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Higher-order Fibonacci numbers ☆

Milan Randić [a], Daniel A. Morales [b] and Oswaldo Araujo [c]

[a] *Department of Mathematics and Computer Science, Drake University, Des Moines, Iowa 50311, USA*
[b] *Departamento de Quimica and* [c] *Departamento de Matematica, Facultad de Ciencias, Universidad de Los Andes, Merida 5101, Venezuela*

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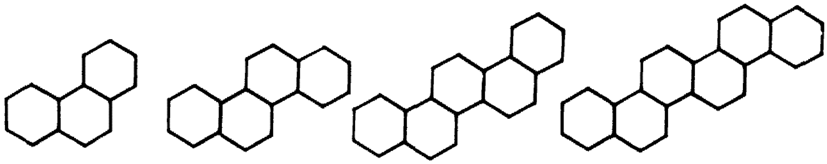
I admired many times the mystical system
of Pythagoras and the magic of the numbers
Thomas Browne
(1605–1682)

We consider a generalization of Fibonacci numbers that was motivated by the relationship of the Hosoya Z topological index to the Fibonacci numbers. In the case of the linear chain structures the new higher order Fibonacci numbers ${}^hF_n$ are directly related to the higher order Hosoya-type Z numbers. We investigate the limits F_n/F_{n-1} and the corresponding equations, the roots of which allow one to write a general expression for ${}^hF_n$. We also report on the ${}^hF$ counting polynomials that give the partition of the ${}^hF$ numbers in contributions arising from k pairs of disjoint paths of length h. It is interesting to see that the partitions of ${}^hF$ are "hidden" in the Pascal triangle in a similar way to the partitions of the Fibonacci numbers that were discovered some time ago by Hoggatt. We end with illustrations of the recursion formulas for the higher order Hosoya numbers for several families of graphs that are based on the corresponding recursions for the higher Fibonacci numbers.

1. Introduction

Fibonacci numbers are ubiquitous, emerging unexpectedly in different problems and in diverse disciplines. In chemistry one finds Fibonacci numbers when counting the Kekule structures in zig-zag fused linear chains of benzenoids:

☆ Dedicated to Professor Haruo Hosoya of Ochanomizu University, Tokyo, Japan, on the occasion of 25 years of the topological index Z.



$K = 5$ $K = 8$ $K = 13$ $K = 21$

Phenathrene Chrysene Picene Fulminene ....

The algorithm for the count of Kekule valence structures of Gordon and Davison [1] is reduced in the case of zig-zag linearly fused benzene rings to the construction of the Fibonacci numbers. Hence, it is not surprising that it was suggested to refer to the zig-zag fused linear benzenes as Fibonaccenes [2]. Balaban and Tomescu [3–5] have in particular studied the relations between the Fibonacci sequence and the numbers of Kekule structures for non-branched cata-condensed polycyclic aromatic hydrocarbons. As a result of their studies these authors have even introduced a particular generalization of Fibonacci numbers, to be mentioned later, which follows from consideration of the number of Kekule valence structures in linearly fused k-benzene rings in a zig-zag fashion.

Fibonacci numbers also occur in connection with the Hosoya Z-topological index [6]. The Z-index of a graph G is based on the count k mutually disjoint edges in a graph. We have been interested in extending the approach of Hosoya and wished to arrive at additional topological indices that are structurally related to the Z index. In doing this we came at the same time across the generalized Fibonacci numbers that we here report on.

The earliest generalization of the Fibonacci numbers, F_n have been reported already over thirty years ago. Horadam considered a generalization in which the recurrence relation of the Fibonacci sequence is preserved but the first two terms are altered [7]. Feinberg extended the summation property $F_n = F_{n-1} + F_{n-2}$ of the Fibonacci sequence to $F_n = F_{n-1} + F_{n-2} + F_{n-3}$ [8]. The new numbers were named "tribonacci" numbers, because now addition of three successive members in the sequence give the next member. More recently several other generalizations of the Fibonacci sequences were reported in the literature [9]. We consider yet another generalization that, as we mentioned, resulted from a consideration of graph-theoretical invariants of interest in chemistry. We should mention, however, that this is not the first generalization of the Fibonacci numbers even in chemical application of graph theory. Balaban and Tomescu [4] selected zig-zag fused benzenoids with longer linear segments and selected the number of the Kekule structures for the fragments ending at a "kink" as generalized Fibonacci numbers. In the case of zig-zag fused anthracene units, the smallest such generalized case, they obtained

$$4, 10, 24, 58, 140, 338, \ldots .$$

This sequence satisfies the recursion: $K_n = 2K_{n-1} + K_{n-2}$. This differs from the recursion for the Fibonacci numbers only in the factor of two, and hence can be viewed as a generalization of the Fibonacci sequence.

Our approach represents a different generalization of the same sequence. We like to think that our generalization produces sequences that are even closer in properties, including recursion relations, to the original Fibonacci sequence. Our generalization, because the properties of the derived higher order Fibonacci numbers are in many ways very closely related to the well-known properties of the Fibonacci numbers [10,11], appears very natural. As we will show the derived generalized Fibonacci numbers have a direct relationship to the recently introduced higher order Hosoya ^kZ indices [12,13]. For a graph G Hosoya defined the Z number, referred to as the topological index of a molecule, in the following way [6]:

$$Z = 1 + p(G,1) + p(G,2) + p(G,3) + p(G,4) + \ldots = \sum_k p(G,k) . \tag{1}$$

Here $p(G,k)$ represents the number of different ways of selecting k nonadjacent edges in the graph. The summation extends over all possible numbers of such edges. By definition $p(G,0) = 1$ and necessarily $p(G,1)$ is equal to the number of edges in the graph. The so derived Z index was subsequently used by Hosoya and coworkers to correlate the boiling points of alkanes (saturated hydrocarbons of the general formula C_nH_{2n+2}) and other physicochemical properties of alkenes with their structure [14].

Hosoya found that for a linear chain the Z indices are the Fibonacci numbers [6]. The relationship is as follows: $Z = F_{n+1}$. Since we generalize the Hosoya number Z, we use the label ^1Z to represent the Hosoya Z index and ^hZ to represent the higher order Z numbers. We wish to design a set of descriptors (^1Z, ^2Z, ^3Z, ^4Z, ^5Z, ..., ^hZ) that are structurally related and that will lead, hopefully, to a satisfactory representation of molecules. As is known many topological indices are combined in an *ad hoc* manner. Many indices, including the Hosoya index Z, also show a high degree of degeneracy. i.e., different structures show the same numerical value for the index. Use of an ordered set of indices, instead of a single index, will lead to a better discrimination among structures while at the same time such indices could be used as molecular descriptors in multivariable regression analyses analogous to the use of the connectivity index $^1\chi$ [15] and the higher connectivity indices $^m\chi$ [16] in the structure-property studies [17].

2. Generalization of the Hosoya Z index

In Table 1 we list for chains of increasing length the initial members of the generalized Hosoya ^hZ numbers that we can also refer to as the "higher order Hosoya numbers". Let us first define the second order Hosoya index ^2Z:

Table 1
The Fibonacci numbers and the higher order Fibonacci numbers.

	^1F	^2F	^3F	^4F
0	1	1	1	1
1	1	1	1	1
2	2	2	2	2
3	3	3	3	3
4	5	4	4	4
5	8	6	5	5
6	13	9	7	6
7	21	13	10	8
8	34	19	14	11
9	55	28	19	15
10	89	41	26	20
11	144	60	36	26
12	233	88	50	34
13	377	129	69	45
14	610	189	95	60

DEFINITION

$$1 + p_2(G,1) + p_2(G,2) + p_2(G,3) + p_2(G,4) + \ldots = \sum p_2(G,k)\,. \tag{2}$$

Here $p_2(G,k)$ represents the number of different ways of selecting k non-adjacent paths of length two in the graph. The summation extends over all possible combinations of disjoint paths of length two. By definition $p_2(G,0) = 1$ and necessarily $p_2(G,1)$ is equal to the number of paths of length two in the graph.

If one compares the definition for ^2Z with the definition for ^1Z given earlier, we note that the only change is the replacement of "edge" (which is a path of length one) by "path of length two". Hence, indeed this is a very natural way of extending the definition of the Hosoya index ^1Z to the higher order index ^2Z. Since the Hosoya index for a linear chain of length n gives the Fibonacci numbers F_{n+1} it is also natural to call the ^2Z numbers for linear chains the Fibonacci numbers of the order two, ^2F_n.

In the same spirit we can generalize the definition (2) and define the Hosoya indices of still higher orders. When the procedure is applied to a chain of length n, we obtain the generalized Fibonacci numbers of higher order:

$$^hZ = \sum p_h(G,k)\,. \tag{3}$$

Here the $p_h(G,k)$ are defined analogously to p_2 but in terms of disjoint paths of length h, with $p_h(G,0)$ by definition being 1 and $p_h(G,1)$ representing the number of paths of length h in the graph. The subscript h and superscript h have been selected to honor *Haruo Hosoya* and at the same time remind us that we deal with *higher* order generalization of the Fibonacci numbers. Formally, our procedure leads to a family of higher order Fibonacci numbers. However, just because the Hosoya index ${}^1Z$ for the linear chains of length n gives the Fibonacci numbers F_{n+1}, this need not be a sufficient, or sufficiently strong, argument to the claim that the numbers ${}^2Z$ for the linear chains of length n have properties that allow us to consider them righteously as the generalized Fibonacci numbers ${}^hF_n$. Similarly, we need yet to fully justify that the numbers ${}^hZ$ for the linear chains of length n should be considered to be generalized Fibonacci numbers ${}^hF_n$. We have to demonstrate that the new numbers exhibit properties similar to those of the Fibonacci numbers F_n.

3. ${}^2F_n$ Fibonacci numbers

Let us consider more closely the sequence

$$1, 1, 2, 3, 4, 6, 9, 13, 19, 28, 41, 60, 88, 129, 189, \dots .$$

Immediately we see that by adding three consecutive members in the series we obtain not the text member in the sequence as is the case with the Fibonacci sequences, but the second next member of the sequence

$$1 + 1 + 2 = 4\,,$$

$$1 + 2 + 3 = 6\,,$$

$$2 + 3 + 4 = 9\,, \quad \text{etc.}$$

Hence we can write the recursion

$${}^2F_n = {}^2F_{n-2} + {}^2F_{n-3} + {}^2F_{n-4}\,. \tag{4}$$

Here we see a similarity to the "tribonacci" sequence of ref. [8]. The additivity property (4) justifies the use of the label "generalized tribonacci sequence" for the sequence ${}^2F_n$. Of course, more than one generalization of a single sequence is possible, but we believe our approach to be the most natural generalization.

In order to derive the generating function and the general formula for ${}^2F_n$ we will use another, even simpler, recursion expression derived from considering only two members of the sequence at a time:

$$1 + 2 = 3\,,$$

$$1 + 3 = 4\,,$$

$$2 + 4 = 6\,,$$

$$3 + 6 = 9\,, \quad \text{etc.}$$

Hence, we can write the recursion

$$^{2}F_n = {}^{2}F_{n-1} + {}^{2}F_{n-3}\,. \tag{5}$$

The apparent similarity with the original Fibonacci sequence is now even more apparent: The next member in the sequence is obtained by adding two previous members, but separated by one place in the sequence. Hence we can refer to the $^{2}F_n$ sequence colloquially as the "jump one" sequence, i.e., to obtain the next member in the sequence we add two preceding members but separated by one place in the sequence. Then the original Fibonacci sequence could be formally referred to as the "jump zero" sequence.

The two recursion equations (4) and (5) can be related using a shift operator that transforms the kth entry of a series of functions or recurrence equations into the corresponding $(k+1)$th entry as outlined by Hosoya and Ohkami [18]. This can be easily seen be replacing F_{n-k} by x^{4-k} that gives for (4) and (5), respectively, $x^4 - x^2 - x - 1 = 0$ and $x^3 - x^2 - 1 - 0$. It is easy to see that

$$(x+1)(x^3 - x^2 - 1) = x^4 - x^2 - x - 1\,,$$

hence the latter, the "tribonacci" recursion, can be simplified using the shift operator, here represented by the factor $(x+1)$.

To obtain the limit for the ratio $^{2}F_n/{}^{2}F_{n-1}$ as n goes to infinity we follow the procedure used to find the limit for F_n/F_{n-1} for the Fibonacci numbers. We then have

$$\begin{aligned} x &= \lim\{^{2}F_n/{}^{2}F_{n-1}\} = \lim\{(^{2}F_{n-1} + {}^{2}F_{n-3})/{}^{2}F_{n-1}\} \\ &= 1 + \lim\{^{2}F_{n-3}/{}^{2}F_{n-1}\} = 1 + \lim\{^{2}F_{n-3}\,{}^{2}F_{n-2}/{}^{2}F_{n-2}\,{}^{2}F_{n-1}\} \\ &= 1 + 1/x^2 \end{aligned} \tag{6}$$

or

$$x^3 - x^2 - 1 = 0\,. \tag{7}$$

We will refer to this as "the limiting equation". One can find that the root of eq. (7) can be expressed as

$$1.46557123\ldots = (1/3)\{2^{1/3}/3(29 + \sqrt{837})^{1/3} + (29 + \sqrt{837})^{1/3}/2^{1/3}\}\,.$$

From eq. (7) we can derive the generating function for the Fibonacci numbers $^{2}F_n$ simply by replacing x with $1/x$ as illustrated below:

$$(1/x)^3 - (1/x)^2 - 1 = 0 \quad \text{or} \quad 1 - x - x^3 = 0\,.$$

From here the generating function for $^{2}F_n$ (starting with $^{2}F_1$) is

$$f(x) = 1/(1 - x - x^3) = 1 + x + x^2 + 2x^3 + 4x^4 + 6x^5 + 13x^6 + 19x^7 + \ldots\,. \tag{8}$$

The above can be compared with the generating function for the Fibonacci numbers:

$$f(x) = 1/(1 - x - x^2) = 1 + x + 2x^2 + 3x^3 + 5x^4 + 8x^5 + 13x^6 + 21x^7 + \dots \tag{9}$$

Again we see great similarity with the Fibonacci sequence and the second order Fibonacci sequence: The generating function for ${}^2F_n$ can be obtained from the generating function for F_n by replacing the quadratic term in the generating function of F_n with the cubic term.

In order to write the general formula for ${}^2F_n$ analogous to the Cauchy–Binet formula [8]: $F_n = [\phi_1^{n+1} - \phi_2^{n+1}]/\sqrt{5}$ for the Fibonacci numbers where $\phi_1 = (1+\sqrt{5})/2$ and $\phi_2 = (1-\sqrt{5})/2$ are the roots of the limiting equation $x^2 - x - 1 = 0$, we have to find all the roots of the limiting equation $x^3 - x - 1 = 0$. The general formula for ${}^2F_n$ is

$$\begin{aligned} {}^2F_n = {} & [\phi_1^{n+2}/(\phi_1 - \phi_2)(\phi_1 - \phi_3) + \phi_2^{n+2}/(\phi_2 - \phi_1)(\phi_2 - \phi_3) \\ & + \phi_3^{n+2}/(\phi_3 - \phi_1)(\phi_3 - \phi_2)] . \end{aligned} \tag{10}$$

with

$$\begin{aligned} \phi_1 &= 1.46557123 , \\ \phi_2 &= -0.2327856 + 0.79255199\mathrm{i} , \\ \phi_3 &= -0.2327856 - 0.79255199\mathrm{i} , \end{aligned} \tag{11}$$

obtained using the Cardano formula for the solution of a cubic.

4. The higher Fibonacci numbers

It is easy to verify from Table 1 that the analogy between F_n and ${}^2F_n$ extends to higher Fibonacci numbers. Thus the members of ${}^3F_n$ can be obtained by adding four consecutive members in the sequence:

$$1 + 1 + 2 + 3 = 7 ,$$

$$1 + 2 + 3 + 4 = 10 ,$$

$$2 + 3 + 4 + 5 = 14 ,$$

$$3 + 4 + 5 + 7 = 19 ,$$

and, generally,

$${}^3F_n = {}^3F_{n-3} + {}^3F_{n-4} + {}^3F_{n-5} + {}^3F_{n-6} . \tag{12}$$

Observe that the derived element ^3F_n is two places away from the last summand $^3F_{n-3}$. The alternative simpler recursion follows from addition of only two preceding members in the sequence, but separated by two places:

$$1+3=4\,,$$

$$1+4=5\,,$$

$$2+5=7\,,$$

$$3+7=10\,,\quad \text{etc.}$$

The recursion

$$^3F_n = {}^3F_{n-1} + {}^3F_{n-4} \tag{13}$$

illustrates the case of the "jump two", i.e., between $^3F_{n-1}$ and $^3F_{n-4}$ there are two members of the sequence. These recursive properties generalize to other higher Fibonacci numbers for which we can write the recursion

$$^hF_n = {}^hF_{n-1} + {}^hF_{n-h-1}\,, \tag{14}$$

which illustrates the "jump $h-1$" case.

Also all the other expressions derived for ^2F_n sequence can be extended to higher order Fibonacci numbers. Thus the limiting equations for F_n and ^2F_n generalize as follows:

$$\begin{aligned}
{}^1F_n &: \; x^2 - x - 1 = 0\,,\\
{}^2F_n &: \; x^3 - x^2 - 1 = 0\,,\\
{}^3F_n &: \; x^4 - x^3 - 1 = 0\,,\\
{}^4F_n &: \; x^5 - x^4 - 1 = 0\,,\\
\ldots & \quad \ldots\\
{}^hF_n &: \; x^{h+1} - x^h - 1 = 0\,.
\end{aligned} \tag{15}$$

Here we use ^1F_n for F_n to emphasize the similarity of the all limiting equations. Derivation of these equations follows the outlined calculation of the limit for $^2F_n/^2F_{n-1}$ by converting the term $^2F_{n-3}/^2F_{n-1}$ to $^2F^2_{n-3}F_{n-2}/^2F_{n-2}\,^2F_{n-1}$. In the case of $^3F_n/^3F_{n-1}$ we obtain the ratio $^3F_{n-4}/^3F_{n-1}$ that is converted to $^3F_{n-4}\,^3F_{n-3}\,^3F_{n-2}/^3F_{n-3}\,^3F_{n-2}\,^3F_{n-1}$, leading to the quartic equation shown. Eqs. (15) have a simple geometrical interpretation that again points to ^kF_n as a natural extension of the Fibonacci sequence. The geometrical interpretation of the Fibonacci numbers can be depicted as the golden ratio relationship of a to b:

$$a/b = (a+b)/a$$

By substituting $a/b = x$ we immediately obtain $1 + 1/x = x$ from which follows $x^2 - x - 1 = 0$. For the ${}^2F_n$ Fibonacci numbers we have a different but similar geometrical relationship:

$$a/b = (a^2 + b^2)/a^2 .$$

Again by substituting $a/b = x$ one immediately obtains $1 + 1/x^2 = x$, from which it follows: $x^3 - x^2 - 1 = 0$. The other higher Fibonacci numbers ${}^kF_n$ lead to the generalization

$$a/b = (a^h + b^h)/a^h .$$

The substitution $a/b = x$ now gives $1 + 1/x^h = x$, from which follows: $x^{h+1} - x^h - 1 = 0$.

The generalized functions for the higher Fibonacci numbers are

$$\begin{aligned}
{}^1f(x) &= 1/(1 - x - x^2) , \\
{}^2f(x) &= 1/(1 - x - x^3) , \\
{}^3f(x) &= 1/(1 - x - x^4) , \\
\ldots & \quad \ldots \\
{}^kf(x) &= 1/(1 - x - x^{k+1}) .
\end{aligned} \tag{16}$$

If we label all the roots (real and complex) of the limiting equations as ϕ_i we can write the general expression for the nth element of the kth generalized Fibonacci sequence, ${}^kF_n$, as

$${}^2F_n = \sum\{\phi_i/\Pi'\phi_i - \phi_j)\} , \quad n = 0, 1, 2, 3, \ldots , \tag{17}$$

where the prime on the product indicates the $j = i$ term is deleted. This is the generalized expression for the higher order Fibonacci sequences analogous to the generalized expressions given by Spickerman [19] for the tribonacci sequence.

5. ${}^hZ$ counting polynomial

The $p(G, k)$ contributions can be viewed as a natural partitioning of the Fibonacci numbers. For a few initial F_n we obtain

$$F_2 = 1 + 1 ,$$

$$F_3 = 1 + 2 ,$$

$$F_4 = 1 + 3 + 1 ,$$

$$F_5 = 1 + 4 + 3 ,$$

$$F_6 = 1 + 5 + 6 + 1\,,$$

$$F_7 = 1 + 6 + 10 + 4\,.$$

These numbers can be recognized as the binomial coefficients. Hoggatt [20] pointed out that Fibonacci numbers are "hidden" in the Pascal triangle. They can be obtained by adding the elements in the Pascal triangle using a slanted line as illustrated in Table 2 (the upper part), which has been also mentioned in ref. [21]. We found that the partitions of the generalized Hosoya numbers for linear chains

Table 2
The Pascal triangle and the Fibonacci numbers. Top: The "hidden" Fibonacci numbers as discovered by Hoggatt. Bottom: The "hidden" second order Fibonacci numbers introduced in this paper.

1
1 1
1 2 1
1 3 3 1
1 4 6 4 1
1 5 10 10 5 1
1 6 15 20 15 6 1
1 7 21 35 35 21 7 1
1 8 28 56 70 56 28 8 1

1
1 1
1 2 1
1 3 3 1
1 4 6 4 1
1 5 10 10 5 1
1 6 15 20 15 6 1
1 7 21 35 35 21 7 1
1 8 28 56 70 56 28 8 1

that we view as the higher order Fibonacci numbers are also "hidden" in the Pascal triangle. For ${}^2F$ we obtain the following partitions (that follows from definition (1)):

$${}^2F_3 = 1 + 1\,,$$

$${}^2F_4 = 1 + 2\,,$$

$${}^2F_5 = 1 + 3\,,$$

$${}^2F_6 = 1 + 4 + 1\,,$$

$${}^2F_7 = 1 + 5 + 3\,,$$

$${}^2F_8 = 1 + 6 + 6\,,$$

$${}^2F_9 = 1 + 7 + 10 + 1\,,$$

$${}^2F_{10} = 1 + 8 + 15 + 4\,,$$

$$\ldots \quad \ldots$$

and so on. The entries in each "column" of the above list are the same as the leading entries of the Pascal triangle. These entries of the Pascal triangle are, however, displaced and have to be combined by drawing slanted lines as shown in the lower part of Table 2. As we see from the upper Pascal triangle in Table 2 the Fibonacci numbers are obtained using the lines with the slope given by joining the first entry in a line with the second entry in the line above. From the lower Pascal triangle of Table 2 we see that the ${}^2F_n$ Fibonacci numbers are obtained from the lines parallel to the line joining the first entry in a line with the second entry two lines above. Similarly the higher order Fibonacci numbers ${}^hF_n$ can be obtained by drawing parallel lines joining the first entries with the second entry in the hth line above. This geometric relationship of the partitions of F and the partitions of ${}^2F_n$ with the binomial coefficients of the Pascal triangle offer strong support that the here introduced ${}^hF_n$ numbers represent the natural generalization of the famed Fibonacci sequence.

There is yet another unique property of the Fibonacci numbers that is also reflected in the here introduced higher order Fibonacci numbers. The reciprocal of the roots $1/\phi$ of the limiting equation for Fibonacci numbers, because they satisfy the equation $x - 1/x = 1$, can be simply obtained as the difference: $1/\phi = \phi - 1$. For the roots associated with the kth order Fibonacci numbers we have a similar expression: $1/\phi = \phi^k - 1$, since now ϕ satisfies the equation $x - 1/x^k = 1$. The numbers ϕ are the only real numbers, which when decreased by one give their own reciprocal to the power k.

6. Application of the higher order Fibonacci recursion expressions

The higher order Fibonacci numbers appear as generalized ${}^hZ$ indices for linear chains. The linear chains represent but very special structures and one may think that the generalized Fibonacci numbers will hardly have other applications. Time will show, but even at this moment we will show a use of the recursions for the higher order Fibonacci numbers in deriving the higher order Hosoya ${}^hZ$ indices for families of branched alkanes.

In Table 3 are listed ${}^hZ$ numbers for several families of alkanes. In all cases we see a simple regularity for the higher order Hosoya numbers for the successive members of each family. The ${}^1Z$ number for $(n+1)$th member of each family is simply obtained by adding the ${}^1Z$ numbers of nth and $(n-1)$th member. The ${}^2Z$ number for $(n+1)$th member of each family is simply obtained by adding the ${}^2Z$ numbers of nth and $(n-2)$th members. The ${}^3Z$ number for $(n+1)$th member of a family is similarly simply obtained by adding the ${}^3Z$ numbers of nth and $(n-3)$th members, and so on.

7. A slightly more general format

In a slightly more general format one can naturally consider generating functions

$$P_h(G,x) = \sum p_n(G,k)x^k .$$

Here $p_n(G,k)$ is the number of ways of disjointedly embedding k copies of the h-site path on the graph G, and x is a variable. Thence $P_h(G,x) = {}^hZ$, but also $P_h(G,x)$ is essentially the partition function for h-unit oligomers on G. Here h-site path represents the h-mer, x is chemical activity for the oligomers, and G might usually be viewed to be regular lattice graphs [22,23].

In a chemical graph-theoretic context, exactly the same sequence of invariants has very recently (since the submission of our manuscript) been suggested by Hermann and Zinn [12]. They, however, use the notation Z_h with the convention that Z_2 is the Hosoya index Z, or our ${}^1Z$, while their Z_1, the smallest index of this type counting nonadjacent atoms, would be in our notation ${}^0Z$. We think that it is better to refer to the original Hosoya index Z as ${}^1Z$ than as Z_2 so we continue to use our notation.

For the case that G is a length-n regular polymer graph, rather than the simple linear chain considered in this paper, linear recursion occurs for many invariants including $P_h(G,x)$ and ${}^hZ$. The results of such linear recursions can be viewed as generalized Fibonacci numbers in some sense. That is, the sequence of ${}^hZ$ satisfies the following:

(i) homogenous linear recurrence relations with constant coefficients;

Table 3
The higher order Hosoya numbers for several families of methyl substituted alkenes.

Molecule	^1Z	^2Z	^3Z	^4Z
2-Methyl-alkanes				
-butane	7	5	3	
-pentane	11	7	4	3
-hexane	18	11	5	4
-heptane	29	16	6	5
-octane	47	23	9	6
-nonane	76	34	13	7
-decane	123	50	18	18
3-Methyl alkanes				
-pentane	12	6	5	2
-hexane	19	9	6	4
-heptane	31	14	8	5
-octane	50	20	11	6
-nonane	81	29	16	7
-decane	131	43	22	9
2,2-Dimethyl alkanes				
-propane	5	7	1	
-butane	9	8	4	
-pentane	14	12	5	4
-hexane	23	19	6	5
-heptane	37	27	7	6
-octane	60	39	11	7
-nonane	97	58	16	8
2,3-Dimethyl alkanes				
-butane	10	8	5	
-pentane	15	13	5	5
-hexane	25	20	6	5
-heptane	40	28	7	6
-octane	65	41	12	7
-nonane	105	61	17	8

(ii) the numbers in the sequence satisfy Cauchy–Binet relations;

(iii) the numbers in the sequence may be expressed in terms of multinomial coefficients; and

(iv) there is a generating functions expressed as the ratio of two polynomials.

The relation between (i) and (ii) for a much wider class of invariants is addressed by Klein et al. [24] still in a chemiscal context. The case (iii) is implied in our identification of the higher order Fibonacci numbers with binomial coefficients of the Pascal triangle. The relation between (i), (ii) and (iii) is illustrated by Živkovič et al. [25], although this applies to another invariant and manipulations that extend beyond this limitation. Also Hosoya has addressed such ideas [18,21,26]. For a purely mathematical view, see several combinatorics texts such as Stanley's Enumerative Combinatorics [27].

Apart from the references in the preceding paragraph, there is a question as to on what one wishes to bestow the "title" the "higher-order Fibonacci numbers". There have been so many different generalizations of Fibonacci numbers starting with the Lucas numbers [4], in which the initial two members of the sequence that define the whole sequence, instead of being 1, 1, are 1, 3, and using three subsequent members to obtain the next member in the sequence (the so-called tribonacci sequence). Recently Lee and Lee [28] considered k-generalized Fibonacci sequence based on the rule (for $n > k > 1$)

$$g_n^{(k)} = g_{n-1}^{(k)} + g_{n-2}^{(k)} + \ldots + g_{n-k}^{(k)}$$

with conditions

$$g_1^{(k)} = g_2^{(k)} = \ldots = g_{k-2}^{(k)} = 0\,; \quad g_{k-1}^{(k)} = g_k^{(k)} = 1\,.$$

For example, if $k = 6$ then 6-generalized Fibonacci numbers are given by

$$0, 0, 0, 0, 1, 1, 2, 4, 8, 16, 32, 63, 125, 248, 477, 961, 1906, \ldots .$$

While such sequences have some interesting properties and parallel Fibonacci numbers, in our view they may better be referred to as generalized k-bonacci numbers in analogy with tribonacci numbers (and consequently are legitimate generalized Fibonacci numbers) rather than *higher order* Fibonacci numbers. We would like to reserve the label *higher order* Fibonacci numbers for members of sequences that parallel Fibonacci numbers more closely than generalized Fibonacci sequences appear to do. For example, in the above case the sequence includes the initial zeros, which are essential for recursion, but the Fibonacci sequences has no zeros (and even if such are formally introduced, they would be redundant, not essential).

We insist on additional constraints besides the already mentioned conditions (i)–(iv), which incidentally are not independent, but are all more-or-less equivalent (as may be deduced from ref. [27]) and which hardly discriminate among many sequences. Just as the Fibonacci numbers involve the recursion including only *two* members of the sequence (not three as in tribonacci, or more as in k-bonacci sequences), we also require recursions involving only two members of the sequence. Under this more stringent requirement most of the generalized Fibonacci numbers mentioned in the literature would be disqualified for the title "higher order Fibonacci numbers" and will remain "only" generalized Fibonacci numbers. The

Lucas numbers would still qualify for the "title" and need be excluded, and we can exclude them on other grounds. One of the reasons for excluding Lucas numbers

$$1, 3, 4, 7, 11, 18, 29, 47, 76, 123, 199, 322, 521, \ldots$$

is that these very numbers themselves can be generalized in "higher order Lucas numbers" by applying the idea of higher order Hosoya numbers to cycles [29]. Because both the Fibonacci numbers and the higher order Fibonacci numbers can be extracted from the Pascal triangle (by summing the entries on the corresponding slanted lines shown in Table 2, which is not the case with Lucas numbers), we may consider this simple regularity as the essential ingredient that justifies the "title" the "higher order Fibonacci numbers".

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Note added in proof

At the recent Seventh International Conference on Fibonacci Numbers and Their Applications (July 15–19, 1996) held in Graz, Austria, A.P. Stakhov reported on his earlier work on generalized Fibonacci numbers which are identical to the ${}^{k}Z$ numbers discussed here. His work was published in his book: Codes of the Golden Proportion (Radio and Communication, Moscow, 1984, in Russian).

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