex set has a common neighbour.

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 these nanostructures (see for example [1, 2, 5]).

In this paper we consider some specific graphs and nanostructures and study their neighborhood polynomials.

2. MAIN RESULTS

In this section we compute the neighbourhood polynomial for some graphs and nanostructures. First we state some properties of neighbourhood polynomial.
We say G is C_4*-free* if G does not contain C_4 as a sub-graph (not necessarily induced).
The following theorem gives the neighborhood polynomial of C_4-free graph.

Theorem 1 ([3]) *Let G be C_4-free with n vertices and m edges. Then*

$$N(G,x)=\sum_{v\in V}(1+x)^{\deg v}-x(2m-n)-(n-1).$$

Proof: Let $N_1,....,N_k$ be the maximal (with respect to containment) neighbourhoods of the vertices of a graph G with n vertices and m edges. Note that in general, $k\leq n$ as some vertices may have the same neighbourhoods, or one might be a subset of the other. A set belongs to the neighbourhood complex of G if and only if it is a subset of one of the N_i s.

By assuming that G has no isolated vertices and is C_4*-free*, a first order approximation for the neighbourhood polynomial is

$$N(G,x)=\sum_{v\in V}(1+x)^{\deg v}-x\sum_{v\in V}(\deg v-1)-(n-1)=\sum_{v\in V}(1+x)^{\deg v}-x(2m-n)-(n-1),$$

Proving the result. ■

Using Theorem 1 we have the neighbourhood polynomials for many graphs.

Corollary 1:

i. If $G=C_n$ is a cycle of length $n>4$, then $N(C_n,x)=1+nx+nx^2$.

ii. If G is an r-regular graph of girth at least 5, then $N(G,x)=n(1+x)^r-n(r-1)x-(n-1)$.

iii. If G is a tree, then $N(G,x)=\sum_{v}(1+x)^{\deg v}-x(n-1)-(n-1)$.

iv. Let F_n be a friendship graph (Figure 1), then $N(F_n,x)=2n(1+x)^2+(1+x)^{2n}-(4n-1)x-2n$.

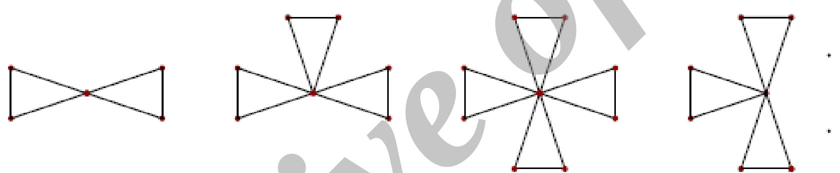

Figure 1: Friendship Graph F_2, F_3, F_4 and F_n.

Here we shall compute the neighbourhood polynomial of some dendrimers. First we compute the neighbourhood polynomial for the first kind of dendrimer of generation 1-3 has grown n stages. We denote this graph by $D_3[n]$. Figure 2 show the first kind of dendrimer of generation 1-3 has grown 3 stages $(D_3[3])$.

Theorem 2. ([1])

(i) The number of vertices of $D_3[n]$ *is* $|V(D_3[n])|=45\times 2^n-26$.

(ii) The number of edges of $D_3[n]$ *is* $|E(D_3[n])=48\times 2^n-24$.

Using Theorems 1 and 2 we have the gollowing theorem for $\mathrm{N}(D_3[n],x)$.

Theorem 3 . *The neighbourhood polynomial of* $D_3[n]$ *is:*

$$N(D_3[n],x)=(15\times 2^n-8)(1+x)^3+12(2^{n+1}-1)(1+x)^2+3\times 2^n(1+x)$$
$$-x(51\times 2^n-22)-(45\times 2^n-27).$$

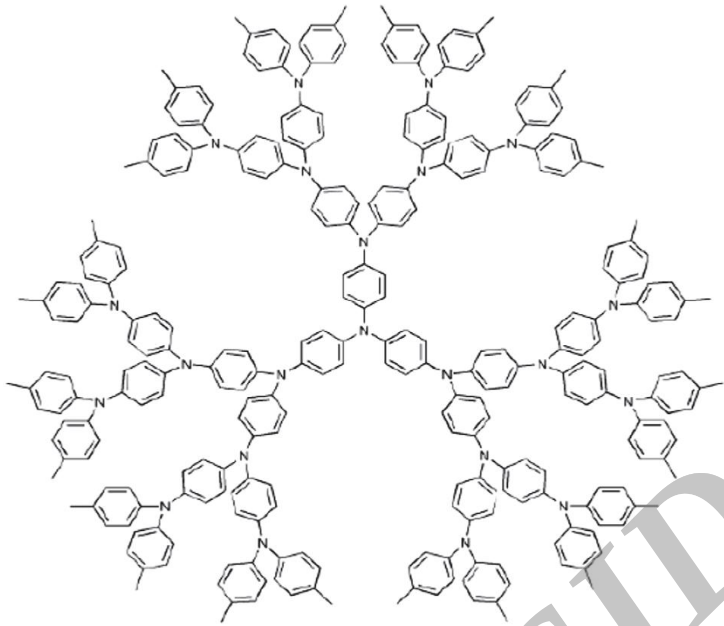

Figure 2: The First Kind of Dendrimer of Generation 1–3 has Grown 3 Stages

Proof. Let n_i be the number of vertices of degree i in $D_3[n]$, where $i = 1,2,3$. It is easy to see that $n_1 = 3\times 2^n$, $n_2 = 12\times(2^{n+1}-1)$ and $n_3 = 15\times 2^n - 8$. Now by Theorems 1 and 2 we have,

$$\begin{aligned} N(D_3[n],x) &= n_1(1+x) + n_2(1+x)^2 + n_3(1+x)^3 \\ &\quad - x(96\times 2^n - 48 - 45\times 2^n + 26) - (45\times 2^n - 27) \\ &= (15\times 2^n - 8)(1+x)^3 + 12(2^{n+1}-1)(1+x)^2 + 3\times 2^n(1+x) \\ &\quad - x(51\times 2^n - 22) - (45\times 2^n - 27). \end{aligned}$$

This completes our argument. ■

Here we shall compute the neighbourhood polynomial of the first kind of dendrimer which has grown n steps denoted $D_1[n]$. Figure 3 show $D_1[4]$. Note that there are three edges between each two cycle C_6 in this dendrimer.

Theorem 4 . ([1])
(i) The order of $D_1[n]$ *is* $2^{n+4} - 9$.
(ii) The size of $D_1[n]$ *is* $9\times 2^{n+1} - 12$.

Using Theorems 1 and 4 we have the following theorem for $N(D_1[n],x)$.

Theorem 5 . *The neighbourhood polynomial of* $D_1[n]$ *is:*

$$\begin{aligned} N(D_1[n],x) &= (6\times 2^{n+1} - 6)(1+x)^3 + (5\times 2^{n+1} - 7)(1+x)^2 + (1+x) \\ &\quad - x(5\times 2^{n+2} - 33) - (2^{n+4} - 10). \end{aligned}$$

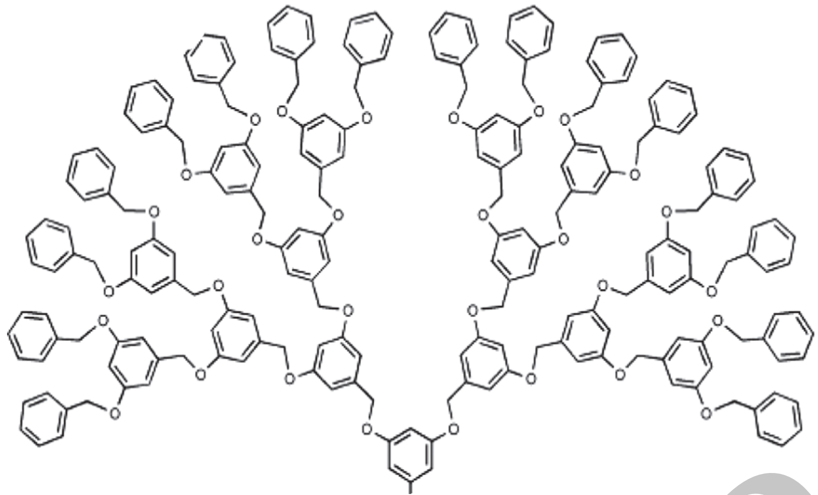

Figure 3. The First Kind of Dendrimer of Generation 1–3 has Grown 4 Stages.

Proof. Let n_i be the number of vertices of degree i in $D_1[n]$, where $i = 1, 2, 3$. It is easy to see that $n_1 = 1$, $n_2 = 5\times 2^{n+1} - 7$ and $n_3 = 6\times 2^{n+1} - 6$. Now by Theorems 1 and 4 we have,

$$\begin{aligned} N(D_1[n], x) &= n_1(1+x) + n_2(1+x)^2 + n_3(1+x)^3 - x(9\times 2^{n+2} - 24 - 2^{n+4} - 9) \\ &\quad - (2^{n+4} - 10) \\ &= (6\times 2^{n+1} - 6)(1+x)^3 + (5\times 2^{n+1} - 7)(1+x)^2 + (1+x) - x(5\times 2^{n+2} - 33) \\ &\quad - (2^{n+4} - 10), \end{aligned}$$

as desired. ■

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