On the Tutte polynomial of benzenoid chains

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ABSTRACT

The Tutte polynomial of a graph $G$, $T(G, x, y)$ is a polynomial in two variables defined for every undirected graph contains information about how the graph is connected. In this paper a simple formula for computing Tutte polynomial of a benzenoid chain is presented.

Keywords: Benzenoid chain, Tutte polynomial, graph.

1. INTRODUCTION

Benzenoid graphs or graph representations of benzenoid hydrocarbons are defined as finite connected plane graphs with no cut-vertices, in which all interior regions are mutually congruent regular hexagons. More details on this important class of molecular graphs can be found in the book of Gutman and Cyvin [1], and in the references cited therein.

Suppose $G$ is an undirected graph, $E = E(G)$ and $v$ is a vertex of $G$. The vertex $v$ is reachable from another vertex $u$ if there is a path in $G$ connecting $u$ and $v$. In this case we write $v \alpha u$. A single vertex is a path of length zero and so $\alpha$ is reflexive. Moreover, we can easily prove that $\alpha$ is symmetric and transitive. So $\alpha$ is an equivalence relation on $V(G)$. The equivalence classes of $\alpha$ is called the connected components of $G$. The Tutte polynomial of a graph $G$ is a polynomial in two variables defined for every undirected graph contains information about how the graph is connected [2-4]. To define we need some notions. The edge contraction $G/uv$ of the graph $G$ is the graph obtained by merging the vertices $u$ and $v$ and removing the edge $uv$. We write $G - uv$ for the graph where the edge $uv$ is merely removed. Then the Tutte polynomial of $G$ is defined by the recurrence relation $T[G; x, y] = T(G - e; x, y) + T(G/e; x, y)$ if $e$ is neither a loop nor a bridge with base case $T(G; x, y) = x^i y^j$ if $G$ contains $i$ bridges and $j$ loops and no other edges. In particular,

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The Tutte polynomial $T(G; x, y) = 1$ if $G$ contains no edges. The importance of the Tutte polynomial $T(G, x, y)$ comes from the algebraic graph theory as a generalization of counting problems related to graph coloring and nowhere-zero flow. It is also the source of several central computational problems in theoretical computer science.

In this paper, the Tutte polynomial of a benzenoid chain $BC(x_1, ..., x_r)$ is computed. This graph is constructed from $r$ linear chains of length $x_1, x_2, ..., x_r$, respectively. Suppose $BC(h)$ denotes the set of all benzenoid chains with $h$ hexagons.

In Figures 1 and 2, the molecular graph of a linear chain $LC(h)$ and $BC(2,3,2,2,4,2,3,2,2)$ is depicted.

Throughout this article our notation is standard and taken mainly from the standard book of graph theory.

2. **Main Results**

In this section the Tutte polynomial of a benzenoid chain $G(h)$ is computed. We first notice that, one can define the Tutte polynomial of a graph $G$ as follows:
\[ T(G; x, y) = \sum_{A \subseteq E(G)} (x - 1)^{c(A)} - c(E) (y - I)^{c(A)} + |A| - |V|. \]

Here, \(c(A)\) denotes the number of connected components of the graph \((V,A)\).

**Theorem 1.** \(T(BC(x_1, x_2, \ldots, x_n); x, y) = T(LBC(x_1 + \ldots + x_n - n + 1); x, y)\).

**Proof.** We proceed by induction on \(n\) to prove

\[ T(BC(x_1, x_2, \ldots, x_n); x, y) = T(LBC(x_1 + \ldots + x_n - n + 1); x, y), \]

and

\[ T(BC(x_1, x_2, \ldots, x_n - C_5); x, y) = T(LBC(x_1 + \ldots + x_n - n + 1 - C_5); x, y). \]

Clearly the result is valid for \(n = 1\). Suppose the validity of result for \(n = k\) and prove it for \(n = k + 1\). Our main proof consider two cases that \(x_{k+1} = 2\) or \(x_{k+1} > 2\). If \(x_{k+1} = 2\) then

\[ T(BC(x_1, x_2, \ldots, x_k, 2); x, y) = x^4 T(BC(x_1, x_2, \ldots, x_k); x, y) + T(BC(x_1, x_2, \ldots, x_k - C_5); x, y) \]
\[ = (x^4 + x^3 + x^2 + x + 1) T(BC(x_1, x_2, \ldots, x_k); x, y) \]
\[ + y T(BC(x_1, x_2, \ldots, x_{k-1}, 1 - C_5); x, y) \]
\[ = T(LBC(x_1 + \ldots + x_k - k + 2); x, y), \]

as desired. On the other hand, by a similar method one can prove that

\[ T(BC(x_1, x_2, \ldots, x_k, 2 - C_5); x, y) = T(LBC(x_1 + \ldots + x_k - k + 2 - C_5); x, y). \]

We now assume that \(m = x_{k+1} > 2\) and the result is valid for \(m\). We have:

\[ T(BC(x_1, x_2, \ldots, x_k, m+1); x, y) = (x^4 + x^3 + x^2 + x + 1) T(BC(x_1, x_2, \ldots, x_k, m); x, y) \]
\[ + y T(BC(x_1, \ldots, x_k, m - C_5); x, y) \]
\[ = (x^4 + x^3 + x^2 + x + 1) T(LBC(x_1 + x_2 + \ldots + x_{k+m-k}); x, y) \]
\[ + y T(LBC(x_1 + \ldots + x_k + m - k - C_5); x, y), \]

which completes our proof.

Before stating the main result of this paper we notice that if \(h = 1, 2\) then

\[ T(G(0), x, y) = x, \text{ where } G(0) \text{ is an edge}, \]
\[ T(G(1), x, y) = x^5 + x^4 + x^3 + x^2 + x + y. \]
Theorem 2. Suppose $G = G(x_1,x_2,...,x_n)$ is an arbitrary benzenoid chain in $BC(h)$, where $h = x_1 + x_2 + \ldots + x_n - n + 1$. Then for $h > 2$

$$T(G, x, y) = \left( \frac{x(J + \sqrt{\Delta}) + 2(1-x)y}{2\sqrt{\Delta}} \right)^n \left( \frac{J + \sqrt{\Delta}}{2} \right)^n + \left( \frac{x(-J + \sqrt{\Delta}) - 2(1-x)y}{2\sqrt{\Delta}} \right)^n \left( \frac{J - \sqrt{\Delta}}{2} \right)^n,$$

where

$$J = x^4 + x^3 + x^2 + x + 1 + y,$$

$$\Delta = (x^4 + x^3 + x^2 + x + 1)^2 + y^2 + 2y(x^4 + x^3 + x^2 + x + 1) - 4x^4y.$$

Proof. By Theorem 1, it is enough to consider the case when $G = G(h)$ is a linear benzenoid chain with exactly $h$ hexagons. Define $S(h) = T(G(h), x, y)$. Consider the following five graphs:

- The Graph $G_1(h)$ constructed from $G$ by replacing the end hexagon of $G$ by a triangle, Figure 3(ii);
- The Graph $G_2(h)$ constructed from $G$ by replacing the end hexagon of $G$ by a quadrangle, Figure 3(iii);
- The Graph $G_3(h)$ constructed from $G$ by replacing the end hexagon of $G$ by a pentagon, Figure 3(iv);
- The Graph $G_4(h)$ constructed from $G$ by replacing the end hexagon of $G$ by an edge, Figure 3(v);
- The Graph $G_5(h)$ constructed from $G_1(h)$ by adding a loop to the middle vertex of the pentagon, Figure 3(vi).

To compute the Tutte polynomial of $G$, we proceed by induction on $h$ and obtain a recurrence relation for $S(h)$. We first notice that $S(1) = x^5 + x^4 + x^3 + x^2 + x + y$. Define $S_i(h) = T(G_i(h-1), x, y), 1 \leq i \leq 5$. By deleting an edge from the end hexagon of $G$ with vertices of degree 2 and applying Theorem 1, we can see that

$$S(h) = x^4S(h-1) + S_1(h-1) = x^4S(h-1) + x^3S(h-1) + S_2(h-1)$$

$$= x^4S(h-1) + x^3S(h-1) + x^2S(h-1) + S_3(h-1)$$

$$= x^4S(h-1) + x^3S(h-1) + x^2S(h-1) + xS(h-1) + S_4(h-1)$$

$$= x^4S(h-1) + x^3S(h-1) + x^2S(h-1) + xS(h-1) + S_5(h-1) + S_5(h-2)$$

$$= (x^4 + x^3 + x^2 + x + 1) S(h-1) + S_5(h-2).$$

Therefore

$$S(h) = (x^4 + x^3 + x^2 + x + 1) S(h-1) + S_5(h-2).$$ (1)
We now calculate $S_5(h - 2)$. To do this, we notice that $S_5(h - 2)$ has a loop. Thus

$$S_5(h - 2) = yS_1(h - 2). \quad (2)$$

To compute $S_1(h - 2)$ we put $h - 1$ in $S(h) = x^4S(h-1) + S_1(h - 1)$. Thus $S(h - 1) = x^4S(h - 2) + S_1(h - 2)$. Therefore $S_1(h - 2) = S(h - 1) - x^4S(h - 2)$. Apply Eqs. (1) and (2), we have:

$$S(h) = (x^4 + x^3 + x^2 + x + 1) S(h-1) + yS_1(h - 2). \quad (3)$$

Hence,

$$S(h) = (x^4 + x^3 + x^2 + x + 1) S(h-1) + y(S(h - 1) - x^4S(h - 2)).$$

This implies that

$$T(G(h), x, y) = \left(y + \frac{x^5 - 1}{x - 1}\right)T(G(h-1), x, y) - x^4yT(G(h-2), x, y).$$

There are several methods in discrete mathematics to solve such a recurrence equation. By applying one of these methods, we have

$$T(G, x, y) = \frac{x(J + \sqrt{A}) + 2(1-x)y}{2\sqrt{A}} \left(\frac{J + \sqrt{A}}{2}\right)^n + \frac{x(-J + \sqrt{A}) - 2(1-x)y}{2\sqrt{A}} \left(\frac{J - \sqrt{A}}{2}\right)^n,$$

where

$$J = x^4 + x^3 + x^2 + x + 1 + y,$$

$$A = (x^4 + x^3 + x^2 + x + 1)^2 + y^2 + 2y(x^4 + x^3 + x^2 + x + 1) - 4x^4y,$$

which completes our proof.
Figure 3. A Graph $G(h)$ and Five Types of Graphs Constructed from $G(h)$.

REFERENCES