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Note

# Equivalence between Clar covering polynomials of single zigzag chains and tiling polynomials of $2 \times n$ rectangles

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The authors would like to celebrate the birthday of Professor Janina Nazarewicz with this article.

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ABSTRACT

This paper offers a formal explanation of a rather puzzling and surprising equivalence between the Clar covering polynomials of single zigzag chains and the tiling polynomials of $2 \times n$ rectangles for tilings using $1 \times 2$, $2 \times 1$ and $2 \times 2$ tiles. It is demonstrated that the set of Clar covers of single zigzag chains $N(n-1)$ is isomorphic to the set of tilings of a $2 \times n$ rectangle. In particular, this isomorphism maps Clar covers of $N(n-1)$ with $k$ aromatic sextets to tilings of a $2 \times n$ rectangle using $k$ square $2 \times 2$ tiles. The proof of this fact is an application of the recently introduced interface theory of Clar covers. The existence of a similar relationship between the Clar covers of more general benzenoid structures and more general tilings of rectangles remains an interesting open problem in chemical graph theory.



## 1. Introduction

This paper offers a formal explanation of a rather puzzling and surprising coincidence between the Clar covering polynomials of a certain class of benzenoid structures and certain tiling polynomials of $2 \times n$ rectangles discovered recently by Sloane [14]. He observed [15] that for $n \leq 12$ the Clar covering polynomials (*aka* Zhang–Zhang polynomials or ZZ polynomials) of single zigzag chains $N(n-1)$ coincide exactly with the tiling polynomials of $2 \times n$ rectangles for tilings with $2 \times 2$, $2 \times 1$ and $1 \times 2$ tiles. It is possible to verify numerically that the equivalence between both families of polynomials extends to much higher values of $n$ but no proof of this fact is known for a general value of $n$ – or even more importantly – no understanding of this phenomenon is available. The main goal of this paper is to establish a direct and lucid correspondence between the Clar covering polynomials of single zigzag chains $N(n)$ and tiling polynomials of $2 \times n$ rectangles. This task might constitute the first step in establishing an analogous relationship between Clar covering polynomials and tiling polynomials of more general classes of benzenoid structures and $m \times n$ rectangles, respectively. Such a result may add to the recently discovered equivalence between the Clar covering polynomials of benzenoid structures and the cube polynomials of resonance graphs [19,1], possibly opening a new avenue in chemical graph theory.

Single zigzag chains are a class of condensed polycyclic aromatic compounds [9]. A single zigzag chain of length $n$, abbreviated as $N(n)$, can be defined as a sequence of $n$ fused benzene rings selected from the hexagonal lattice in the armchair direction, as shown in Fig. 1 [7,3].

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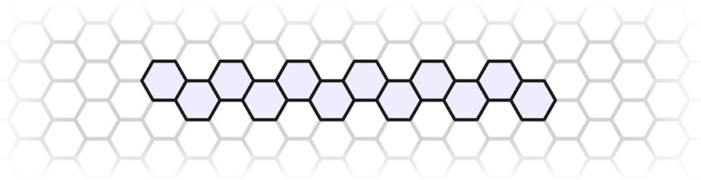

**Fig. 1.** An example of a single zigzag chain $N(n)$ with $n = 12$ depicted on the underlying hexagonal lattice.

A *Clar cover* of a benzenoid $S$ can be defined [6] from two different viewpoints. In chemical terminology, a Clar cover is a resonance structure of $S$, such that every carbon atom maintains tetravalent character by participating either in a double bond or in an aromatic sextet. From the graph-theoretical perspective, a Clar cover is a spanning subgraph of $S$ that has only hexagons and edges as its components. The *order* of a given Clar cover $C$ is defined as the number of aromatic rings (hexagons) present in $C$. The number of conceivable Clar covers of $S$ can be conveniently expressed in form of a *Clar covering polynomial* (*aka Zhang–Zhang polynomial* or *ZZ polynomial*) [20,22,18,21],

$$\mathrm{ZZ}\,(S, x) = \sum_{k=0}^{Cl} c_k x^k, \tag{1}$$

where the *Clar number* $Cl$ is the maximal number of aromatic rings that can appear in $S$ [6,8], $x$ is a dummy variable keeping track of the order $k$, and $c_k$ is the number of possible Clar covers of order $k$.

The number of conceivable tilings of a $2 \times n$ rectangle using $2 \times 2$, $2 \times 1$ and $1 \times 2$ tiles (briefly: $2 \times n$ *tilings*) [13] can be conveniently expressed in form of a *tiling polynomial*

$$\mathrm{TP}\,(n, x) = \sum_{k=0}^{\lfloor n/2 \rfloor} t_k x^k, \tag{2}$$

where $t_k$ is the number of possible tilings using exactly $k$ tiles of dimension $2 \times 2$ and $n - 2k$ tiles of dimensions $2 \times 1$ or $1 \times 2$. Sloane [14,15] discovered that $\mathrm{TP}\,(n, x) = \mathrm{ZZ}\,(N(n-1), x)$ for $n \le 12$ [3,2]. An illustration of this fact for $n = 4$ is given in Fig. 2, where we arrange all the conceivable Clar covers of $N(n-1)$ and all the conceivable $2 \times n$ tilings in a way demonstrating explicitly the equality of both polynomials. Careful inspection of these structures reveals that the Clar covers and tilings do not only agree in their respective numbers, but also share certain structural properties. Specifically, it is possible to relate the position of the aromatic sextets in the Clar covers to the position of the $2 \times 2$ tiles in the corresponding tilings. A further similarity is given by the fact that, just like any always can be replaced by either or to yield another Clar cover, any $2 \times 2$ tile always can be replaced by either or to yield another tiling.

In the following sections, the reasons responsible for these analogies will be derived. Indeed, it will become clear that there exists a one-to-one correspondence not only between both polynomials, but also between the Clar covers of $N(n-1)$ and $2 \times n$ tilings.

## 2. Basic theory

ZZ polynomials are usually computed using recursive decomposition algorithms [10,3,5,2,4,17,16]. In [12], we have developed an alternative method for representing and enumerating Clar covers of single zigzag chains by introducing the concepts of interfaces and connectivity graphs. In this section, some important definitions and results pertaining to these concepts and relevant to the problem at hand are summarized. For a more detailed step-by-step introduction, see [12].

First, we define an interface, which can be perceived as a descriptor of a local structure of a Clar cover.

**Definition 1** (*[12, Def. 9]*)**.** Assume that a single zigzag chain $N(n)$ is horizontally oriented as depicted in Fig. 1. Each hexagon $h_j$ in $N(n)$ then possesses a pair of horizontal edges, specifically, an *outer edge*, which connects two vertices that do not belong to any hexagon other than $h_j$, and an *inner edge*, which has at least one vertex belonging to an adjacent hexagon $h_{j-1}$ or $h_{j+1}$. The Clar covering character of this pair of horizontal edges, denoted as $(kl)$, will be referred to as an *interface*. In the symbol $(kl)$, $k$ refers to the outer edge and $l$ refers to the inner edge. The indices $k$ and $l$ can take the values s, d and a, corresponding to single, double and aromatic bonds, respectively. In graph-theoretical terminology, the values s, d and a correspond to no covering, edge covering and hexagon covering, respectively.

Every Clar cover of a single zigzag chain can be expressed as a sequence of interfaces in the following way.

**Definition 2.** Let $\kappa$ be the map that assigns to each Clar cover of $N(n)$ the sequence of interfaces $I = (i_1, i_2, \ldots, i_n)$, where $i_j$ is the interface of the $j$th hexagon of $N(n)$. An example for this map is given in Fig. 3.