Informaticae Abstracta
Año 2023, Vol. 1, No. 1, pp. 20-29 JUL | DIC 2023

Independent sets on n-polygonal regular arrays

Hernández-Servín, J.A.; Marcial-Romero, J.R.; De Ita Luna, G.

Article info

Recibido: 10-feb-2023
Aceptado: 15-jun-2023

Keywords: Merrifield-Simmons index, Polygonal arrays, Independent sets, Graph theory

Abstract

On this paper, we present a closed formula to compute the Merrifield-Simmons index on polygonal arrays at distance 1. The proof of our main theorem establishes a method to solve the recurrences derived from a decomposition of the original polygonal array at any distance. Hence, closed formulas for any polygonal array can be obtained. Closed formulas had previously been exhibited when polygons were vertex's joined however for edge's joined it has not been previously presented.

1 Introduction

Hexagonal chain graphs have been widely investigated. They represent a relevant area of interest in mathematical chemistry, since they are molecular graphs used to represent the structural formula of chemical benzenoid compounds. Thus, the unbranched catacondensed benzenoid molecules play an important role for the theoretical chemistry of benzenoid hydrocarbons [1].

The Merrifield-Simmons index of a molecular graph G, that is the number of independent sets of G, denoted as $\sigma(G)$, is a typical example of an invariant used in mathematical chemistry for quantifying relevant details of molecular structures. Merrifield and Simmons showed the correlation between $\sigma(G)$ and boiling points for polygonal chain graphs representing chemical molecules.

Hexagonal chains have been widely investigated and represent a relevant area of interest in mathematical chemistry, since they are used for quantifying relevant details of the molecular structure of the benzenoid hydrocarbons [2, 1, 3].

In recent years, a lot of work has been done on the extremal problem for the Merrifield-Simmons index, i. e., on determining the graphs within a prescribed class that minimize or maximize the value of the index. Gutman [4] discussed the extremal hexagonal chains according to three topological invariants: Hosoya index, largest eigenvalue, and Merrified-Simmons index. His work greatly motivated the study of extremal polygonal chains.

On his seminal paper, Gutman showed that the linear chain has the maximum value for the Merrifield-Simmons index for the particular case of hexagonal chains. Afterward, L.Zhang [5] showed that the minimum value for the Merrifield-Simmons index is achieved by the zig-zag polyphenegraph, which we denote as H^1.

These results were further generalized in various directions: the second-smallest (-largest) values were determined [6] as well as the corresponding extremal chains, and it was shown that the linear chain is still optimal if catacondensed benzenoids are considered (which allow branching, as opposed to chains). A very surprising result due to Zhang and Zhang [7] states that the linear chain and the zigzag chain are even extremal, when the number of independent sets or edges of any fixed size k (and not just the sum over all k) are considered.

Several works have been developed for searching closed formulas to compute the Merrifield-Simmon index on different class of graphs. For example, Döslić et.al [9] showed closed formulas based on the independence polynomials of polyphenylene uniform chains. De Ita et.al [8] presented some recurrence equations to compute the Merrifield-Simmons index on polygonal uniform chains.

In this paper, we develop initial recurrence equations expressing the Merrifield-Simmons index on a polygonal uniform chain at distance 1. Our objective is to find closed formulas for computing $\sigma(H^1)$, we also show that the computation of $\sigma(H^1)$ can be done in poly-logarithmic time, and in fact, for any polygonal uniform chain at distance 1.

2 Preliminaries

Let $G = (V, E)$ be an undirected simple graph with set of vertices V and set of edges E. The *neighborhood* of a vertex $v \in V$ is defined as the set of vertices adjacent to v, that is $N(v) = \{y \in V \mid vy \in E\}$. The *closed neighborhood* of V is defined as $N[v] = N(v) \cup \{v\}$.

A simple path of length n between two vertices v and y , denoted as P_n, is a sequence of distinct edges in E of the form $v_0v_1, v_1v_2, \ldots, v_{n-1}v_n$, such that $v_0 = v$ and $v_n = y$. A simple cycle C_n is a non-empy simple path P_n, where the first and last vertices are identical. The distance $d_G(v; y)$ from a vertex v to another vertex y is the minimum number of edges in an $v - y$ path of G.

An *independent set* of V is a subset $S \subseteq V$ such that when $v, y \in S$, then $vy \notin E$. The number of independent sets of a graph G is denoted as $\sigma(G)$. We restrict our attention to particular cases of molecular graphs. An m-gon is a simple cycle C_m. Meanwhile, an n, m-gon chain graph consists of a set of n, m-gons $C^1, C^2, \ldots C^n$ such that $E(C^i) \cap E(C^{i+1}) = \{e_i\}$, e.g. the intersection of two consecutive m-gons is a single edge. Figure 1 shows a 5, 6-gon chain graph, which is also called an hexagonal chain graph. From now on, we will call an nm-gon chain graph as an array of n, m-gons.

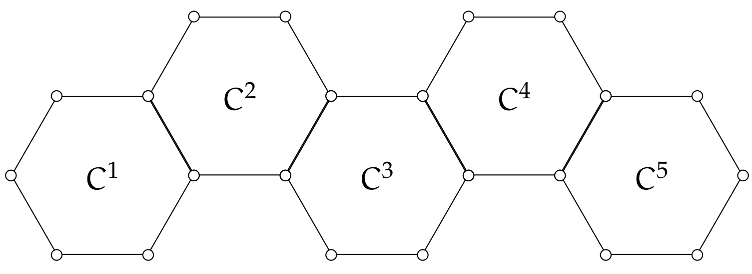

Figure 1: Hexagonal chain graph

Let $\mathcal{H}_n^m$ be an array of n, m-gons. By definition, each par of adjacent m-gons C^i and C^{i+1} are joined by a common edge, lets say e_i. If each pair of consecutive sharing edges e_i and e_{i+1} of the array holds that $d_{H_n}(e_i, e_{i+1}) = r$, then we say that $\mathcal{H}_n^m$ is an array at distance r. For example, for hexagonal chain graphs with $r = 1$, then $\mathcal{H}_n^6$ is known as the zig-zag hexagonal chain (Z_n), Figure 1.

The following rules have been useful to count independent sets on a graph G:

1. Vertex reduction rule: Let $v \in V(G)$,

$$\sigma(G) = \sigma(G - v) + \sigma(G - N[v]) \tag{1}$$

2. Edge division rule : let $e = \{x, y\} \in E(G)$,

$$\sigma(G) = \sigma(G - e) - \sigma(G - N[x] \cup N[y]) \tag{2}$$

Therefore, in order to count the number of independent sets on an $\mathcal{H}_n^m$ array at distance 1, we find a recurrence which represents that number. Afterward, we calculate a closed formula using a matrix method.

3 Posing the problem

In this section, we formally establish the problem we want to solve. The question we want to answer in this paper is how to calculate $\sigma(\mathcal{H}_n^m)$, that is

Question 1. *What's $\sigma(\mathcal{H}_n^m)$, where $\mathcal{H}_n^m$ is an n, m-gon?*

For simplicity, we drop the index m as the proof the main theorem and set of recurrences is independent of m. Part of the answer is to calculate the set of recurrences that are inferred using vertex and edge division rules. For that, we are using the decomposition of a $6, 4$–gon, which is shown in Figure 2.

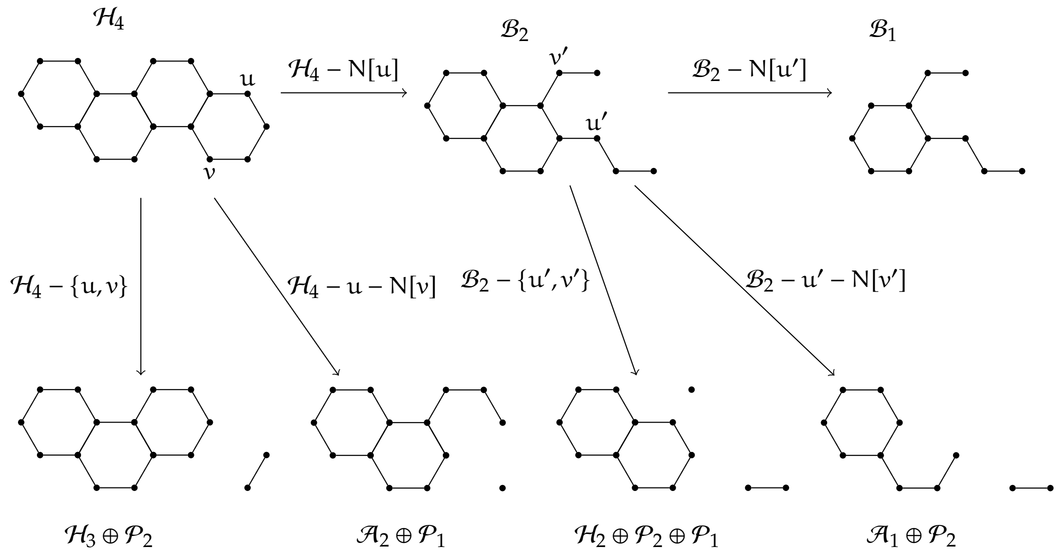

Figure 2: Decomposition of $\mathcal{H}_4$ in order to get the graphs $\mathcal{H}_3$, $\mathcal{A}_2$, $\mathcal{B}_2$, etc., which lead to the set of recurrences.

Let $\mathcal{H}_n$ be and array of n, m-gons, we ommit the superscript in $\mathcal{H}_n$ since it is composed uniquely of m-gons. Let $C^1, C^2, \ldots, C^n$ be the m-gons of $\mathcal{H}_n$. Let e_{n-1} be the edge that joins the m-gons C^{n-1} and C^n. Let v and y be the neighbours of the vertices e_{n-1} in C^n. We use Equation 1 to decompose $\mathcal{H}_n$ in order to calculate $\sigma(\mathcal{H}_n)$.

$$\begin{aligned}\sigma(\mathcal{H}_n) &= \sigma(\mathcal{H}_n - v) + \sigma(\mathcal{H}_n - N[v]) \\ &= \sigma(\mathcal{H}_n - v - y) + \sigma(\mathcal{H}_n - v - N[y]) + \sigma(\mathcal{H}_n - N[v])\end{aligned}$$

It is easy to see that $\sigma(\mathcal{H}_n - v - y) = \sigma(\mathcal{H}_{n-1}) \cdot \sigma(\mathcal{P}_{m-4})$. On the other hand, $\sigma(\mathcal{H}_n - v - N[y])$ can be computed as $\sigma(\mathcal{A}_{n-2}) \cdot \sigma(\mathcal{P}_{m-5})$, where $\mathcal{A}_{n-2}$ is the graph formed by the union of $\mathcal{H}_{n-2}$ and a path of length $m-3$ joined to a vertex of C^{n-2}. Figure 2 shows an example of $\mathcal{A}_{n-2}$ for hexagonal arrays. We call the graph $\mathcal{H}_n - (N[v])$ as $\mathcal{B}_{n-2}$, since it is the union of $\mathcal{H}_{n-2}$ and two paths of length $m-3$ and $m-4$ to the vertices of an edge e of $\mathcal{H}_2$. Figure 2 shows and example of $\mathcal{B}_{n-2}$.

The computation of $\sigma(\mathcal{A}_{n-2})$ is achieved by applying Equation 1 to the first vertex of the path, lets say v, which joins it with $\mathcal{H}_{n-2}$. The result is:

$$\begin{aligned}\sigma(\mathcal{A}_{n-2}) &= \sigma(\mathcal{A}_{n-2} - v) + \sigma(\mathcal{A}_{n-2}-(N[v])) \\ &= \sigma(\mathcal{P}_{m-4}) \cdot \sigma(\mathcal{H}_{n-2}) + \sigma(\mathcal{P}_{m-5}) \cdot \sigma(\mathcal{A}_{n-3})\end{aligned}$$

The calculation of $\sigma(B_{n-2})$ is done by applying Equation 1 to the first vertices of the paths, lets say v and y, which join them with H_{n-2}. The result is:

$$\begin{aligned}\sigma(\mathcal{B}_{n-2}) &= \sigma(\mathcal{B}_{n-2} - v) + \sigma(\mathcal{B}_{n-2} - N[v]) \\ &= \sigma(\mathcal{B}_{n-2} - v - y) + \sigma(\mathcal{B}_{n-2} - v - N[y]) + \sigma(\mathcal{B}_{n-2} - N[v]) \\ &= \sigma(\mathcal{P}_{m-5}) \cdot \sigma(\mathcal{P}_{m-4}) \cdot \sigma(\mathcal{H}_{n-2}) + \sigma(\mathcal{P}_{m-4}) \cdot \sigma(\mathcal{P}_{m-6}) \cdot \sigma(\mathcal{A}_{n-2}) + \\ &\quad \sigma(\mathcal{P}_{m-5}) \cdot \sigma(\mathcal{B}_{n-2})\end{aligned}$$

It is well known that $\sigma(\mathcal{P}_n) = F_{n+2}$, where F_n is the $n-th$ Fibonacci number. Hence, the final recurrences are as follows:

$$\begin{aligned}H_{n+1} &= F_{m-2} \cdot H_n + F_{m-3} \cdot A_{n-1} + B_{n-1} \\ A_{n+1} &= F_{m-2} \cdot H_{n+1} + F_{m-3} \cdot A_n \\ B_{n+1} &= F_{m-2} \cdot F_{m-3} \cdot H_{n+1} + F_{m-2} \cdot F_{m-4} \cdot A_n + F_{m-3} \cdot B_n\end{aligned}$$

where we have simplified the notation $\sigma(\mathcal{H}_n) = H_n$, $\sigma(\mathcal{A}_n) = A_n$ and $\sigma(\mathcal{B}_n) = B_n$. Now, if we make $p = F_{m-2}$, $q = F_{m-3}$ and $r = F_{m-4}$, then the recurrences for an array of n, m-gons at distance one become a reduced sets of recurrences:

$$\begin{aligned}H_{n+1} &= pH_n + qA_{n-1} + B_{n-1} \\ A_{n+1} &= pH_{n+1} + qA_n \\ B_{n+1} &= pqH_{n+1} + prA_n + qB_n\end{aligned} \tag{3}$$

Thus, Question (1) has been reduced to solve the above set of recurrences, which we are going established as the main theorem of this paper.

Theorem 1. *Let us define* a_n, c_n *two sequences as* $a_{-1} = 0$, $a_0 = 0$, *and* $a_n = n$ *for all* n, *and* $c_0 = 1$ *and* $c_n = -(a_{n-2}P + a_nQ)$, *where* $P = p(pr - q^2)/q^2$ *and* $Q = p/q$. *Let* T *be the upper triangular matrix*

$$\begin{pmatrix} 1 & c_1 & \cdots & c_n \\ 0 & 1 & \cdots & c_{n-1} \\ \vdots & & \cdots & \vdots \\ 0 & 0 & \cdots & c_1 \\ 0 & 0 & \cdots & 1 \end{pmatrix}$$

and $\Lambda = (\delta_{ij}t_{ij})$. *If* $y_n = H_n/q^n$, *then we have that*

$$\begin{pmatrix} y_n \\ \vdots \\ y_5 \end{pmatrix} = \left(\sum_{j=0}^{n} \left(-\Lambda^{-1}T_u\right)^j \right) \begin{pmatrix} z_n \\ \vdots \\ z_4 \end{pmatrix} \tag{4}$$

gives a solution to the system of recurrences (3) for H_n, *where* $z_n = x_n - \sum_{s=2}^{4} c_{4-s+1}y_s$ *and the sequence* x_n *is given by*

$$x_n = \frac{A_1}{q^2} + \frac{D}{q} + \frac{A_1(n-2)}{q} + \frac{A_1(pr-q^2)(n-3)}{q^3}$$

with $D = B_1/q + A_1(pr - q^2)/q^2$.

Proof. We want to solve A_n, B_n and the back substitution of (3) after finding out an equation for H_n. Starting with (3), we can apply a well known generalized procedure to solve these type of recurrences by taking as input data the recurrence H_n. Thus, if $f_n = q$ for all n, we have the recurrence $A_{n+1} - f_nA_n = pH_{n+1}$. The recurrence is therefore equivalent to

$$\frac{A_{n+1}}{\prod_{k=0}^{n} f_k} - \frac{A_n}{\prod_{k=0}^{n-1} f_k} = \frac{pH_{n+1}}{\prod_{k=0}^{n} f_k}, \tag{5}$$

which after taking the sums we end up with

$$A_{n+1} = q^{n+1}\left(\frac{A_1}{q} + p\sum_{k=1}^{n} \frac{H_{k+1}}{q^{k+1}}\right) \tag{6}$$

$$A_{n+1} = q^nA_1 + pq^{n+1}\sum_{k=1}^{n} \frac{H_{k+1}}{q^{k+1}}$$

$$A_{n-1} = q^{n-2}A_1 + pq^{n-1}\sum_{k=1}^{n-2} \frac{H_{k+1}}{q^{k+1}}$$

If now we solve for B_{n+1}, using (3), we have the recurrence $B_{n+1} - qB_n = qA_{n+1} - q^2A_n + prA_n$ and by using the same procedure as for A_n, we have

$$\begin{aligned} B_{n+1} &= q^{n+1}\left(\frac{B_1}{q} + \sum_{s=1}^{n} \frac{qA_{s+1} + (pr - q^2)A_s}{q^{s+1}}\right) \qquad (7) \\ &= q^n B_1 + q^{n+1}\sum_{s=1}^{n} \frac{qA_{s+1} + (pr - q^2)A_s}{q^{s+1}} \\ B_{n-1} &= q^{n-2}B_1 + q^{n-1}\sum_{s=1}^{n-2} \frac{qA_{s+1} + (pr - q^2)A_s}{q^{s+1}} \end{aligned}$$

For B_{n-1} we obtain,

$$\begin{aligned} B_{n-1} &= q^{n-2}B_1 + q^{n-1}\sum_{s=1}^{n-2}\frac{A_{s+1}}{q^s} + (pr - q^2)q^{n-1}\sum_{s=1}^{n-2}\frac{A_s}{q^{s+1}} \\ &= q^{n-2}B_1 + q^{n-1}\sum_{s=1}^{n-2}\frac{A_{s+1}}{q^s} + (pr - q^2)q^{n-1}\sum_{s=1}^{n-2}\frac{A_s}{q^{s+1}} \\ &= q^{n-2}B_1 + (pr - q^2)q^{n-3}A_1 + q^{n-1}\sum_{s=1}^{n-2}\frac{A_{s+1}}{q^s} + (pr - q^2)q^{n-1}\sum_{s=2}^{n-2}\frac{A_s}{q^{s+1}} \\ &= D + q^{n-1}\sum_{s=1}^{n-2}\frac{A_{s+1}}{q^s} + (pr - q^2)q^{n-1}\sum_{s=2}^{n-2}\frac{A_s}{q^{s+1}} \end{aligned}$$

where we have made

$$D(p, q, r, n) = q^{n-2}B_1 + (pr - q^2)q^{n-3}A_1 \qquad (8)$$

From Equation (6) we have that,

$$\begin{aligned} \frac{A_{s+1}}{q^s} &= A_1 + pq\sum_{k=1}^{n}\frac{H_{k+1}}{q^{k+1}} \\ \sum_{s=1}^{n-2}\frac{A_{s+1}}{q^s} &= A_1(n-2) + pq\sum_{s=1}^{n-2}\sum_{k=1}^{s}\frac{H_{k+1}}{q^{k+1}} \\ q^{n-1}\sum_{s=1}^{n-2}\frac{A_{s+1}}{q^s} &= A_1(n-2)q^{n-1} + pq^n\sum_{s=1}^{n-2}\sum_{k=1}^{s}\frac{H_{k+1}}{q^{k+1}} \end{aligned}$$

and

$$\begin{aligned}
\sum_{s=2}^{n-2} \frac{A_s}{q^{s+1}} &= \frac{A_1(n-3)}{q^2} + \frac{p}{q}\sum_{s=2}^{n-2}\sum_{k=1}^{s-1} \frac{H_{k+1}}{q^{k+1}} \\
q^{n-1}\sum_{s=2}^{n-2} \frac{A_s}{q^{s+1}} &= A_1(n-3)q^{n-3} + pq^{n-2}\sum_{s=2}^{n-2}\sum_{k=1}^{s-1} \frac{H_{k+1}}{q^{k+1}} \\
(pr-q^2)q^{n-1}\sum_{s=2}^{n-2} \frac{A_s}{q^{s+1}} &= A_1(pr-q^2)(n-3)q^{n-3} + p(pr-q^2)q^{n-2}\sum_{s=2}^{n-2}\sum_{k=1}^{s-1} \frac{H_{k+1}}{q^{k+1}}
\end{aligned}$$

Therefore,

$$\begin{aligned}
B_{n-1} &= D + q^{n-1}A_1(n-2) + pq^n \sum_{s=1}^{n-2}\sum_{k=1}^{s} \frac{H_{k+1}}{q^{k+1}} \\
&\quad + A_1(pr-q^2)(n-3)q^{n-3} + p(pr-q^2)q^{n-2}\sum_{s=2}^{n-2}\sum_{k=1}^{s-1} \frac{H_{k+1}}{q^{k+1}}
\end{aligned} \tag{9}$$

Substitution of (8) by using the above equations and also A_{n-1} from (6) into the original recurrence for H_n in the Formula (3). We obtain a recurrence for H_n, as follows:

$$\begin{aligned}
H_{n+1} = pH_n& \\
&+ q^{n-1}A_1 + pq^n \sum_{k=1}^{n-2} \frac{H_{k+1}}{q^{k+1}} \\
&+ D + A_1 q^{n-1}(n-2) \\
&+ pq^n \sum_{s=1}^{n-2}\sum_{k=1}^{s} \frac{H_{k+1}}{q^{k+1}} + A_1(pr-q^2)(n-3)q^{n-3} \\
&+ p(pr-q^2)q^{n-2}\sum_{s=2}^{n-2}\sum_{k=1}^{s-1} \frac{H_{k+1}}{q^{k+1}}.
\end{aligned} \tag{10}$$

Dividing by q^{n+1} and making $y_n = H_n/q^n$ we have

$$\begin{aligned}
\frac{H_{n+1}}{q^{n+1}} = \frac{p}{q}\frac{H_n}{q^n}& \\
&+ \frac{A_1}{q^2} + \frac{p}{q}\sum_{k=1}^{n-2} \frac{H_{k+1}}{q^{k+1}} \\
&+ \frac{D}{q^{n+1}} + \frac{A_1(n-2)}{q^2} \\
&+ \frac{p}{q}\sum_{s=1}^{n-2}\sum_{k=1}^{s} \frac{H_{k+1}}{q^{k+1}} + \frac{A_1(pr-q^2)(n-3)}{q^4} \\
&+ \frac{p(pr-q^2)}{q^3}\sum_{s=2}^{n-2}\sum_{k=1}^{s-1} \frac{H_{k+1}}{q^{k+1}}.
\end{aligned} \tag{11}$$

In oredr to simplify the equation, we will make

$$\begin{aligned}
\frac{D(p,q,r,n)}{q^{n+1}} &= \frac{B_1}{q^3} + \frac{(pr-q^2)A_1}{q^4} \\
x_n &= \frac{A_1}{q^2} + \frac{D}{q^{n+1}} + \frac{A_1(n-2)}{q^2} + \frac{A_1(pr-q^2)(n-3)}{q^4} \\
P &= \frac{p(pr-q^2)}{q^3} \\
Q &= \frac{p}{q}
\end{aligned}$$

Equation (11) reduces to

$$y_{n+1} = Qy_n + Q\sum_{k=1}^{n-2} y_{k+1} + Q\sum_{s=1}^{n-2}\sum_{k=1}^{s} y_{k+1} + P\sum_{s=2}^{n-2}\sum_{k=1}^{s-1} y_{k+1} + x_n. \tag{12}$$

Or,

$$y_{n+1} = Q\sum_{k=1}^{n-1} y_{k+1} + Q\sum_{s=1}^{n-2}\sum_{k=1}^{s} y_{k+1} + P\sum_{s=2}^{n-2}\sum_{k=1}^{s-1} y_{k+1} + x_n. \tag{13}$$

And also,

$$y_{n+1} = Q\sum_{s=1}^{n-1}\sum_{k=1}^{s} y_{k+1} + P\sum_{s=2}^{n-2}\sum_{k=1}^{s-1} y_{k+1} + x_n. \tag{14}$$

Let us calculate the double sum,

$$\begin{aligned}
\sum_{s=1}^{n-1}\sum_{k=1}^{s} y_{k+1} &= y_2, n = 2 \\
&\quad + y_2 + y_3, n = 3 \\
&\quad + y_2 + y_3 + y_4, n = 4 \\
&\quad + y_2 + y_3 + y_4 + y_5, n = 5 \\
&\quad + y_2 + y_3 + y_4 + y_5 + y_6, n = 6 \\
&\vdots \\
&\quad + y_2 + y_3 + y_4 + y_5 + y_6 + \cdots + y_n, n-1 \\
&= (n-1)y_2 + (n-2)y_3 + (n-3)y_4 + \cdots + \\
&\quad 4y_{n-3} + 3y_{n-2} + 2y_{n-1} + y_n, n-1 \\
&= \sum_{j=1}^{n-1}(n-j)y_{j+1}
\end{aligned}$$

Now for the second summation,

$$\sum_{s=2}^{n-2}\sum_{k=1}^{s-1} y_{k+1} \quad = \quad \sum_{j=1}^{n-3}(n-j-2)y_{j+1}$$

Then, we obtain the reduced recurrences,

$$y_{n+1} \quad = \quad Q\sum_{j=1}^{n-1}(n-j)y_{j+1} + P\sum_{j=1}^{n-3}(n-j-2)y_{j+1} + x_n \tag{15}$$

Or after making $s = j+1$

$$y_{n+1} \quad = \quad Q\sum_{s=2}^{n}(n-s+1)y_s + P\sum_{s=2}^{n-2}(n-s-1)y_s + x_n \tag{16}$$

$$\begin{aligned}
c_0y_8 + c_1y_7 + c_2y_6 + c_3y_5 + c_4y_4 + c_5y_3 + c_6y_2 &= x_7, \quad n = 7\\
c_0y_7 + c_1y_6 + c_2y_5 + c_3y_4 + c_4y_3 + c_5y_2 &= x_6, \quad n = 6\\
c_0y_6 + c_1y_5 + c_2y_4 + c_3y_3 + c_4y_2 &= x_5, \quad n = 5\\
c_0y_5 + c_1y_4 + c_2y_3 + c_3y_2 &= x_4, \quad n = 4
\end{aligned}$$

Now, if we make $z_n = x_n - \sum_{s=2}^{4} c_{4-s+1}y_s$, then

$$\begin{pmatrix} c_0 & c_1 & \cdots & c_{n-5}\\ 0 & c_0 & \cdots & c_{n-4}\\ \vdots & & & \vdots\\ 0 & \cdots & 0 & c_0 \end{pmatrix}\begin{pmatrix} y_n\\ y_{n-1}\\ \vdots\\ y_5 \end{pmatrix} = \begin{pmatrix} z_{n-1}\\ z_{n-2}\\ \vdots\\ z_4 \end{pmatrix}$$

In order to solve the above system of equations, we use the following lemma, where the proof can be found elsewhere. For completeness, we are reproducing it on its more general form:

Lemma 1. *Let* $T = \Lambda + T_u$ *be an upper triangular matrix, where* $\Lambda = (\delta_{ij}t_{ij})$ *then* $T^{-1} = \left(I + \Lambda^{-1}T_u\right)^{-1}\Lambda^{-1}$ *and*

$$\left(I + \Lambda^{-1}T_u\right)^{-1} \quad = \quad \sum_{j=0}^{m}\left(-\Lambda^{-1}T_u\right)^{j} \tag{17}$$

Thus from lemma (1), the theorem follows.

Conclusions

We have presented a closed formula for computing the Merrifield-Simmons index of polygonal array graphs at distance 1, and a method to compute the closed formula for a polygonal array at any distance based on its associated recurrence. Although the Merrifield-Simmons index has been previously exhibited for polygonal edge joining, it has not been tackled with its associated closed formula.

Bibliography

[1] W.C. Shiu, Extremal Hosoya index and Merrifield-Simmons index of hexagonal spiders, Discrete Applied Mathematics 156 (2008) 2978–2985.

[2] T. Došli'c, F. Måløy, Chain hexagonal cacti: Matchings and independent sets, Discrete Mathematics, 310 (2010) 1676–1690.

[3] S. Wagner, I. Gutman, Maxima and minima of the Hosoya index and the Merrifield-Simmons index: A survey of results and techniques, Acta Applicandae Mathematicae 112(3) (2010) 323–346.

[4] I. Gutman, Extremal hexagonal chains, J. of Mathematical Chemistry, 12 (1993) 197–210.

[5] L. Zhang, The proof of Gutman's conjectures concerning extremal hexagonal chains, Jour. Systems Sci. Math. Sci., 18(4) (1998) 460–465.

[6] L.-Z. Zhang. On the ordering of a class of hexagonal chains with respect to Merrifield-Simmons index, Systems Sci. Math. Sci., 13(2) (2000) 219–224.

[7] L.-Z. Zhang and F.-J. Zhang. Extremal hexagonal chains concerning k-matchings and k-independent sets, J. Math. Chem., 27(4), (2000) 319–329.

[8] G. De Ita, J.R. Marcial-Romero, P. Bello, M. Contreras, Linear-time algorithms for computing the Merrifield-Simmons index on polygonal trees, MATCH Comm. in Math. Comp. Chem. 69:1 (2018) 55–78.

[9] T. Došli'c, M. S. Litz, Matching and independent sets in polyphenylene chains, MATCH Comm. in Math. Comp. Chem. 67 (2012) 313–330.

email from authors

Hernández-Servín, J.A.: xoseahernandez@uaemex.mx

Marcial-Romero, J.R.: jrmarcialr@uaemex.mx

De Ita Luna, G.: email@example.com