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Counting Matchings in Caterpillar Graphs with an Application to a Class of Benzenoid Chains

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Abstract

Total number of matchings is called Hosoya index in graph theory. Although Hosoya index was introduced in 1971, the relations between the Hosoya index of caterpillar graphs and Euler's continuants were introduced in 2007. In this paper, we show that the Hosoya index of caterpillar graphs can be computed as product of 2×2 matrices. Moreover, we obtain that Hosoya index of the caterpillar graphs $Z(C_n(x,\ldots,x))$ equals to $(n+1)-th$ Fibonacci polynomial and we show that the Hosoya index of the caterpillar graphs $Z(C_n(x+1,\ldots,x+1))$ can be shown in a polynomial form with the coefficients as a Pell triangle of Reference number A038137 in OEIS. Finally, we use these relations in the computation of the Kekulé number of a class $\mathcal{H}_{n,x}$ of benzenoid chains which have n segments of length x.

1 Introduction

Hosoya index of caterpillar graphs can be computed using Euler's continuants. This relationship was presented in a series of articles by Hosoya [7,

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8, 10]. This relation is important in two ways. It is known that benzenoid chains can be represented by caterpillar graphs, and the Kekulé number of benzenoid chains can be computed using the Hosoya index of caterpillars [9].

The Hosoya index (or Z-index) was defined by Hosoya in 1971 [6] and the Hosoya index of a graph G is denoted by $Z(G)$. A matching of the graph G is a subset of $E(G)$ such that no two edges share a common vertex. The number of matchings which have k edges is denoted by $p(G,k)$ and the Hosoya index of a graph G of order n is defined as

$$Z(G) = \sum_{k=0}^{\lfloor n/2 \rfloor} p(G,k).$$

with empty set $p(G,0) = 1$.

The results reported in this paper deal with some open problems of the paper [1]. In the paper [1], the authors obtained the Hosoya index of some classes of unbranched polymers. Hosoya index of unbranched polymers was also studied in [5].

In this paper, we show that the Hosoya index of caterpillar graphs can be computed as product of 2×2 matrices. Moreover, we obtain that Hosoya index of the caterpillar graphs $Z(C_n(x,\ldots,x))$ equals to $(n+1)-th$ Fibonacci polynomial and we show that the Hosoya index of the caterpillar graphs $Z(C_n(x+1,\ldots,x+1))$ can be shown in a polynomial form with the coefficients as a Pell triangle of Reference number A038137 in OEIS. Finally, we use these relations in the computation of the Kekulé number of a class $\mathcal{H}_{n,x}$ of benzenoid chains which have n segments of length x.

The relations between Kekulé number of benzenoid chains and Fibonacci numbers were obtained many years ago as in the papers of the authors Tošić and Stojmenović [15, 16]. Since caterpillar graphs are very related to benzenoid chains, these relations are current for the Hosoya index of caterpillar graphs.

Our starting point is the Pell triangle of the page 9 which is obtained from the Hosoya index of caterpillars. This triangle represents the coefficients of the polynomial $P_n(x)$ and it has no relation with the matchings of graphs in OEIS. We prove that $P_n(x)$ equals to $F_{n+1}\ (x+1)$ which is the $(n+1)-th$ Fibonacci polynomial and use the equation for the computation of the Kekulé number of a class of benzenoid chains.

2 Preliminaries

We give some essential theorems in this section.

Lemma 1. *The Z-counting polynomial of a path P_n is presented by the following equation:*

$$Q(P_n, x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n-k}{k} x^k.$$

Hosoya's Z-counting polynomial and matching polynomial are related but not equal. Matching polynomial is a generalization of Z-counting polynomial. Recall that matching polynomial equals to acyclic polynomial which was studied by Gutman and Hosoya [4].

Lemma 2. *Let H be a graph. Then ([8])*

1. *If $H_1, H_2, \ldots, H_m$ are the components of graph H, then*

$$Z(H) = \prod_{k=1}^{m} Z(H_k).$$

2. *If $e = uv \in E(H)$, then $Z(H) = Z(H - uv) + Z(H - \{u, v\})$.*

   It means that the Hosoya index of a big graph can be calulated by this recurrence relation. The Hosoya index of a graph H equals to production of Hosoya indices of subgraphs after the removing an edge e plus production of Hosoya indices of subgraphs after the removing of all adjacent edges to first removed edge e.

3. *If the paths, cycles and stars of order n are denoted P_n,C_n and S_n respectively, we obtain that $Z(P_n) = F_{n+1}, Z(C_n) = L_n$ and $Z(S_n) = n$.*

Caterpillar graphs are usually used in chemistry and graph theory because they represent benzenoid hydrocarbon molecules. In the chemistry literature, caterpillar trees are also known as Gutman trees. A caterpillar graph G is consisted of an n vertex path $v_1v_2\ldots v_n$ and the leaves $x_1, x_2, \ldots, x_n$ which are attached to the $v_1, v_2, \ldots, v_n$, respectively. G is denoted with $G = C_n(x_1+1, x_2+1, \ldots, x_n+1)$ as in Figure 1.

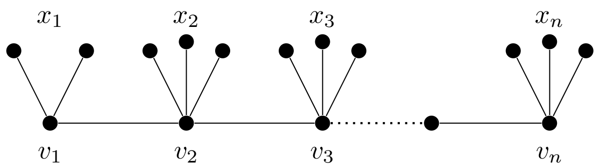

Figure 1. The caterpillar graph G

Caterpillar graphs is important not only for chemical graph theory but also statistical graph theory. Several topological indices of random caterpillars were studied Zhang and Wang [17]. The authors gave an open problem about Hosoya index of random graphs including the caterpillars. We think our results about caterpillar graphs can help to solve of this problem.

3 Matchings in caterpillar

Definition 1. The nth convergent of a continued fraction is given by

$$\frac{p_n}{q_n} = a_1 + \cfrac{b_2}{a_2 + \cfrac{b_3}{a_3 + \cdots + \cfrac{b_n}{a_n}}}.$$

It is known that p_n and q_n can be obtained as the product of n 2×2 matrices by Milne–Thomson [13] as follows:

$$\begin{bmatrix} p_n & p_{n-1} \\ q_n & q_{n-1} \end{bmatrix} = \begin{bmatrix} a_1 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} a_2 & 1 \\ b_2 & 0 \end{bmatrix} \cdots \begin{bmatrix} a_n & 1 \\ b_n & 0 \end{bmatrix}.$$

Definition 2. Assume that x_i $(1 \leq i \leq n)$ are positive integers. The continuant is defined recursively as follows [11]:

$$K_0() = 1,$$

$$K_1(x_1) = x_1,$$

$$K_2(x_1, x_2) = x_1 x_2 + 1,$$

$$K_n(x_1, x_2, \ldots, x_n) = x_n K_{n-1}(x_1, x_2, \ldots, x_{n-1}) + K_{n-2}(x_1, x_2, \ldots, x_{n-2}).$$

Definition 3. If we combine the continued fraction and continuant concepts, we obtain the nth convergent as follows [10]. Assume that a_i $(1 \leq i \leq n)$ are positive integers. Then

$$p_n = K_n(a_1, \ldots, a_n),$$

$$q_n = K_{n-1}(a_2, \ldots, a_n),$$

and therefore

$$\frac{p_n}{q_n} = \frac{K_n(a_1, \ldots, a_n)}{K_{n-1}(a_2, \ldots, a_n)}.$$

Moreover, the following recursive relations and initial conditions hold:

$$p_n = a_n p_{n-1} + p_{n-2}, \qquad (p_1 = a_1,\ p_2 = a_2 a_1 + 1),$$

$$q_n = a_n q_{n-1} + q_{n-2}, \qquad (q_1 = 1,\ q_2 = a_2).$$

Lemma 3. *The Hosoya index of the caterpillar graph $C_n(x_1, x_2, \ldots, x_n)$ is equal to the continuant of $(x_1, x_2, \ldots, x_n)$ [7], that is,*

$$Z\big(C_n(x_1, x_2, \ldots, x_n)\big) = K(x_1, x_2, \ldots, x_n).$$

By Lemma 3 and Definitions 1-3, we obtain the nth convergent of the Hosoya index of caterpillars of two consecutive terms as follows:

$$\frac{p_n}{q_n} = \frac{Z\big(C_n(x_1, x_2, \ldots, x_n)\big)}{Z\big(C_{n-1}(x_2, \ldots, x_n)\big)}.$$

This implies that

$$p_n = Z\big(C_n(x_1, x_2, \ldots, x_n)\big),$$

$$q_n = Z\big(C_{n-1}(x_2, \ldots, x_n)\big),$$

$$p_{n-1} = Z\big(C_{n-1}(x_1, x_2, \ldots, x_{n-1})\big),$$

$$q_{n-1} = Z\big(C_{n-2}(x_2, \ldots, x_{n-1})\big).$$

In the following theorem, the Hosoya index of the caterpillar graph $C_n(x_1, x_2, \ldots, x_n)$ is expressed, following Milne–Thomson [13], as the product of n 2×2 matrices.

Theorem 1. *The Hosoya index of the caterpillar graph $C_n(x_1, x_2, \ldots, x_n)$ can be represented as*

$$\begin{bmatrix} Z\big(C_n(x_1, x_2, \ldots, x_n)\big) & Z\big(C_{n-1}(x_1, x_2, \ldots, x_{n-1})\big) \\ Z\big(C_{n-1}(x_2, \ldots, x_n)\big) & Z\big(C_{n-2}(x_2, \ldots, x_{n-1})\big) \end{bmatrix} = \begin{bmatrix} x_1 & 1 \\ 1 & 0 \end{bmatrix} \cdots \begin{bmatrix} x_n & 1 \\ 1 & 0 \end{bmatrix}.$$

The following theorem was given by Hosoya [10] under the name Cassini's identity *(see Theorem 6, p. 19). We provide an alternative proof of this identity.*

Theorem 2. ***(Cassini's identity).***

$$\begin{aligned} &Z(C_n(x_1, x_2, \ldots, x_n))\, Z(C_{n-2}(x_2, \ldots, x_{n-1})) \\ &-Z(C_{n-1}(x_1, x_2, \ldots, x_{n-1}))\, Z(C_{n-1}(x_2, \ldots, x_n)) = (-1)^n \end{aligned}$$

Proof. If we take the determinant of the matrix given in Theorem 1, we obtain

$$\begin{vmatrix} Z(C_n(x_1, \ldots, x_n)) & Z(C_{n-1}(x_1, \ldots, x_{n-1})) \\ Z(C_{n-1}(x_2, \ldots, x_n)) & Z(C_{n-2}(x_2, \ldots, x_{n-1})) \end{vmatrix} = \begin{vmatrix} x_1 & 1 \\ 1 & 0 \end{vmatrix} \cdots \begin{vmatrix} x_n & 1 \\ 1 & 0 \end{vmatrix}$$
$$= (-1)^n$$

Result 1. Assume that $x_1 = x_2 = \cdots = x_n = x$. Then

$$\begin{bmatrix} Z\big(C_n(x,\ldots,x)\big) & Z\big(C_{n-1}(x,\ldots,x)\big) \\ Z\big(C_{n-1}(x,\ldots,x)\big) & Z\big(C_{n-2}(x,\ldots,x)\big) \end{bmatrix} = \begin{bmatrix} x & 1 \\ 1 & 0 \end{bmatrix}^n .$$

Theorem 3. *The nth convergent*

$$\frac{p_n}{q_n} = \frac{Z\big(C_n(x_1,x_2,\ldots,x_n)\big)}{Z\big(C_{n-1}(x_2,\ldots,x_n)\big)}$$

can be computed in $O(\log n)$ *time using* $O\Big(\frac{n}{\log n}\Big)$ *processors.*

Proof. Since the Hosoya index of caterpillars can be represented as a continued fraction whose nth convergent is

$$\frac{p_n}{q_n} = \frac{Z\big(C_n(x_1,x_2,\ldots,x_n)\big)}{Z\big(C_{n-1}(x_2,\ldots,x_n)\big)},$$

it follows that all convergents $\frac{p_n}{q_n}$ can be computed in $O(\log n)$ time using $O\Big(\frac{n}{\log n}\Big)$ processors by Theorem 2 of Eğecioğlu et al. [2].

Now we use Lemma 2. (2) for the caterpillar graph G of Figure 1.

$$Z(G) = Z(G \setminus \{v_{n-1}v_n\}) + Z\left(H \setminus \{v_{n-1}v_n\} - \{v_{n-2}v_{n-1}, x_{n-1}, x_n\}\right)$$

If the edge $v_{n-1}v_n$ is removed from $G = C_n(x_1+1, x_2+1, \ldots, x_n+1)$, we obtain the caterpillar $C_{n-1}(x_1+1, x_2+1, \ldots, x_{n-1}+1)$ and the star graph S_{x_n+1}. Then the Hosoya index of $Z(G \setminus v_{n-1}v_n)$ equals to

$$Z(G \setminus \{v_{n-1}v_n\}) = Z(S_{x_n+1})Z(C_{n-1}(x_1+1, x_2+1, \ldots, x_{n-1}+1))$$

$$= (x_n+1)Z(C_{n-1}(x_1+1, x_2+1, \ldots, x_{n-1}+1))$$

Moreover, if the adjacent edges of $v_{n-1}v_n$ (the edge $v_{n-2}v_{n-1}$ and the edges which are attached to v_{n-1} and v_n), we obtain the caterpillar graph

$C_{n-2}(x_1+1, x_2+1, \ldots, x_{n-2}+1)$. Therefore, we obtain that

$$
\begin{aligned}
Z(G) &= (x_n+1)\cdot Z(C_{n-1}(x_1+1,\ldots,x_{n-1}+1)) \\
&\quad + Z(C_{n-2}(x_1+1,\ldots,x_{n-2}+1)) \qquad (*)
\end{aligned}
$$

By this equation (*), we can calculate the Hosoya index of caterpillar graphs. We know that $Z(C_0)=1, C_1(x_1+1)$ is a star and the Hosoya index of a star S_{x_1+1} equals to

$$Z(C_1(x_1+1)) = x_1+1.$$

Now we can calculate the Hosoya index of following caterpillars by the equation (*)

$$
\begin{aligned}
Z(C_2(x_1+1,x_2+1)) &= (x_2+1)Z(C_1(x_1+1)) + Z(C_0) \\
&= (x_2+1)(x_1+1)+1 \\
&= x_1x_2+x_1+x_2+2
\end{aligned}
$$

$$
\begin{aligned}
Z(C_3(x_1+1,x_2+1,x_3+1)) &= (x_3+1)Z(C_2(x_1+1,x_2+1)) + Z(C_1(x_1+1)) \\
&= (x_3+1)\big[(x_2+1)(x_1+1)+1\big] + x_1+1 \\
&= x_1x_2x_3+x_1x_2+x_1x_3+x_2x_3 \\
&\quad + 2x_1+x_2+2x_3+3
\end{aligned}
$$

$$
\begin{aligned}
&Z(C_4(x_1+1,x_2+1,x_3+1,x_4+1)) \\
&\quad = (x_4+1)Z(C_3(x_1+1,x_2+1,x_3+1)) + Z(C_2(x_1+1,x_2+1)) \\
&\quad = (x_4+1)\Big[(x_3+1)\left[(x_2+1)(x_1+1)+1\right] + x_1+1\Big] \\
&\qquad + (x_2+1)(x_1+1)+1 \\
&\quad = (x_4+1)(x_1x_2x_3+x_1x_2+x_1x_3+x_2x_3+2x_1+x_2+2x_3+3) \\
&\qquad + x_1x_2+x_1+x_2+2 \\
&\quad = x_1x_2x_3x_4+x_1x_2x_3+x_1x_2x_4+x_1x_3x_4+x_2x_3x_4
\end{aligned}
$$

$$+ 2x_1x_2 + x_1x_3 + 2x_1x_4 + x_2x_3 + x_2x_4 + 2x_3x_4$$
$$+ 3x_1 + 2x_2 + 2x_3 + 3x_4 + 5$$

Assume that $x_1 = x_2 = \cdots = x_n = x$. By this way, we obtain the following polynomials of the caterpillar graphs C_n for $n = 0, 1, \ldots, 5$ below.

$$\begin{aligned}
P_0(x) &= 1\\
P_1(x) &= x + 1\\
P_2(x) &= x^2 + 2x + 2\\
P_3(x) &= x^3 + 3x^2 + 5x + 3\\
P_4(x) &= x^4 + 4x^3 + 9x^2 + 10x + 5\\
P_5(x) &= x^5 + 5x^4 + 14x^3 + 22x^2 + 20x + 8
\end{aligned}$$

It is generalized with

$$P_n(x) = Z(C_n((x+1, \ldots, x+1)) = \sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n-k}{k} (x+1)^{n-2k}$$

If we use the coefficients of this polynomials, we obtain a Pascal like triangle as follows.

$$\begin{array}{c}
1\\
1 \quad 1\\
1 \quad 2 \quad 2\\
1 \quad 3 \quad 5 \quad 3\\
1 \quad 4 \quad 9 \quad 10 \quad 5\\
1 \quad 5 \; 14 \; 22 \; 20 \; 8
\end{array}$$

The $n-th$ row and r-column element of the triangle is denoted by

$$\begin{bmatrix} n \\ r \end{bmatrix}$$

By this way we obtain the following equations for each rows,

1.
$$\begin{bmatrix} n \\ 0 \end{bmatrix} = 1.$$

2.
$$\begin{bmatrix} n \\ 1 \end{bmatrix} = n.$$

3.
$$\begin{bmatrix} n \\ n \end{bmatrix} = F_{n+1}$$

which is the $(n+1)$-th Fibonacci number.

4. For $3 \leq r \leq n-1$,
$$\begin{bmatrix} n \\ r \end{bmatrix} = \begin{bmatrix} n-1 \\ r \end{bmatrix} + \begin{bmatrix} n-1 \\ r-1 \end{bmatrix} + \begin{bmatrix} n-2 \\ r-2 \end{bmatrix}.$$

5. Sums of rows of the triangles equal to the Pell sequence 1, 2, 5, 12, 29, 70...

which is obtained by the relation a+2b with initial conditons a=1 and b=2. It means that we obtain a Pell triangle.This Pell triangle was listed with reference number A038137 in OEIS [14], but the relations with matchings of graphs are not appeared. Detailed information about Pell triangels can be found in the book [12], Section 13.

Theorem 4. *The Hosoya index of the caterpillar graph $C_n(x,\ldots,x)$ is given by the following equation*

$$Z(C_n(x,\ldots,x)) = F_{n+1}(x)$$

which is given by the $(n+1)-th$ Fibonacci polynomial $F_{n+1}(x) = xF_n(x) + F_{n-1}(x)$ with initial conditions $F_2(x) = x$ and $F_1(x) = 1$.

Proof. Since $C_1(x)$ is a star and $Z(C_1(x)) = x$, $Z(C_1(x))$ is identity function. Moreover, the Hosoya index of caterpillar $C_n(x,\ldots,x)$ is computed by the following recurrence relation

$$Z(C_n(x,\ldots,x)) = x(Z(C_{n-1}(x,\ldots,x) + Z(C_{n-2}(x,\ldots,x))$$

with initial conditions $Z(C_1(x)) = x$ and $Z(C_0()) = 1$. It implies that the initial conditions equal to the initial conditions of Fibonacci polynomial as $Z(C_1(x)) = x = F_2(x)$ and $Z(C_0()) = 1 = F_1(x)$.

The first recurrence relation is attained as

$$Z(C_2(x,x)) = xZ(C_1(x) + Z(C_0()) = x^2 + 1 = F_3(x)$$

Finally this goes to the $Z(C_n(x,\ldots,x))$ and we obtain that

$$Z(C_n(x,\ldots,x)) = F_{n+1}(x).$$

We know that $C_n(1,\ldots,1)$ is a path and by the Theorem 4. We obtain for $x = 1$,

$$Z(C_n(1,\ldots,1)) = F_{n+1}(1) = F_{n+1}.$$

As a qonsequence of Theorem 4, we can give the following theorem which shows the Hosoya index of regular caterpillar $C_n(x+1,\ldots,x+1)$ of Pell triangle in the page 9.

Theorem 5. *The polynomial $P_n(x)$ which equals to Hosoya index of*

$$Z(C_n(x+1,\ldots,x+1))$$

is expressed by

$$P_n(x) = F_{n+1}(x+1)$$

as $F_{n+1}(x+1)$ is $(n+1)-th$ Fibonacci polynomial.

4 An application to chemistry

Perfect matching or Kekulé number is widely studied in graph theory and chemistry [9]. Moreover, it is known that a benzenoid chain is represented by a caterpillar by its LA-sequence. The LA-sequence is obtained by the number of linear hexagons in each segment of the benzenoid. Each segment is seperated from the others by the angular hexagons. More information about the benzenoid systems can be found in the paper [9]. Gutman obtained an identity about the characteristic polynomials of trees by using the LA-sequence of the nonbranched catacondensed benzenoid molecules [3]. In this section we are interested in a class of benzenoid chains which have n segments of equal lenghth. As an example, the family $\mathcal{H}_{5,3}$ of all hexagonal chains with five segments of length three is given in Figure 2. We take the family $\mathcal{H}_{n,x}$ of all hexagonal chains with n segments of length x. This is a class of unbranched catacondensed benzenoids.

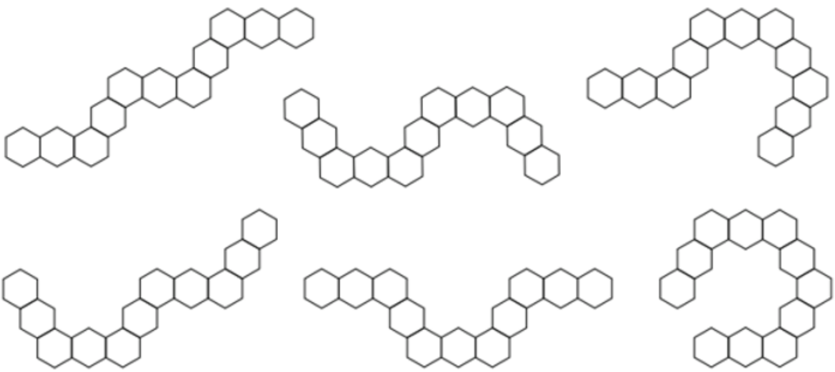

Figure 2. All hexagonal chains $\mathcal{H}_{5,3}$ with five segments of length three

The LA-sequence of the benzenoid chains with n segments of length x is

$$L^{x-1}AL^{x-2}AL^{x-2}A\ldots AL^{x-2}AL^{x-1}$$

and the corresponding caterpillar is

$$C_n(x, x-1, \ldots, x-1, x).$$

Theorem 6. *For a hexagonal chain H whose LA-sequence is $L^{x_1}AL^{x_2}A\ldots AL^{x_{n-1}}AL^{x_n}$, it is known that the Kekulé number of H equals the Hosoya index of the caterpillar $C_n(x_1+1, \ldots, x_{n+1})$ as [9]:*

$$K(H) = Z\big(C_n(x_1+1,\dots,x_{n+1})\big).$$

Theorem 7. *The Kekulé number of the family $\mathcal{H}_{n,x}$ of all hexagonal chains with n segments of length x equals*

$$K(\mathcal{H}_{n,x}) = F_{n+1}(x-1).$$

Proof. The Kekulé number of the family $\mathcal{H}_{n,x}$ (Hosoya index of the corresponding caterpillar) is

$$\begin{aligned} Z\big(C_n(x,x-1,\dots,x-1,x)\big) &= x\,Z\big(C_{n-1}(x,x-1,\dots,x-1)\big)\\ &\quad + Z\big(C_{n-2}(x,x-1,\dots,x-1)\big). \end{aligned}$$

We can compute the first and the second terms on the right-hand side of the equation by Theorem 4:

$$\begin{aligned} Z\big(C_{n-1}(x,x-1,\dots,x-1)\big) &= x\,Z\big(C_{n-2}(x-1,\dots,x-1)\big)\\ &\quad + Z\big(C_{n-3}(x-1,\dots,x-1)\big)\\ &= xF_{n-1}(x-1) + F_{n-2}(x-1)\\ &= F_n(x-1), \end{aligned}$$

$$\begin{aligned} Z\big(C_{n-2}(x,x-1,\dots,x-1)\big) &= x\,Z\big(C_{n-3}(x-1,\dots,x-1)\big)\\ &\quad + Z\big(C_{n-4}(x-1,\dots,x-1)\big)\\ &= xF_{n-2}(x-1) + F_{n-3}(x-1)\\ &= F_{n-1}(x-1). \end{aligned}$$

If we write these terms in the main equation, we obtain that

$$\begin{aligned} Z\big(C_n(x,x-1,\dots,x-1,x)\big) &= x\,Z\big(C_{n-1}(x,x-1,\dots,x-1)\big)\\ &\quad + Z\big(C_{n-2}(x,x-1,\dots,x-1)\big)\\ &= xF_n(x-1) + F_{n-1}(x-1)\\ &= F_{n+1}(x-1). \end{aligned}$$

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