Flow Polynomial of some Dendrimers

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ABSTRACT. Suppose G is an n–vertex and m–edge simple graph with edge set E(G). An integer–valued function f: E(G) → Z is called a flow. Tutte was introduced the flow polynomial F(G, λ) as a polynomial in an indeterminate λ with integer coefficients by $F(G,\lambda) = (-1)^{|E(G)|}\sum_{S\subset E(G)}(-1)^{|S|}\lambda^{n-m+c(G:S)}$, where c(G:S) is the number of connected components of G and (G : S) denotes the spanning subgraph of G with edge set S. In this paper the Flow polynomial of some dendrimers are computed.

Keywords: Flow polynomial, dendrimer, graph.

1 INTRODUCTION

A simple graph $G = (V, E)$ is a finite nonempty set $V(G)$ of objects called vertices together with a set $E(G)$ of unordered pairs of distinct vertices of G called edges. In chemical graphs, the vertices correspond to the atoms and the edges represent the chemical bonds. If $x, y \in V(G)$ then the distance $d(x, y)$ between x and y is defined as the length of a minimum path connecting x and y.

For a simple graph G, integer–valued function f: E(G) → Z is called a flow. Tutte was introduced the flow polynomial F(G, λ) as a graph function and as a polynomial in an indeterminate λ with integer coefficients by

$$F(G,\lambda) = (-1)^{|E(G)|}\sum_{S\subset E(G)}(-1)^{|S|}\lambda^{n-m+c(G:S)},$$

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where c(G:S) is the number of connected components of G and (G : S) denotes the spanning subgraph of G with edge set S [1, 5–8]. At x = 0, the Tutte polynomial specializes to the flow polynomial studied in combinatorics. He proved that $F(G,\lambda) = (-1)^{|E|+|V|+c(G)}T(G,0,1-\lambda)$, where T(G, x,y) is the Tutte polynomial of graph G.

We denote the complete graph, the cycle and the path of order n by K_n, C_n and P_n, respectively.

2 THE FLOW POLYNOMIAL OF GRAPHS

In this section we compute the flow polynomial of an infinite class of a special type D of dendrimers. Dendrimers are complex macromolecules with very well–defined chemical structures. They consist of three major architectural components: core, branches and end groups. The topological study of these macromolecules is the subject of some recent papers [2–4]. For the sake of completeness, we mention here six results from [5] which are important in our calculations.

Theorem A. F(G, λ) is a polynomial of degree t = t(G). The coefficient of λ^t is $(-1)^t$ and all terms in F(G, λ) have the same sign.

Theorem B. If G has no edges, then F(G, λ) = 1 and If G has a bridge, then F(G, λ) = 0.

Theorem C. If G consists of two graphs H and K which are either disjoint or have a single vertex in common, then F(G, λ) = F(H, λ) F(K, λ).

Theorem D. If G is a cycle, then F(G, λ) = λ – 1.

Theorem E. F(G, λ) is a topological invariant and hence any two homeomorphic graphs will have the same flow polynomial.

Theorem F. If e is any edge of G, then F(G, λ) = F(G–e, λ) − F(G.e, λ), where G.e contracting the edge e.

Theorem 1. Let G be a graph with two induced cycles C_m and C_n containing a common path P_t without bridge edge. Then the Flow polynomial of G is obtained as follows:

$$F(G,\lambda) = \left(F(C_{m-t+1},\lambda)F(C_{n-t+1},\lambda) + F(C_{m+n-2t+2},\lambda)\right).$$

Proof. The graph H has two induced cycles, C_m and C_n, such that they have a path P_t in common, see Figure 1. Let P_t: $v_1e_1v_2e_2 \ldots v_{t-1}e_{t-1}v_t$ be a common path

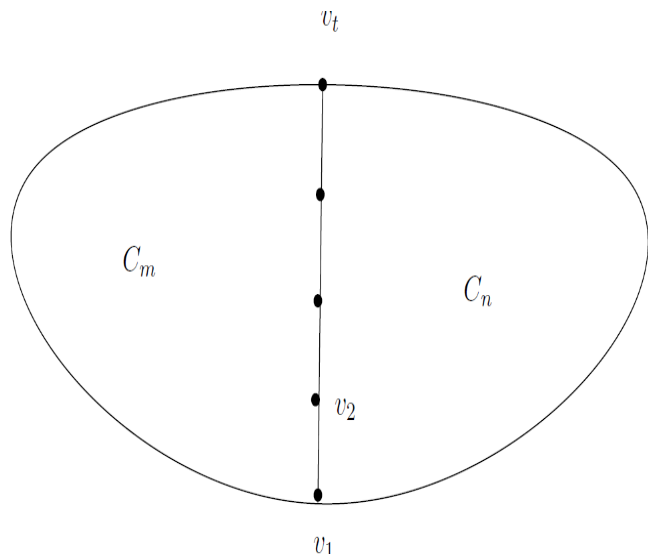

Figure 1. The bicycle graph.

between C_m and C_n. Then we have

$$F(H,\lambda) = F(H/e_1,\lambda) + F(H-e_1,\lambda).$$

Since H–e_1 is a unicycle graph, then $F(H-e_1,\lambda) = F(C_{m+n-2t+2},\lambda)$. By continuing this process, we have

$$\begin{aligned} F(H,\lambda) &= F(H/e_1/e_2,\lambda) + F(H/e_1-e_2,\lambda) + F(H-e_1,\lambda) \\ &= F(H/e_1/e_2/e_3,\lambda) + F(H/e_1/e_2-e_3,\lambda) + F(H/e_1-e_2,\lambda) + F(H-e_1,\lambda) \\ &\vdots \\ &= F(H/e_1/e_2/e_3/\cdots/e_{t-1},\lambda) + F(H/e_1/e_2/e_3/\cdots/e_{t-2}-e_{t-1},\lambda) \\ &\quad + F(H/e_1/e_2/e_3/\cdots/e_{t-3}-e_{t-2},\lambda) \\ &\vdots \\ &\quad + F(H/e_1/e_2-e_3,\lambda) + F(H/e_1-e_2,\lambda) + F(H-e_1,\lambda) \\ &= F(C_m,\lambda)T(C_{n;},\lambda) + F(C_{m+n-2t+2},\lambda) \\ &= F(C_{m-t+1},\lambda)F(C_{n-t+1},\lambda) + F(C_{m+n-2t+2},\lambda). \end{aligned}$$

By above argument the proof is completed. ■

Theorem 2. Let G be a simple graph with edge disjoint cycles without bridge edge. Then the flow polynomial of G is obtained as follows:

$$F(G,\lambda) = (\lambda - 1)^t.$$

where t is the number of cycles of G.

Proof. Apply Theorems C and D. ■

Corollary 3. Let D be a dendrimer with a bridge edge then $F(G,\lambda) = 0$.

Proof. Apply Theorems F. ■

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