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Branched Continued Fractions Associated with Hosoya Index of the Tree Graph

Takao Komatsu

Department of Mathematical Sciences, School of Science
Zhejiang Sci-Tech University
Hangzhou 310018, China
komatsu@zstu.edu.cn

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Abstract

In this paper, we give graphs whose topological index are exactly equal to the number u_n, satisfying the three term recurrence relation

$$u_n = au_{n-1} + bu_{n-2} \quad (n \ge 2) \quad u_0 = 0 \quad \text{and} \quad u_1 = u\,,$$

where a, b and u are positive integers. We show an interpretation from the continued fraction expansion in a more general case, so that the topological index can be computed easily. On the contrary, for any given positive integer N, we can find the graphs (trees) whose topological indices are exactly equal to N. We also show how to calculate Hosoya index of the given tree graph or the graph including circle type graphs, by using the branched continued fractions.

1 Introduction

The concept of the *topological index* was first introduced by Haruo Hosoya in 1971 [8]. As more different types of topological indices have been discovered in chemical graph theory (e.g., see [5]), the first topological index is also called *Hosoya index* or the Z *index* nowadays. Topological indices are used for example in the development of quantitative structure-activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure. The integer $Z := Z(G)$

is the sum of a set of the numbers $p(G,k)$, which is the number of ways for choosing k disjoin edges from G. By using the set of $p(G,k)$, the topological index Z is defined by

$$Z = \sum_{k=0}^{m} p(G,k)\,.$$

The topological index is closely related to Fibonacci F_n [9] and related numbers [10]. For the path graph S_n, we have $Z(S_n) = F_{n+1}$, where $F_n = F_{n-1} + F_{n-2}$ $(n \geq 2)$ with $F_0 = 0$ and $F_1 = 1$. For the monocyclic graph C_n, we have $Z(C_n) = L_n$, where L_n is the Lucas number, defined by $L_n = L_{n-1} + L_{n-2}$ $(n \geq 2)$ with $L_0 = 2$ and $L_1 = 1$.

In [11], manipulation of continued fraction, either finite and infinite, was shown to be greatly simplified and systematized by introducing the topological index Z and caterpillar graph $C_n(x_1, x_2, \ldots, x_n)$. The continuant which was introduced by Euler in 18 century for solving continued fraction problems was shown to be identical to the Z-index of the caterpillar graph derived from the continued fraction concerned. Then the fastest algorithm for solving the Pell equations was obtained. Further, graph-theoretical interpretation for Fibonacci and Lucas numbers and generalized Fibonacci numbers was obtained. A *caterpillar graph* is a tree containing a path graph such that every edge has one or more endpoints in that path. In [11], it is shown that for $n \geq 1$

$$Z\big(C_n(a_0, a_1, \ldots, a_{n-1})\big) = p_{n-1}\,, \tag{1}$$

where

$$\frac{p_{n-1}}{q_{n-1}} = a_0 + \cfrac{1}{a_1 + \cfrac{1}{\ddots + \cfrac{1}{a_{n-1}}}} \quad \text{with} \quad \gcd(p_{n-1}, q_{n-1}) = 1,\ a_i \geq 1\ (0 \leq i \leq n-1)\,.$$

In [12], the three series of numbers, Fibonacci F_n, Lucas L_n and generalized Fibonacci G_n are defined to have the same recursive relation, $u_n = u_{n-1} + u_{n-2}$. By imposing the following set of initial conditions, $f_0 = f_1 = 1$, $L_1 = 1$ and $L_2 = 3$, and $G_1 = a > 0$ and $G_2 = b > 0$ with $b > 2a$, a number of novel identities were found which systematically relate f_n, L_n, and G_n with each other. Further, graph-theoretical interpretation for these relations was obtained by the aid of the continuant, caterpillar graph, and topological index Z which was proposed and developed by Hosoya. In [13], the conventional algorithm for solving the linear Diophantine equation in two variables is greatly improved graph-theoretically by using the Z-caterpillars, namely, by substituting all the relevant series of integers with the caterpillar graphs whose topological indices represent those integers. By this graph-theoretical analysis, the mathematical structure of the linear Diophantine equation and its relation with Euclid's algorithm, continued fraction, and Euler's continuant is clarified.

The numbers u_n, satisfying the three term recurrence relation $u_n = au_{n-1} + u_{n-2}$, are entailed from the topological index of caterpillar graphs. In particular, Pell numbers P_n, where $a = 2$, are yielded from the comb graph [10], which is the special case of the caterpillar graphs. In addition, the numbers u_n appear in the convergents p_n/q_n of the simple continued fraction expansion. However, it does not seem that the numbers u_n, satisfying the three-term recurrence relation $u_n = u_{n-1} + bu_{n-2}$, have not been recognized as any special graph yet.

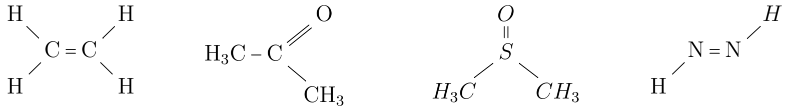
In this paper, we give graphs whose topological index are exactly equal to the number u_n, satisfying the three-term recurrence relation

$$u_n = au_{n-1} + bu_{n-2} \quad (n \geq 2) \quad u_0 = 0 \quad \text{and} \quad u_1 = u\,,$$

where a, b and u are positive integers. We show an interpretation from the continued fraction expansion in a more general case, so that the topological index can be computed easily. On the contrary, for any given positive integer N, we can find the graphs (trees) whose topological indices are exactly equal to N. We also show how to calculate Hosoya index of the given tree graph or the graph including circle type graphs, by using the branched continued fractions.

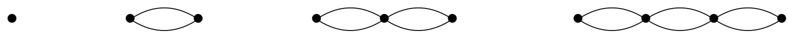
2 Double bonds

We explain double bonds in order to understand the structure of the sequence $\{u_n\}_{n\geq 0}$, satisfying the three term recurrence relation $u_n = u_{n-1} + 2u_{n-2}$. In Chemistry, double bonds are chemical bonds between two chemical elements involving four bonding electrons instead of the usual two, and found in ethylene (carbon-carbon double bond C=C), acetone (carbon-oxygen double bond C=O), dimethyl sulfoxide (sulfur-oxygen double bond S=O), diazene (nitrogen-nitrogen double bond N=N) and so on (see, e.g., [19]).



ethylene　　acetone　　dimethyl sulfoxide　　diazene

Though there does not seem to exist any concrete example, we shall consider the connected graph of double bonds as B_n.



B_0　　B_1　　B_2　　B_3

Then the topological index of B_n coincides with the Jacobsthal number, whose sequence is given by

$$0, 1, 1, 3, 5, 11, 21, 43, 85, 171, 341, 683, 1365, 2731, 5461, 10923, 21845, 43691, 87381, 174763, \ldots$$

([20, A001045]).

Theorem 1. *For* $n \geq 0$

$$Z(B_n) = J_{n+2},$$

where J_n *are the Jacobsthal numbers defined by*

$$J_n = J_{n-1} + 2J_{n-2} \quad (n \geq 2) \quad \textit{with} \quad J_0 = 0 \quad \textit{and} \quad J_1 = 1\,.$$

Theorem 1 is a special case of the main result in the later section. Theorem 1 holds for small n by the following table.

	$k = 0$	$k = 1$	$k = 2$	$Z(B_n)$
$p(B_0, k)$	1			1
$p(B_1, k)$	1	2		3
$p(B_2, k)$	1	4		5
$p(B_3, k)$	1	6	4	11

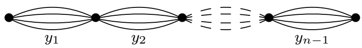
There exist stronger bonds in chemistry. Triple bonds are of order 3. Some chemical compounds with a triple bond are acetylene and cyanogen.

$\mathrm{H - C \equiv C - H}$　　　$\mathrm{N \equiv C - C \equiv N}$

acetylene　　cyanogen

Quadruple bond (e.g., chromium(II) acetate), Quintuple bond and Sextuple bond have been also known as of order 4, 5 and 6, respectively.

In Mathematics, define a *bond graph* denoted by $B_n(y_1, y_2, \ldots, y_{n-1})$, a connected graph with bonds order y_1, y_2, $\ldots$, y_{n-1}, where $y_1, y_2, \ldots, y_{n-1}$ are positive integers.



If $y_1 = y_2 = \cdots = y_{n-1} = 1$, $S_n = B_n(1, 1, \ldots, 1)$ is the path graph. If $y_1 = y_2 = \cdots = y_{n-1} = 2$, $B_n = B_n(2, 2, \ldots, 2)$ yields Jacobsthal numbers in its topological indices above. Similarly, if $y_1 = y_2 = \cdots = y_{n-1} = b$, $B_n(b, b, \ldots, b)$ is related with the number u_n, satisfying the three term recurrence relation $u_n = u_{n-1} + bu_{n-2}$ $(n \geq 3)$ with $u_1 = b$ and $u_2 = b + 1$. In fact, we shall discuss more general cases in the later section.

3 Continued fraction

Any real number α is expressed as the regular (or simple) continued fraction expansion

$$\alpha := [a_0; a_1, a_2, \ldots] = a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \ddots}},$$

where

$$\begin{aligned} \alpha &= a_0 + \theta_0, \quad a_0 = \lfloor \alpha \rfloor, \\ 1/\theta_{n-1} &= a_n + \theta_n, \quad a_n = \lfloor 1/\theta_{n-1} \rfloor \quad (n \geq 1). \end{aligned}$$

The n-th convergent of the continued fraction expansion of α is given by

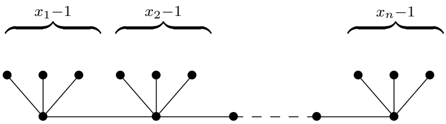
$$\frac{p_n}{q_n} := [a_0; a_1, a_2, \ldots, a_n] = a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \ddots + \cfrac{1}{a_n}}}.$$

It is well-known that p_n and q_n satisfy the recurrence relation:

$$p_n = a_n p_{n-1} + p_{n-2} \quad (n \geq 0), \qquad p_{-1} = 1, \qquad p_{-2} = 0, \tag{2}$$

$$q_n = a_n q_{n-1} + q_{n-2} \quad (n \geq 0), \qquad q_{-1} = 0, \qquad q_{-2} = 1. \tag{3}$$

In Graph theory, a caterpillar graph (or tree), denoted by $C_n(x_1, x_2, \ldots, x_n)$, is a tree in which all the vertices are within distance 1 of a central path.



If $x_1 = \cdots = x_n = 1$, $S_n = C_n(1, \ldots, 1)$ is a path graph.

In [11], it is shown that for $n \geq 1$

$$Z\big(C_n(a_0, a_1, \ldots, a_{n-1}\big) = p_{n-1}\,, \tag{4}$$

where

$$\frac{p_{n-1}}{q_{n-1}} = a_0 + \cfrac{1}{a_1 + \ddots + \cfrac{1}{a_{n-1}}} \quad \text{with} \quad \gcd(p_{n-1}, q_{n-1}) = 1,\ a_i \geq 1\ (0 \leq i \leq n-1)\,.$$

4 Caterpillar-bond graphs and continued fractions

Any real number can be expressed as a generalized continued fraction expansion of the form

$$\alpha = a_0 + \cfrac{b_1}{a_1 + \cfrac{b_2}{a_2 + \ddots}}\,.$$

In this paper, we assume that all numbers $a_0, a_1, a_2, \ldots$ and $b_1, b_2, \ldots$ are positive integers. The n-th convergent p_n/q_n is given by

$$\frac{p_n}{q_n} = a_0 + \cfrac{b_1}{a_1 + \cfrac{b_2}{a_2 + \ddots + \cfrac{b_n}{a_n}}}\,.$$

Here, p_n and q_n satisfy the recurrence relation:

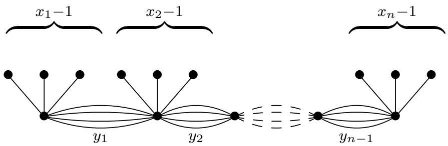
$$p_n = a_n p_{n-1} + b_n p_{n-2} \quad (n \geq 2), \qquad p_0 = a_0, \qquad p_1 = a_0 a_1 + b_1, \tag{5}$$

$$q_n = a_n q_{n-1} + b_n q_{n-2} \quad (n \geq 2), \qquad q_0 = 1, \qquad q_1 = a_1\,. \tag{6}$$

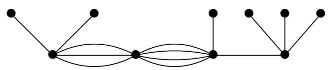
Notice that the expression of the generalized continued fraction expansion is not unique, and p_n and q_n are not necessarily coprime.

Now, we introduce a combined graph of the caterpillar graph and the bond graph as their generalization.

Caterpillar-bond graph $D_n(x_1, x_2, \dots, x_n; y_1, y_2, \dots, y_{n-1})$



Example I. For example, the caterpillar-bond graph $D_4(3,1,2,4;3,4,1)$ is given by the following.



Notice that

$$D_n(2, x_2, \dots, x_n; y_1, \dots, y_{n-1}) = D_{n+1}(1, 1, x_2, \dots, x_n; 1, y_1, \dots, y_{n-1})\,, \tag{7}$$

$$D_n(x_1, \dots, x_{n-1}, 2; y_1, \dots, y_{n-1}) = D_{n+1}(x_1, \dots, x_{n-1}, 1, 1; y_1, \dots, y_{n-1}, 1)\,. \tag{8}$$

Our first main result can be stated as follows.

Theorem 2. *For $n \ge 1$,*

$$Z\big(D_n(a_0, a_1, \dots, a_{n-1}; b_1, \dots, b_{n-1})\big) = p_{n-1}\,,$$

where p_{n-1} is the numerator of the convergent of the continued fraction expansion

$$\frac{p_{n-1}}{q_{n-1}} = a_0 + \cfrac{b_1}{a_1 + \cfrac{b_2}{a_2 + \ddots + \cfrac{b_{n-1}}{a_{n-1}}}} \tag{9}$$

and p_j's and q_j's satisfy the recurrence relations in (5) and (6), respectively.

Remark. Since

$$\ddots + \cfrac{b}{1 + \cfrac{1}{1}} = \ddots + \frac{b}{2}$$

with two continued fraction expansions of p/q and $p/(p-q)$ $(p > q)$, we can recognize the relations (7) and (8), and their topological indices are the same.

Example II. Since

$$3 + \cfrac{3}{1 + \cfrac{4}{2 + \cfrac{1}{4}}} = \frac{102}{25}\,,$$

the topological index is given by $Z\big(D_4(3,1,2,4;3,4,1)\big) = 102$.

In order to prove our main result, we need the known relations, which were first suggested by Hosoya [8,9] and were elaborated by Gutman and Polansky [7]. Though we need only the first one in this paper, we also list related relations for convenience.

Lemma 1. *1. If $e = uv$ is an edge of a graph G, then $Z(G) = Z(G-e) + Z(G-\{u,v\})$.*

2. If v is a vertex of a graph G, then $Z(G) = Z(G-v) + \sum_{uv} Z(G-uv)$, where the summation extends over all vertices adjacent to v.

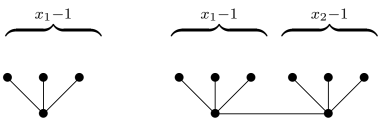
3. If $G_1, G_2, \dots, G_k$ are connected components of G, then $Z(G) = \prod_{i=1}^{k} Z(G_i)$.

Proof of Theorem 2. We can show that for $n \ge 3$

$$\begin{aligned} &Z\big(D_n(x_1,x_2,\dots,x_n;y_1,\dots,y_{n-1})\big) \\ &= x_n Z\big(D_{n-1}(x_1,x_2,\dots,x_{n-1};y_1,\dots,y_{n-2})\big) + y_{n-1} Z\big(D_{n-2}(x_1,x_2,\dots,x_{n-2};y_1,\dots,y_{n-3})\big)\,. \end{aligned} \tag{10}$$

Manually, we can compute

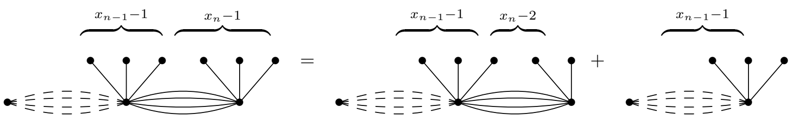
$$Z\big(D_1(x_1)\big) = x_1 \quad \text{and} \quad Z\big(D_2(x_1,x_2,y_1)\big) = x_1x_2 + y_1\,.$$



On the other hand, for this general continued fraction expansion, we know that

$$a_0 = \frac{a_0}{1} = \frac{p_0}{q_0} \quad \text{and} \quad a_0 + \frac{b_1}{a_1} = \frac{a_0a_1 + b_1}{a_1} = \frac{p_1}{q_1}$$

with the recurrence relation (2). By setting $x_k = a_{k-1}$ $(k \ge 1)$ and $y_k = b_k$ $(k \ge 1)$, the structures of $Z\big(D_n(x_1,x_2,\dots,x_n;y_1,\dots,y_{n-1})\big)$ and p_{n-1} are completely the same. Therefore, we obtain $Z\big(D_n(x_1,x_2,\dots,x_n;y_1,\dots,y_{n-1})\big) = p_{n-1}$ $(n \ge 1)$.



$D_n(x_1,\dots,x_n;y_1,\dots,y_{n-1})$ $D_n(x_1,\dots,x_n-1;y_1,\dots,y_{n-1})$ $D_{n-1}(x_1,\dots,x_{n-1};y_1,\dots,y_{n-2})$

Finally, we prove (10). By using the first relation in Lemma 1 repeatedly,

$$
\begin{aligned}
&Z\big(D_n(x_1,x_2,\dots,x_n;y_1,\dots,y_{n-1})\big)\\
&=Z\big(D_{n-1}(x_1,x_2,\dots,x_{n-1};y_1,\dots,y_{n-2})\big)+Z\big(D_n(x_1,x_2,\dots,x_n-1;y_1,\dots,y_{n-1})\big)\\
&=\cdots\\
&=(x_n-1)Z\big(D_{n-1}(x_1,x_2,\dots,x_{n-1};y_1,\dots,y_{n-2})\big)+Z\big(D_n(x_1,x_2,\dots,1;y_1,\dots,y_{n-1})\big)\\
&=(x_n-1)Z\big(D_{n-1}(x_1,x_2,\dots,x_{n-1};y_1,\dots,y_{n-2})\big)\\
&\quad+Z\big(D_{n-2}(x_1,x_2,\dots,x_{n-2};y_1,\dots,y_{n-3})\big)\\
&\quad+Z\big(D_n(x_1,x_2,\dots,x_{n-1},1;y_1,\dots,y_{n-2},y_{n-1}-1)\big)\\
&\cdots\\
&=(x_n-1)Z\big(D_{n-1}(x_1,x_2,\dots,x_{n-1};y_1,\dots,y_{n-2})\big)\\
&\quad+(y_{n-1}-1)Z\big(D_{n-2}(x_1,x_2,\dots,x_{n-2};y_1,\dots,y_{n-3})\big)\\
&\quad+Z\big(D_n(x_1,x_2,\dots,x_{n-1},1;y_1,\dots,y_{n-2},1)\big)\\
&=x_nZ\big(D_{n-1}(x_1,x_2,\dots,x_{n-1};y_1,\dots,y_{n-2})\big)+y_{n-1}Z\big(D_{n-2}(x_1,x_2,\dots,x_{n-2};y_1,\dots,y_{n-3})\big)\,.
\end{aligned}
$$

■

Additional proof. We can recognize the desired result by a tridiagonal determinantal expression.

$$
K_n(x_1,\dots,x_n;y_1,\dots,y_{n-1}):=\begin{vmatrix}
x_1 & y_1 & 0 & & \\
-1 & x_2 & y_2 & \ddots & \\
0 & -1 & \ddots & \ddots & 0\\
 & \ddots & \ddots & x_{n-1} & y_{n-1}\\
 & & 0 & -1 & x_n
\end{vmatrix}
$$

$$
\begin{aligned}
&=x_n\begin{vmatrix}
x_1 & y_1 & 0 & & \\
-1 & x_2 & y_2 & \ddots & \\
0 & -1 & \ddots & \ddots & 0\\
 & \ddots & \ddots & x_{n-2} & y_{n-2}\\
 & & 0 & -1 & x_{n-1}
\end{vmatrix}
-y_{n-1}\begin{vmatrix}
x_1 & y_1 & 0 & & \\
-1 & x_2 & y_2 & \ddots & \\
0 & \ddots & \ddots & \ddots & 0\\
 & & -1 & x_{n-2} & y_{n-2}\\
0 & \cdots & \cdots & 0 & -1
\end{vmatrix}\\
&=x_nK_n(x_1,\dots,x_n;y_1,\dots,y_{n-1})+y_{n-1}K_{n-2}(x_1,\dots,x_{n-2};y_1,\dots,y_{n-3})
\end{aligned}
$$

with

$$
K_1(x_1)=|x_1|=x_1\quad\text{and}\quad K_2(x_1,x_2;y_1)=\begin{vmatrix}x_1 & y_1\\ -1 & x_2\end{vmatrix}=x_1x_2+y_1\,.
$$

■

4.1 Special cases with recurrence relations

If $x_1=\dots=x_n=a$ and $y_1=\dots=y_{n-1}=b$ in Theorem 2, we have the following.

Corollary 1. *Let a and b be positive integers. Then for a positive integer n,*

$$\begin{aligned} Z\big(D_n(\underbrace{a,\ldots,a}_{n};\underbrace{b,\ldots,b}_{n-1})\big) &= u_{n+1} \\ &= au_n + bu_{n-1} \end{aligned}$$

with $u_0 = 0$ and $u_1 = 1$.

If the initial values are also arbitrary, then we have the following.

Corollary 2. *For a positive integer n,*

$$\begin{aligned} Z\big(D_n(v_1,\underbrace{a,\ldots,a}_{n-1};bv_0,\underbrace{b,\ldots,b}_{n-2})\big) &= v_n \\ &= av_{n-1} + bv_{n-2} \quad (n \ge 2)\,. \end{aligned}$$

More specific cases are for Fibonacci F_n, Lucas L_n, Pell P_n, Pell-Lucas Q_n and Jacobsthal numbers J_n, where

$$\begin{aligned} &F_n = F_{n-1} + F_{n-2} \quad (n \ge 2) \quad \text{with} \quad F_0 = 0 \quad \text{and} \quad F_1 = 1\,, \\ &L_n = L_{n-1} + L_{n-2} \quad (n \ge 2) \quad \text{with} \quad L_0 = 2 \quad \text{and} \quad L_1 = 1\,, \\ &P_n = 2P_{n-1} + P_{n-2} \quad (n \ge 2) \quad \text{with} \quad P_0 = 0 \quad \text{and} \quad P_1 = 1\,, \\ &Q_n = 2Q_{n-1} + Q_{n-2} \quad (n \ge 2) \quad \text{with} \quad Q_0 = 2 \quad \text{and} \quad Q_1 = 2\,, \\ &J_n = J_{n-1} + 2J_{n-2} \quad (n \ge 2) \quad \text{with} \quad J_0 = 0 \quad \text{and} \quad J_1 = 1\,. \end{aligned}$$

$$\begin{aligned} Z\big(D_n(\underbrace{1,\ldots,1}_{n};\underbrace{1,\ldots,1}_{n-1})\big) &= F_{n+1}\,, \\ Z\big(D_n(\underbrace{1,\ldots,1}_{n};2,\underbrace{1,\ldots,1}_{n-2})\big) &= L_n\,, \\ Z\big(D_n(\underbrace{2,\ldots,2}_{n};\underbrace{1,\ldots,1}_{n-1})\big) &= P_{n+1}\,, \\ Z\big(D_n(\underbrace{2,\ldots,2}_{n};2,\underbrace{1,\ldots,1}_{n-2})\big) &= Q_{n+1}\,, \\ Z\big(D_n(\underbrace{1,\ldots,1}_{n};\underbrace{2,\ldots,2}_{n-1})\big) &= Z\big(B_{n-1}\big) = J_{n+1}\,. \end{aligned}$$

The first four cases can be seen in [10–12]. The last case is exactly the same as Theorem 1. In [10] more numbers with corresponding graphs are presented, and graphs of L_n and Q_n are different. Another graph of L_n by Hosoya is the monocyclic graph C_n, where $Z(C_n) = L_n$.

$L_2 = 3$ $L_3 = 4$ $L_4 = 7$ $Q_3 = 6$ $Q_4 = 14$ $Q_5 = 34$

4.2 Applications

Using the continued fraction expansion, we can compute the topological index of the graph by Theorem 2.

On the other hand, we can constitute the graph (without any ring) whose topological index is given. For example, we shall find the graphs whose topological index are 17. Then, concerning the continued fractions we get

$$17,\quad \frac{17}{2} = 8 + \frac{1}{2},\quad \frac{17}{3} = 5 + \frac{2}{3},\quad \frac{17}{4} = 4 + \frac{1}{4},\quad \frac{17}{5} = 3 + \frac{2}{5},\quad \frac{17}{6} = 2 + \frac{5}{6},$$

$$\frac{17}{7} = 2 + \frac{3}{7},\quad \frac{17}{8} = 2 + \frac{1}{8},\quad \frac{17}{9} = 1 + \cfrac{1}{1 + \cfrac{1}{8}},\quad \frac{17}{10} = 1 + \cfrac{1}{1 + \cfrac{3}{7}},\quad \frac{17}{11} = 1 + \cfrac{1}{1 + \cfrac{5}{6}},$$

$$\frac{17}{12} = 1 + \cfrac{1}{2 + \cfrac{2}{5}},\quad \frac{17}{13} = 1 + \cfrac{1}{3 + \cfrac{1}{4}},\quad \frac{17}{14} = 1 + \cfrac{1}{4 + \cfrac{2}{3}},\quad \frac{17}{15} = 1 + \cfrac{1}{7 + \cfrac{1}{2}},\quad \frac{17}{16} = 1 + \frac{1}{16}.$$

If we allow (7) and (8), we still have different expressions with the same value. For example,

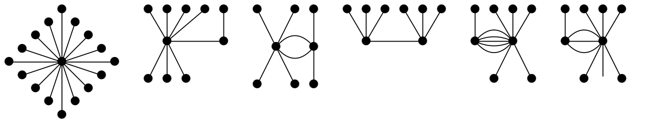
$$\frac{17}{3} = 5 + \frac{2}{3} = 5 + \cfrac{1}{1 + \cfrac{1}{2}} = 5 + \cfrac{1}{1 + \cfrac{1}{1 + \cfrac{1}{1}}}$$

and

$$\frac{17}{14} = 1 + \frac{3}{14} = 1 + \cfrac{1}{4 + \cfrac{2}{3}} = 1 + \cfrac{1}{4 + \cfrac{1}{1 + \cfrac{1}{2}}} = 1 + \cfrac{1}{4 + \cfrac{1}{1 + \cfrac{1}{1 + \cfrac{1}{1}}}}.$$

However, the graph structures of $\frac{17}{3}$ and $\frac{17}{14}$ are essentially the same. It is similar for $\frac{17}{q}$ and $\frac{17}{17-q}$. Therefore, the essentially different graphs whose topological indices are equal to 17 are given as follows.

$$17 \qquad \frac{17}{2} \qquad \frac{17}{3} \qquad \frac{17}{4} \qquad \frac{17}{6} \qquad \frac{17}{7}$$



Notice that other continued fraction expansions are the essentially the same as one of the above 6 graphs. Namely,

$$17 \sim \frac{17}{16}, \quad \frac{17}{2} \sim \frac{17}{8} \sim \frac{17}{9} \sim \frac{17}{15}, \quad \frac{17}{3} \sim \frac{17}{5} \sim \frac{17}{12} \sim \frac{17}{14}, \quad \frac{17}{4} \sim \frac{17}{13},$$
$$\frac{17}{6} \sim \frac{17}{11}, \quad \frac{17}{7} \sim \frac{17}{10}$$

4.3 Examples in chemistry

Ethylene, acetone (or dimethyl sulfoxide) and diazene correspond to the continued fraction expansions

$$3 + \frac{2}{3} = \frac{11}{3}, \quad 3 + \frac{2}{1} = \frac{5}{1} \quad \text{and} \quad 2 + \frac{2}{2} = \frac{6}{2},$$

respectively. These topological indices are given by 11, 5 and 6, respectively. In fact, the structure of diazene can be explained by Pell-Lucas number Q_3.

Acetylene can be written as $D_4(1,1,1,1;1,3,1)$, $D_3(2,1,1;3,1)$ (or $D_3(1,1,2;1,3)$) or $D_2(2,2;3)$. Then the corresponding continued fractions are

$$1 + \cfrac{1}{1 + \cfrac{3}{1 + \cfrac{1}{1}}} = \frac{7}{5}, \quad 2 + \cfrac{3}{1 + \cfrac{1}{1}} = \frac{7}{2} \quad \text{or} \quad 2 + \frac{3}{2} = \frac{7}{2}.$$

In any case its topological index is given by 7.

For cyanogen, by the continued fraction expansion

$$1 + \cfrac{3}{1 + \cfrac{1}{1 + \cfrac{3}{1}}} = \frac{17}{5},$$

its topological index is given by $Z\bigl(D_4(1,1,1,1;3,1,3)\bigr) = 17$.

5 Awful graphs and branched continued fractions

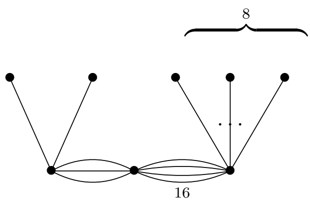
Caterpillar-bond graphs associated with general continued fractions are not only mere extensions of caterpillar graphs with simple continued fractions, but also yield more availabilities. For example, by using several expressions of the same value by general continued fractions

$$3+\cfrac{3}{1+\cfrac{4}{2+\cfrac{1}{4}}}=3+\cfrac{3}{1+\cfrac{16}{9}}=3+\frac{27}{25}=\frac{102}{25}\,,$$

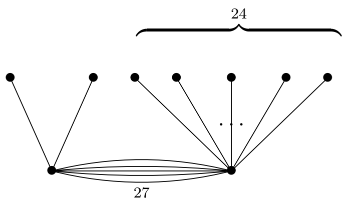
the topological indices are given by

$$Z\bigl(D_4(3,1,2,4;3,4,1)\bigr)=Z\bigl(D_3(3,1,9;3,16)\bigr)=Z\bigl(D_2(3,25;27)\bigr)=102\,.$$

Although the appearance may be bad, the techniques used here are useful for calculating the topological index of more complex graphs.



$D_3(3,1,9;3,16)$



$D_2(3,25;27)$

Namely, the given graph cannot be reduced to any of caterpillar-bond graphs, the method in Theorem 2 cannot be used directly. In [3], it is shown that the largest topological indices of $(n,n+1)$-graphs is $F_{n+1}+F_{n-1}+2F_{n-3}$, where F_n are Fibonacci numbers, defined by $F_n=F_{n-1}+F_{n-2}$ $(n\ge 2)$ with $F_0=0$ and $F_1=1$. In [4], the lower bound for the topological index in $(n,n+1)$-graphs is determined.

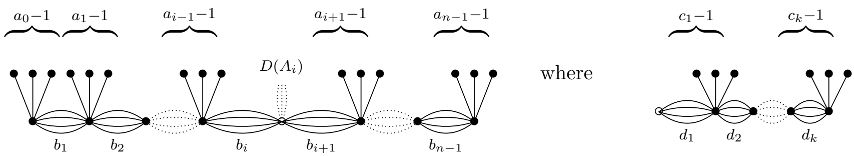
In this section, we show how to calculate Hosoya index of the given tree graph or the graph which includes circle type graphs, by using the continued fraction expansions. In fact, totally, we would calculate the continued fraction including other continued fractions like

$$1+\cfrac{1}{1+\cfrac{2}{2}+\cfrac{2}{1+\cfrac{2}{1+\cfrac{1}{2}}+\cfrac{1}{1}}}$$

(see Subsection 6.1). Such continued fractions are sometimes called *branched continued fractions* (see, e.g., [2, 18]), or *Two-dimensional continued fraction* (see, e.g. [16, 17]) if they are divided into 2 parts. These continued fractions were proposed by Kuchmins'ka in the late of 1970's.

5.1 Combined caterpillar-bond graph

The main and basic result explains how to calculate Hosoya index of the caterpillar-bond graph attached with another caterpillar-bond graph.



$\mathrm{D}_n(a_0, \ldots, a_{i-1}, A_i, a_{i+1}, \ldots, a_{n-1}; b_1, \ldots, b_{n-1})$ $\qquad$ $\mathrm{D}(A_i) := \mathrm{D}_{k+1}(1, c_1, \ldots, c_k; d_1, \ldots, d_k)$

Theorem 3. *For some i, let A_i be a positive rational number which continued fraction is given by*

$$A_i = \frac{P_i}{Q_i} = 1 + \cfrac{d_1}{c_1 + \ddots + \cfrac{d_k}{c_k}}$$

for positive integers c_j and d_j $(j \geq 1)$, according to the similar recurrence relation (5) and (6). Then, for positive integers a_h $(h \neq i)$ and b_h, the Hosoya index of above combined caterpillar-bond graph is equal to

$$\mathrm{Z}\big(\mathrm{D}_n(a_0, \ldots, a_{i-1}, A_i, a_{i+1}, \ldots, a_{n-1}; b_1, \ldots, b_{n-1})\big) = p_{n-1}\,,$$

where a positive integer a_i in (9) is replaced by A_i.

An important remark. Because of the recurrence relations (5) and (6), P_i/Q_i and fractional calculations that appear in the middle do not reduce. For example, we keep the unreduced form as

$$\frac{7}{4} + \frac{5}{8} = \frac{7 \cdot 8 + 5 \cdot 4}{4 \cdot 8} = \frac{76}{32}$$

though it can be reduced to 19/8. In other words, after usual calculation the greatest common divisor is multiplied. That is, as $\gcd(4, 8) = 4$ we calculate as

$$\frac{7}{4} + \frac{5}{8} = \frac{19}{8} = \frac{19 \times 4}{8 \times 4} = \frac{76}{32}\,.$$

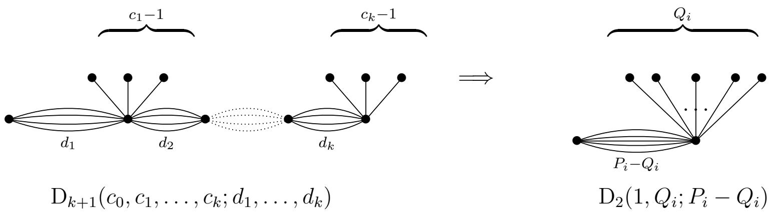
In order to prove Theorem 3, we need the known relations, which were first suggested by Hosoya [8,9] and were elaborated by Gutman and Polansky [7]. Though we need only the first one in this paper, we also list related relations for convenience.

Lemma 2. *1. If $e = uv$ is an edge of a graph G, then $\mathrm{Z}(G) = \mathrm{Z}(G-e)+\mathrm{Z}(G-\{u,v\})$.*

2. If v is a vertex of a graph G, then $\mathrm{Z}(G) = \mathrm{Z}(G-v) + \sum_{uv} \mathrm{Z}(G-uv)$, where the summation extends over all vertices adjacent to v.

3. If $G_1, G_2, \ldots, G_k$ are connected components of G, then $\mathrm{Z}(G) = \prod_{i=1}^{k} \mathrm{Z}(G_i)$.

Proof of Theorem 3. Notice that the caterpillar-bond graph $\mathrm{D}_{k+1}(c_0, c_1, \ldots, c_k; d_1, \ldots, d_k)$ can be transformed into the most reduced caterpillar-bond graph $\mathrm{D}_2(1, Q_i; P_i - Q_i)$ without changing its Hosoya index as P_i.



First, consider the case

$$\mathrm{Z}\big(\mathrm{D}_n(A_0, a_1, \ldots, a_{n-1}; b_1, \ldots, b_{n-1})\big)\,,$$

where

$$A_0 = \frac{P_0}{Q_0} = 1 + \cfrac{d_1}{c_1 + \ddots + \cfrac{d_k}{c_k}}\,.$$

By applying Lemma 2 (1) repeatedly,

$$\begin{aligned}
&\mathrm{Z}\big(\mathrm{D}_n(A_0, a_1, \ldots, a_{n-1}; b_1, \ldots, b_{n-1})\big)\\
&= Q_0 \cdot \mathrm{Z}\big(\mathrm{D}_n(1, a_1, \ldots, a_{n-1}; b_1, \ldots, b_{n-1})\big) + (P_0 - Q_0) \cdot \mathrm{Z}\big(\mathrm{D}_{n-1}(a_1, \ldots, a_{n-1}; b_2, \ldots, b_{n-1})\big)\\
&= Q_0(P' + b_1 Q') + (P_0 - Q_0)P' = P_0 P' + b_1 Q_0 Q'\,,
\end{aligned}$$

where

$$\frac{P'}{Q'} := a_1 + \cfrac{b_2}{a_2 + \ddots + \cfrac{b_{n-1}}{a_{n-1}}}\,,$$

where P' and Q' are positive integers that are not necessarily coprime after applying the similar relation in (5) and (6). On the other hand,

$$A_0 + \cfrac{b_1}{a_1 + \ddots + \cfrac{b_{n-1}}{a_{n-1}}} = \frac{P_0}{Q_0} + \frac{b_1 Q'}{P'} = \frac{P_0 P' + b_1 Q_0 Q'}{Q_0 P'} .$$

Therefore, Hosoya index can be calculated as the numerator from the continued fraction expansion

$$A_0 + \cfrac{b_1}{a_1 + \ddots + \cfrac{b_{n-1}}{a_{n-1}}} ,$$

where

$$A_0 = 1 + \cfrac{d_1}{c_1 + \ddots + \cfrac{d_k}{c_k}} .$$

The simple continued fraction expansion, where $b = 1$ in (9), for a real number can be represented using 2×2 matrices. The use of such matrices to represent continued fractions is apparently due to Hurwitz and appears in Frame [6] and Kolden [15], independently, but popularized by van der Poorten (e.g., see [21, 22]). For the general case, we use the matrices' relation of the continued fraction expansion in (9) as

$$\begin{pmatrix} a_0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a_1 & 1 \\ b_1 & 0 \end{pmatrix} \cdots \begin{pmatrix} a_{n-1} & 1 \\ b_{n-1} & 0 \end{pmatrix} = \begin{pmatrix} p_{n-1} & p_{n-2} \\ q_{n-1} & q_{n-2} \end{pmatrix} .$$

By applying Lemma 2 (1) repeatedly, we have

$$\begin{aligned} & \mathrm{Z}\big(\mathrm{D}_n(a_0, \dots, a_{i-1}, A_i, a_{i+1}, \dots, a_{n-1}; b_1, \dots, b_{n-1})\big) \\ & = \mathrm{Z}\big(\mathrm{D}_n(a_0, \dots, a_{i-1}, P_i - Q_i + 1, a_{i+1}, \dots, a_{n-1}; b_1, \dots, b_{n-1})\big) \\ & \quad + (Q_i - 1) \cdot \mathrm{Z}\big(\mathrm{D}_n(a_0, \dots, a_{i-1}, 1, a_{i+1}, \dots, a_{n-1}; b_1, \dots, b_{n-1})\big) . \end{aligned}$$

Put

$$\frac{P'}{Q'} := a_{i+1} + \cfrac{b_{i+2}}{a_{i+2} + \ddots + \cfrac{b_{n-1}}{a_{n-1}}} ,$$

where P' and Q' are positive integers that are not necessarily coprime after applying the similar relation in (5) and (6). Then by the matrices' calculation, we get for a positive real number α

$$\begin{pmatrix} a_0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a_1 & 1 \\ b_1 & 0 \end{pmatrix}\cdots\begin{pmatrix} a_{i-1} & 1 \\ b_{i-1} & 0 \end{pmatrix}\begin{pmatrix} \alpha & 1 \\ b_i & 0 \end{pmatrix}\begin{pmatrix} a_{i+1} & 1 \\ b_{i+1} & 0 \end{pmatrix}\cdots\begin{pmatrix} a_{n-1} & 1 \\ b_{n-1} & 0 \end{pmatrix}$$
$$= \begin{pmatrix} p_{i-1} & p_{i-2} \\ q_{i-1} & q_{i-2} \end{pmatrix}\begin{pmatrix} \alpha & 1 \\ b_i & 0 \end{pmatrix}\begin{pmatrix} P' & S \\ b_{i+1}Q' & R \end{pmatrix}$$
$$= \begin{pmatrix} (\alpha p_{i-1} + b_i p_{i-2})P' + b_{i+1}p_{i-1}Q' & S' \\ (\alpha q_{i-1} + b_i q_{i-2})P' + b_{i+1}q_{i-1}Q' & R' \end{pmatrix},$$

where S, R, S' and R' are some positive integers. Then

$$\begin{aligned} &= \mathrm{Z}\big(\mathrm{D}_n(a_0,\dots,a_{i-1},P_i-Q_i+1,a_{i+1},\dots,a_{n-1};b_1,\dots,b_{n-1})\big) \\ &\quad + (Q_i-1)\cdot \mathrm{Z}\big(\mathrm{D}_n(a_0,\dots,a_{i-1},1,a_{i+1},\dots,a_{n-1};b_1,\dots,b_{n-1})\big) \\ &= \big((P_i-Q_i+1)p_{i-1}+b_ip_{i-2}\big)P' + b_{i+1}p_{i-1}Q' + (Q_i-1)\big(\alpha p_{i-1}+b_ip_{i-2})P' + b_{i+1}p_{i-1}Q'\big) \\ &= (P_ip_{i-1}+Q_ib_ip_{i-2})P' + Q_ib_{i+1}p_{i-1}Q'\,. \end{aligned}$$

On the other hand,

$$a_0 + \cfrac{b_1}{a_1 + \ddots + a_{i-1} + \cfrac{b_i}{A_i + \cfrac{b_{i+1}}{a_{i+1} + \ddots + \cfrac{b_{n-1}}{a_{n-1}}}}}$$
$$= \frac{(A_ip_{i-1}+b_ip_{i-2})P' + b_{i+1}p_{i-1}Q'}{(A_iq_{i-1}+b_iq_{i-2})P' + b_{i+1}q_{i-1}Q'}$$
$$= \frac{(P_ip_{i-1}+Q_ib_ip_{i-2})P' + Q_ib_{i+1}p_{i-1}Q'}{(P_iq_{i-1}+Q_ib_iq_{i-2})P' + Q_ib_{i+1}q_{i-1}Q'}\,.$$

Hence,

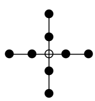
$$\begin{aligned} &\mathrm{Z}\big(\mathrm{D}_n(a_0,\dots,a_{i-1},A_i,a_{i+1},\dots,a_{n-1};b_1,\dots,b_{n-1})\big) \\ &= (P_ip_{i-1}+Q_ib_ip_{i-2})P' + Q_ib_{i+1}p_{i-1}Q'\,. \end{aligned}$$

■

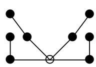
5.2 Examples

Theorem 3 can be extensively more applicable. If the part A_i cannot be written as a caterpillar-bond graph, then it is resolved into more subgraphs further until all the parts are caterpillar-bond graphs.

Suppose that we want to calculate Hosoya index of the following tree graph.



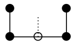
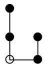
or



Here $\circ$ denotes the disjoint vertex. This graph does not have the corresponding general continued fraction, but a branched continued fraction

$$2+\cfrac{1}{A_1+\cfrac{1}{2}}.$$

This graph can be factorized by separating the part of A_1 as follows.

 and 

A_1 still does not have the corresponding caterpillar graph. The second graph of A_1 part corresponds to the continued fraction

$$A_1 = B_0 + \frac{1}{2}$$

respectively, where

$$B_0 = 1 + \frac{1}{2} = \frac{3}{2}.$$

Since the denominators are not coprime,

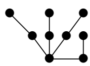
$$A_1 = B_0 + \frac{1}{2} = \frac{4}{2} = \frac{8}{4}$$

and

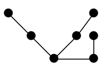
$$2+\cfrac{1}{A_1+\cfrac{1}{2}} = 2+\cfrac{1}{\cfrac{8}{4}+\cfrac{1}{2}} = 2+\cfrac{1}{\cfrac{20}{8}} = \frac{48}{20}.$$

Therefore, Hosoya index of the given graph is 48.

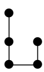
There is not only one way to interpret or factorize the original graph. One of other ways is as follows.



$$A_0 + \frac{1}{2}$$



$$A_0 = \tilde{A}_0 + \frac{1}{2}$$



$$\tilde{A}_0 = B_0 + \frac{1}{2}$$

By noticing the denominators are not coprime,

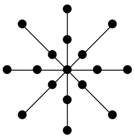
$$\tilde{A}_0 = \frac{3}{2} + \frac{1}{2} = \frac{8}{4}, \quad A_0 = \frac{8}{4} + \frac{1}{2} = \frac{20}{8}$$

and

$$\frac{20}{8} + \frac{1}{2} = \frac{48}{16}.$$

Therefore, Hosoya index of the given graph is 48. The denominator is different because the factorization is different.

Repeating this process, we can get Hosoya index of the following graph as 1280.



Indeed,

$$\frac{48}{16} + \frac{1}{2} = \frac{112}{32}, \quad \frac{112}{32} + \frac{1}{2} = \frac{112}{32}, \quad \frac{112}{32} + \frac{1}{2} = \frac{256}{64}, \quad \frac{256}{64} + \frac{1}{2} = \frac{576}{128}$$

and

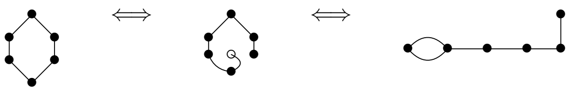
$$\frac{576}{128} + \frac{1}{2} = \frac{1280}{256}.$$

Hence, Hosoya index is equal to 1280.

6 Graphs with cycles

In the case of tree graphs, by resolving the tree, it would be possible to calculate Hosoya index from its corresponding continued fraction expansion. However, if the graph includes a cycle, we cannot calculate Hosoya index by using the continued fractions. Nevertheless, some graphs with cycles can be converted into the caterpillar-bond graphs.

In this section, we show how to calculate Hosoya index if the graph contains one cycle graph C_n, which represents cycloraraffin $\mathrm{C}_n\mathrm{H}_{2n}$. It is known that $\mathrm{Z}(\mathrm{C}_n) = L_n$ ([10]), where L_n are Lucas numbers, defined by $L_n = L_{n-1} + L_{n-2}$ $(n \ge 2)$ with $L_0 = 2$ and $L_1 = 1$.



C_6 cyclohexane $\qquad$ $D_5(1,1,1,1,2;2,1,1,1)$

Theorem 4. *The cycle graph C_n can be transformed into the caterpillar-bond graph*

$$\mathrm{D}_{n-1}(\underbrace{1,\dots,1}_{n-2},2;2,\underbrace{1,\dots,1}_{n-3})\,.$$

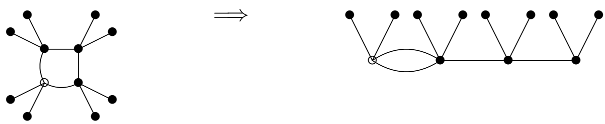
Proof. First, notice that the numbers of edges and vertices are unchanged. Since the corresponding continued fraction expansion is

$$1+\cfrac{2}{1+\cfrac{1}{1+\ddots+1+\cfrac{1}{1+\cfrac{1}{2}}}}=1+\cfrac{2}{\cfrac{F_n}{F_{n-1}}}$$
$$=\frac{F_n+2F_{n-1}}{F_n}=\frac{F_{n+1}+F_{n-1}}{F_n}=\frac{L_n}{F_n}\,,$$

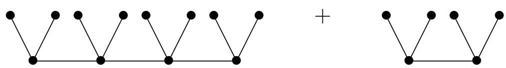
Hosoya index is given by $\mathrm{Z}\big(\mathrm{D}_{n-1}(\underbrace{1,\dots,1}_{n-2},2;2,\underbrace{1,\dots,1}_{n-3})\big)=L_n$. ■

In addition, comb related graphs, including monocycle graphs C_n and cyclic comb graphs CU_n [10], can be converted into the caterpillar-bond graphs.

Indeed, CV_n can be converted into $\mathrm{D}_n(\underbrace{3,\dots,3}_{n};2,\underbrace{1,\dots,1}_{n-2})$ by cutting one edge to another edge into bond edges by turning around.



For, by the first relation in Lemma 2, both graphs can be factorized into the same graphs.



For instance,

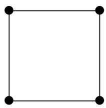
$$\mathrm{Z}(\mathrm{CV}_4)=\mathrm{Z}\big(\mathrm{D}_4(3,3,3,3;2,1,1)\big)=119$$

because

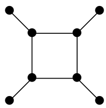
$$3+\cfrac{2}{3+\cfrac{1}{3+\cfrac{1}{3}}}=\frac{119}{33}\,.$$

Similarly,

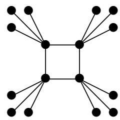
$$\begin{aligned}
\mathrm{Z}(\mathrm{C}_n) &= \mathrm{Z}\big(\mathrm{D}_n(\underbrace{1,\dots,1}_{n};2,\underbrace{1,\dots,1}_{n-2})\big)\,,\\
\mathrm{Z}(\mathrm{CU}_n) &= \mathrm{Z}\big(\mathrm{D}_n(\underbrace{2,\dots,2}_{n};2,\underbrace{1,\dots,1}_{n-2})\big)\,,\\
\mathrm{Z}(\mathrm{CV}_n) &= \mathrm{Z}\big(\mathrm{D}_n(\underbrace{3,\dots,3}_{n};2,\underbrace{1,\dots,1}_{n-2})\big)\,,\\
\mathrm{Z}(\mathrm{CW}_n) &= \mathrm{Z}\big(\mathrm{D}_n(\underbrace{4,\dots,4}_{n};2,\underbrace{1,\dots,1}_{n-2})\big)\,.
\end{aligned}$$



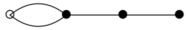
C_4



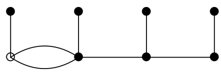
CU_4



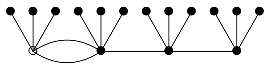
CW_4



$\mathrm{D}_4(1,1,1,1;2,1,1)$



$\mathrm{D}_4(2,2,2,2;2,1,1)$



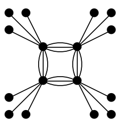
$\mathrm{D}_4(4,4,4,4;2,1,1)$

In general, let $\mathrm{C}_{n,a,b}$ be the graph which each vertex has a additional branches and each edge is b-tupled on the monocycle C_n. When $a=0$ and $b=1$, $\mathrm{C}_n=\mathrm{C}_{n,0,1}$. When $a=1$ and $b=1$, $\mathrm{CU}_n=\mathrm{C}_{n,1,1}$. When $a=2$ and $b=1$, $\mathrm{CV}_n=\mathrm{C}_{n,2,1}$. When $a=3$ and $b=1$, $\mathrm{CW}_n=\mathrm{C}_{n,3,1}$.

Then, $\mathrm{C}_{n,a,b}$ can be transformed into the caterpillar-bond graph

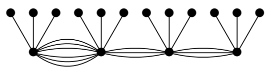
$$\mathrm{D}_n(\underbrace{a+1,\dots,a+1}_{n};2b,\underbrace{b,\dots,b}_{n-2})$$

without changing of the numbers of vertices and edges.



$\mathrm{C}_{4,3,3}$

$\Longrightarrow$



$\mathrm{D}_4(4,4,4,4;6,3,3)$

Theorem 5. *We have*

$$\mathrm{Z}(\mathrm{C}_{n,a,b}) = \mathrm{Z}\big(\mathrm{D}_n(\underbrace{a+1,\dots,a+1}_{n}; 2b, \underbrace{b,\dots,b}_{n-2})\big)\,.$$

Proof. By using Lemma 2 (1) repeatedly,

$$\begin{aligned}
&\mathrm{Z}(\mathrm{C}_{n,a,b})\\
&= \mathrm{Z}(\mathrm{C}_{n,a,b-1}) + \mathrm{Z}\big(\mathrm{D}_{n-2}(\underbrace{a+1,\dots,a+1}_{n-2}; \underbrace{b,\dots,b}_{n-3})\big)\\
&= \cdots\\
&= \mathrm{Z}(\mathrm{C}_{n,a,1}) + (b-1)\mathrm{Z}\big(\mathrm{D}_{n-2}(\underbrace{a+1,\dots,a+1}_{n-2}; \underbrace{b,\dots,b}_{n-3})\big)\\
&= \mathrm{Z}(\mathrm{D}_n(\underbrace{a+1,\dots,a+1}_{n}; \underbrace{b,\dots,b}_{n-1})\big) + b\cdot\mathrm{Z}\big(\mathrm{D}_{n-2}(\underbrace{a+1,\dots,a+1}_{n-2}; \underbrace{b,\dots,b}_{n-3})\big)\\
&= \mathrm{Z}(\mathrm{D}_n(a,\underbrace{a+1,\dots,a+1}_{n-1}; \underbrace{b,\dots,b}_{n-1})\big) + \mathrm{Z}\big(\mathrm{D}_{n-1}(\underbrace{a+1,\dots,a+1}_{n-1}; \underbrace{b,\dots,b}_{n-2})\big)\\
&\quad + b\cdot\mathrm{Z}\big(\mathrm{D}_{n-2}(\underbrace{a+1,\dots,a+1}_{n-2}; \underbrace{b,\dots,b}_{n-3})\big)\\
&= \cdots\\
&= \mathrm{Z}(\mathrm{D}_n(1,\underbrace{a+1,\dots,a+1}_{n-1}; \underbrace{b,\dots,b}_{n-1})\big) + a\cdot\mathrm{Z}\big(\mathrm{D}_{n-1}(\underbrace{a+1,\dots,a+1}_{n-1}; \underbrace{b,\dots,b}_{n-2})\big)\\
&\quad + b\cdot\mathrm{Z}\big(\mathrm{D}_{n-2}(\underbrace{a+1,\dots,a+1}_{n-2}; \underbrace{b,\dots,b}_{n-3})\big)\\
&= \mathrm{Z}(\mathrm{D}_n(1,a,\underbrace{a+1,\dots,a+1}_{n-1}; b-1,\underbrace{b,\dots,b}_{n-2})\big) + a\cdot\mathrm{Z}\big(\mathrm{D}_{n-1}(\underbrace{a+1,\dots,a+1}_{n-1}; \underbrace{b,\dots,b}_{n-2})\big)\\
&\quad + (b+1)\cdot\mathrm{Z}\big(\mathrm{D}_{n-2}(\underbrace{a+1,\dots,a+1}_{n-2}; \underbrace{b,\dots,b}_{n-3})\big)\\
&= \cdots\\
&= \mathrm{Z}(\mathrm{D}_n(1,a,\underbrace{a+1,\dots,a+1}_{n-1}; 1,\underbrace{b,\dots,b}_{n-2})\big) + a\cdot\mathrm{Z}\big(\mathrm{D}_{n-1}(\underbrace{a+1,\dots,a+1}_{n-1}; \underbrace{b,\dots,b}_{n-2})\big)\\
&\quad + (2b-1)\cdot\mathrm{Z}\big(\mathrm{D}_{n-2}(\underbrace{a+1,\dots,a+1}_{n-2}; \underbrace{b,\dots,b}_{n-3})\big)\\
&= (a+1)\cdot\mathrm{Z}\big(\mathrm{D}_{n-1}(\underbrace{a+1,\dots,a+1}_{n-1}; \underbrace{b,\dots,b}_{n-2})\big) + 2b\cdot\cdot\mathrm{Z}\big(\mathrm{D}_{n-2}(\underbrace{a+1,\dots,a+1}_{n-2}; \underbrace{b,\dots,b}_{n-3})\big)\,.
\end{aligned}$$

On the other hand,

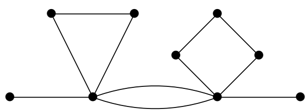
$$\mathrm{Z}\big(\mathrm{D}_n(\underbrace{a+1,\dots,a+1}_{n}; 2b, \underbrace{b,\dots,b}_{n-2})\big)$$

$$
\begin{aligned}
&= \mathrm{Z}\big(\mathrm{D}_n(a, \underbrace{a+1,\ldots,a+1}_{n-1}; 2b, \underbrace{b,\ldots,b}_{n-2})\big) + \mathrm{Z}\big(\mathrm{D}_{n-1}(\underbrace{a+1,\ldots,a+1}_{n-1}; \underbrace{b,\ldots,b}_{n-2})\big) \\
&= \cdots \\
&= \mathrm{Z}\big(\mathrm{D}_n(1, \underbrace{a+1,\ldots,a+1}_{n-1}; 2b, \underbrace{b,\ldots,b}_{n-2})\big) + a\cdot\mathrm{Z}\big(\mathrm{D}_{n-1}(\underbrace{a+1,\ldots,a+1}_{n-1}; \underbrace{b,\ldots,b}_{n-2})\big) \\
&= \mathrm{Z}\big(\mathrm{D}_n(1, \underbrace{a+1,\ldots,a+1}_{n-1}; 2b-1, \underbrace{b,\ldots,b}_{n-2})\big) + a\cdot\mathrm{Z}\big(\mathrm{D}_{n-1}(\underbrace{a+1,\ldots,a+1}_{n-1}; \underbrace{b,\ldots,b}_{n-2})\big) \\
&\quad + \mathrm{Z}\big(\mathrm{D}_{n-2}(\underbrace{a+1,\ldots,a+1}_{n-2}; \underbrace{b,\ldots,b}_{n-3})\big) \\
&= \cdots \\
&= \mathrm{Z}\big(\mathrm{D}_n(1, \underbrace{a+1,\ldots,a+1}_{n-1}; 1, \underbrace{b,\ldots,b}_{n-2})\big) + a\cdot\mathrm{Z}\big(\mathrm{D}_{n-1}(\underbrace{a+1,\ldots,a+1}_{n-1}; \underbrace{b,\ldots,b}_{n-2})\big) \\
&\quad + (2b-1)\mathrm{Z}\big(\mathrm{D}_{n-2}(\underbrace{a+1,\ldots,a+1}_{n-2}; \underbrace{b,\ldots,b}_{n-3})\big) \\
&= (a+1)\cdot\mathrm{Z}\big(\mathrm{D}_{n-1}(\underbrace{a+1,\ldots,a+1}_{n-1}; \underbrace{b,\ldots,b}_{n-2})\big) + 2b\cdot\cdot\mathrm{Z}\big(\mathrm{D}_{n-2}(\underbrace{a+1,\ldots,a+1}_{n-2}; \underbrace{b,\ldots,b}_{n-3})\big)\,.
\end{aligned}
$$

■

6.1 One more example

Consider the following graph with one double bond and two cycles.



This can be written as the graph $\mathrm{D}_4(1, \mathrm{C}_3, \mathrm{C}_4, 1; 1, 2, 1) := G$, which continued fraction expansion is

$$1 + \cfrac{1}{c_3 + \cfrac{2}{c_4 + \cfrac{1}{1}}}\,.$$

Now, C_3 and C_4 can be transformed into the caterpillar-bond graphs $\mathrm{D}_2(1, 2; 2)$ and $\mathrm{D}_3(1, 1, 2; 2, 1)$, respectively. Their continued fractions are

$$1 + \frac{2}{2} = \frac{4}{2} := c_3 \quad \text{and} \quad 1 + \cfrac{2}{1 + \cfrac{1}{2}} = \frac{7}{3} := c_4\,,$$

respectively. Hence, the original continued fraction can be calculated as

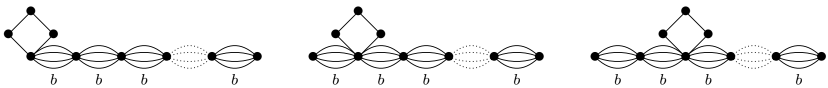
$$1+\cfrac{1}{c_3+\cfrac{2}{c_4+\cfrac{1}{1}}}=1+\cfrac{1}{\frac{4}{2}+\cfrac{2}{\frac{7}{3}+\frac{1}{1}}}$$
$$=\frac{72}{56}\,.$$

Therefore, Hosoya index of the given graph is 72. Indeed,

$$\begin{aligned}\mathrm{Z}(G)&=p(G,0)+p(G,1)+p(G,2)+p(G,3)+p(G,4)\\&=1+11+31+25+4=72\,.\end{aligned}$$

7 Continued fractions with one additional branch

In [3, 4], some transformations are used by changing the connected position or resolving the original graph. In this section, we show the exact situation of the gap change of Hosoya index by changing the position on the path or bond graph.



$\mathrm{D}_n(\alpha,1,\dots,1;b,\dots,b)$ $\mathrm{D}_n(1,\alpha,1,\dots,1;b,\dots,b)$ $\mathrm{D}_n(1,1,\alpha,1,\dots,1;b,\dots,b)$

Note that $\alpha\ge 1$ (in this example, $\alpha=7/3$).

For simplicity, put $D_{n,k}(b):=\mathrm{Z}\big(\mathrm{D}_n(\underbrace{1,\dots,1}_{k-1},\alpha,\underbrace{1,\dots,1}_{n-k};\underbrace{b,\dots,b}_{n-1})\big)$. Then, we have the complete arrangement of sizes of Hosoya indices.

Let $\{r_n\}$ and $\{s_n\}$ be sequences, satisfying the recurrence relations

$$r_n=r_{n-1}+br_{n-2}\quad(n\ge 0)\quad\text{with}\quad r_{-1}=0,\quad r_{-2}=\frac{1}{b}$$

and

$$s_n=s_{n-1}+bs_{n-2}\quad(n\ge 2)\quad\text{with}\quad s_0=2\quad\text{and}\quad s_1=1\,,$$

respectively. In addition, r_n can be written as

$$r_n=\sum_{j=0}^{\lfloor n/2\rfloor}\binom{n-j}{j}b^j\,.$$

Notice that $r_n=F_{n+1}$ and $s_n=L_n$ if $b=1$.

Now, we have some different expressions of Hosoya index.

Theorem 6. *If α is a positive integer, then*

$$\begin{aligned} D_{n,k}(b) &= \alpha r_{k-1}r_{n-k} + b(r_{k-1}r_{n-k-1} + r_{k-2}r_{n-k}) \quad (k \ge 1) && (11)\\ &= \frac{\alpha s_{n+1} + 2bs_n + (-1)^{k-1}b^k(\alpha-1)s_{n-2k+1}}{4b+1} \quad (k \ge 1) && (12)\\ &= \alpha(r_{n-1} - br_{n-3} + b^2 r_{n-5} - \cdots + (-1)^{k-1}b^{k-1}r_{n-2k+1})\\ &\quad + br_{n-2} + br_{n-3} - b^2 r_{n-5} + \cdots + (-1)^k b^{k-1} r_{n-2k+1} \quad (k \ge 2)\,. && (13) \end{aligned}$$

If $\alpha = p/q$ is a rational number, where p and q are positive integers which are not necessarily coprime, then

$$\begin{aligned} D_{n,k}(b) &= pr_{k-1}r_{n-k} + bq(r_{k-1}r_{n-k-1} + r_{k-2}r_{n-k}) \quad (k \ge 1) && (14)\\ &= \frac{ps_{n+1} + 2qbs_n + (-1)^{k-1}b^k(p-q)s_{n-2k+1}}{4b+1} \quad (k \ge 1) && (15)\\ &= p(r_{n-1} - br_{n-3} + b^2 r_{n-5} - \cdots + (-1)^{k-1}b^{k-1}r_{n-2k+1})\\ &\quad + q\big(br_{n-2} + br_{n-3} - b^2 r_{n-5} + \cdots + (-1)^k b^{k-1} r_{n-2k+1}\big) \quad (k \ge 2)\,. && (16) \end{aligned}$$

In particular, when $b = 1$, we have the following Fibonacci-Lucas identities.

Corollary 3. *If α is a positive integer, then*

$$\begin{aligned} D_{n,k}(1) &= \alpha F_k F_{n-k+1} + F_k F_{n-k} + F_{k-1}F_{n-k+1}\\ &= \frac{\alpha L_{n+1} + 2L_n + (-1)^{k-1}(a-1)L_{n-2k+1}}{5}\\ &= \alpha\big(F_n - F_{n-2} + F_{n-4} - \cdots + (-1)^{k-1}F_{n-2k+2}\big)\\ &\quad + \big(F_{n-1} + F_{n-2} - F_{n-4} + \cdots + (-1)^k F_{n-2k+2}\big)\,. \end{aligned}$$

If $\alpha = p/q$ is a positive rational number, then

$$\begin{aligned} D_{n,k}(1) &= pF_k F_{n-k+1} + q(F_k F_{n-k} + F_{k-1}F_{n-k+1})\\ &= \frac{pL_{n+1} + 2qL_n + (-1)^{k-1}(p-q)L_{n-2k+1}}{5}\\ &= p\big(F_n - F_{n-2} + F_{n-4} - \cdots + (-1)^{k-1}F_{n-2k+2}\big)\\ &\quad + q\big(F_{n-1} + F_{n-2} - F_{n-4} + \cdots + (-1)^k F_{n-2k+2}\big)\,. \end{aligned}$$

Remark. When $\alpha = 1$ in Corollary 3, as is well-known,

$$[\underbrace{1;1,\dots,1}_{n}] = \frac{F_{n+1}}{F_n}\,.$$

Then, $D_{n,k}(1) = F_{n+1} = (L_{n+1} + 2L_n)/5$.

Proof of Theorem 6. First, by the matrices' relation of the continued fraction, we have

$$\underbrace{\begin{pmatrix}1&1\\1&0\end{pmatrix}\begin{pmatrix}1&1\\b&0\end{pmatrix}\cdots\begin{pmatrix}1&1\\b&0\end{pmatrix}}_{k-1}\begin{pmatrix}\alpha&1\\b&0\end{pmatrix}\underbrace{\begin{pmatrix}1&1\\b&0\end{pmatrix}\cdots\begin{pmatrix}1&1\\b&0\end{pmatrix}}_{n-k}$$
$$=\begin{pmatrix}1&1\\1&0\end{pmatrix}\begin{pmatrix}r_{k-2}&r_{k-3}\\br_{k-3}&br_{k-4}\end{pmatrix}\begin{pmatrix}\alpha&1\\b&0\end{pmatrix}\begin{pmatrix}r_{n-k}&r_{n-k-1}\\br_{n-k-1}&br_{n-k-2}\end{pmatrix}$$
$$=\begin{pmatrix}r_{k-1}&r_{k-2}\\r_{k-2}&r_{k-3}\end{pmatrix}\begin{pmatrix}\alpha r_{n-k}+br_{n-k-1}&\alpha r_{n-k-1}+br_{n-k-2}\\br_{n-k}&br_{n-k-1}\end{pmatrix}$$
$$=\begin{pmatrix}\alpha r_{k-1}r_{n-k}+b(r_{k-1}r_{n-k-1}+r_{k-2}r_{n-k})&*\\\alpha r_{k-2}r_{n-k}+b(r_{k-2}r_{n-k-1}+r_{k-3}r_{n-k})&**\end{pmatrix}.$$

Hence, we obtain that

$$1+\cfrac{b}{1+\ddots+\cfrac{b}{1+\cfrac{b}{\alpha+\cfrac{b}{1+\ddots+\cfrac{b}{1}}}}}=\frac{\alpha r_{k-1}r_{n-k}+b(r_{k-1}r_{n-k-1}+r_{k-2}r_{n-k})}{\alpha r_{k-2}r_{n-k}+b(r_{k-2}r_{n-k-1}+r_{k-3}r_{n-k})}.$$

Thus, we get (11) and (14).

Second, since

$$r_n=\frac{\theta^{n+1}-\phi^{n+1}}{\theta-\phi}\quad(n\ge 0)$$

with

$$\theta=\frac{1+\sqrt{4b+1}}{2}\quad\text{and}\quad\phi=\frac{1-\sqrt{4b+1}}{2},$$

satisfying $\theta+\phi=1$, $\theta\phi=-b$ and $\theta-\phi=\sqrt{4b+1}$, we have for $1\le k\le\lceil n/2\rceil$,

$$r_{k-1}r_{n-k}=\frac{s_{n+1}+(-1)^{k-1}b^k s_{n-2k+1}}{4b+1},$$
$$r_{k-1}r_{n-k-1}+r_{k-2}r_{n-k}=\frac{2s_n+(-1)^k b^{k-1}s_{n-2k+1}}{4b+1},$$

where $s_n=\theta^n+\phi^n$ $(n\ge 0)$. Thus, we get (12) and (15).

Third, we use the first identity (11). If k increases as $k+1$, Hosoya index becomes

$$\frac{\alpha s_{n+1}+2s_n+(-1)^k b^{k+1}(\alpha-1)s_{n-2k-1}}{4b+1}.$$

Hence, the gap between them is given by

$$\frac{(-1)^{k-1}b^k(\alpha-1)(s_{n-2k+1}+bs_{n-2k-1})}{4b+1}$$
$$=(-1)^{k-1}b^k(\alpha-1)r_{n-2k-1}.$$

Thus, we get (13) and (16). This means that Hosoya index increases (or decreases) by r_{n-2k-1} if the position of an additional branch is changed to the next vertex. ∎

By Theorem 6 (11), we have the complete arrangement of Hosoya indices of $D_{n,k}(b)$ $(k=1,2,\dots,n)$. It is clear that $D_{n,k}(b)=D_{n,n-k}(b)$. So, it is good enough to show the cases for $1\le k\le\lceil n/2\rceil$.

Corollary 4. *If $n=2m$ is even, then*

$$D_{2m,1}(b)\ge D_{2m,3}(b)\ge\cdots\ge D_{2m,2\lceil m/2\rceil-1}(b)\ge D_{2m,2\lfloor m/2\rfloor}(b)\ge\cdots\ge D_{2m,4}(b)\ge D_{2m,2}(b)\,.$$

If $n=2m-1$ is even, then

$$\begin{aligned}D_{2m-1,1}(b)\ge D_{2m-1,3}(b)\ge\cdots\ge D_{2m-1,2\lceil m/2\rceil-1}(b)&\\ \ge D_{2m-1,2\lfloor m/2\rfloor}(b)\ge\cdots\ge D_{2m-1,4}(b)\ge D_{2m-1,2}(b)\,.&\end{aligned}$$

The equation signs hold if and only if $\alpha=1$.

Proof. By Theorem 6 (11), for $\ell\ge 1$

$$\begin{aligned}D_{n,2\ell-1}(b)-D_{n,2\ell+1}(b)&=(\alpha-1)(b^{2\ell-1}r_{n-4\ell+1}-b^{2\ell}r_{n-4\ell-1})\\&=(\alpha-1)b^{2\ell-1}r_{n-4\ell}\ge 0\end{aligned}$$

and

$$\begin{aligned}D_{n,2\ell}(b)-D_{n,2\ell+2}(b)&=-(\alpha-1)(b^{2\ell}r_{n-4\ell-1}-b^{2\ell+1}r_{n-4\ell-3})\\&=-(\alpha-1)b^{2\ell}r_{n-4\ell-2}\le 0\,.\end{aligned}$$

In addition, from Theorem 6 (12), $(-1)^{k-1}b^k(\alpha-1)s_{n-2k+1}\ge 0$ if k is odd; $(-1)^{k-1}b^k(\alpha-1)s_{n-2k+1}\le 0$ if k is even. Hence, $D_{n,2\kappa-1}\ge D_{n,2\lambda}$. If α is not an integer, that is, any subgraph is attached with the path graph with one point, the situation is similar. ∎

For example, let $\alpha=a$ be a positive integer. Since

$$\begin{aligned}&[a;1,1,1,1,1,1]=\frac{13a+8}{13}, \quad [1,a,1,1,1,1,1]=\frac{8a+13}{8a+5},\\&[1,1,a,1,1,1,1]=\frac{10a+11}{5a+8}, \quad [1,1,1,a,1,1,1]=\frac{9a+12}{6a+7},\\&[1,1,1,1,a,1,1]=\frac{10a+11}{6a+7}, \quad [1,1,1,1,1,a,1]=\frac{8a+13}{5a+8},\\&[1,1,1,1,1,1,a]=\frac{13a+8}{8a+5}\,,\end{aligned}$$

we have

$$D_{7,1}(1) = 13a + 8, \quad D_{7,2}(1) = 8a + 13, \quad D_{7,3}(1) = 10a + 11, \quad D_{7,4}(1) = 9a + 12,$$
$$D_{7,5}(1) = 10a + 11, \quad D_{7,6}(1) = 8a + 13, \quad D_{7,7}(1) = 13a + 8\,.$$

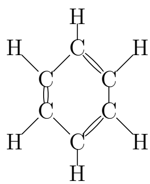
Thus, for $a \geq 1$,

$$13a + 8 \geq 10a + 11 \geq 9a + 12 \geq 8a + 13\,.$$

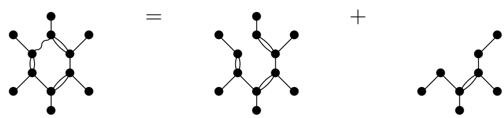
The equation sign holds only for $a = 1$.

8 Final remarks

For the moment, there is no way to transform a circle type graph without uniform pattern into a caterpillar-bond graph directly. In other words, there is no method to calculate Hosoya index of a circle type graph without uniform pattern directly by using continued fractions. For example, consider the very famous benzene C_6H_6.



Though we cannot calculate this Hosoya index directly by using continued fractions, we can calculate it as the sum of Hosoya indices of two caterpillar-bond graphs by Lemma 2 (1). For example,



Therefore,

$$\begin{aligned} \mathrm{Z}(\mathrm{C_6H_6}) &= \mathrm{Z}\big(\mathrm{D}_6(2,2,2,2,2,2;2,1,2,1,2)\big) + \mathrm{Z}\big(\mathrm{D}_4(2,2,2,2;1,2,1)\big) \\ &= 268 + 33 = 301 \end{aligned}$$

because

$$2+\cfrac{2}{2+\cfrac{1}{2+\cfrac{2}{2+\cfrac{1}{2+\cfrac{2}{2}}}}}=\frac{268}{24}\quad\text{and}\quad 2+\cfrac{1}{2+\cfrac{2}{2+\cfrac{1}{2}}}=\frac{33}{14}\,.$$

Indeed,

$$\begin{aligned}
Z(C_6H_6) &= p(C_6H_6,0)+p(C_6H_6,1)+p(C_6H_6,2)+p(C_6H_6,3)\\
&\quad +p(C_6H_6,4)+p(C_6H_6,5)+p(C_6H_6,6)\\
&= 1+15+72+125+72+15+1=301\,.
\end{aligned}$$

Any complicated graph can be done similarly by resolving it into the sum of caterpillar graphs.

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