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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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:
\[ T(G; x, y) = \sum_{A \subseteq E(G)} (x - 1)^{c(A)} (y - 1)^{|A| - |V|}. \]

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

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

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

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

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

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

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

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

which completes our proof. \( \Box \)

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

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

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

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

where

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

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

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 $S(l) = x^5 + x^4 + x^3 + x^2 + x + y$. 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

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

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

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

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

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

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

$$S_5(h - 2) = yS_1(h - 2).$$  \hspace{1cm} (2)$$

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

$$S(h) = (x^4 + x^3 + x^2 + x + 1) S(h - 1) + yS_1(h - 2).$$ \hspace{1cm} (3)

Hence,

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

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

This implies that $T(G(h), x, y) = \left( y + \frac{x^5 - 1}{x - 1} \right) T(G(h - 1), x, y) - x^4y T(G(h - 2), x, y)$. There are several methods in discrete mathematics to solve such a recurrence equation. By applying one of these methods, we have

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

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

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. \hfill \square
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**Figure 3.** A Graph $G(h)$ and Five Types of Graphs Constructed from $G(h)$.

**REFERENCES**