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REVIEW

THEORY AND COMPUTATIONAL APPLICATIONS OF FIBONACCI GRAPHS+

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Abstract

The concept of Fibonacci graphs introduced and developed by this author is critically reviewed. The concept has been shown to provide an easy *pencil-and-paper* method of calculating characteristic, matching, counting, sextet, rook, color and king polynomials of graphs of quite large size with limited connectivities. For example, the coefficients of the matching polynomial of 18-annuleno – 18-annulene can be obtained *by hand* using the definition of Fibonacci graphs. They are (in absolute magnitudes): 1, 35, 557, 5337, 34 361, 157 081, 525 296, 1 304 426, 2 416 571, 3 327 037, 3 362 528, 2 440 842, 1 229 614, 407 814, 81 936, 8652, 361, 3. The theory of Fibonacci graphs is reviewed in an easy and detailed language. The theory leads to modulation of the polynomial of a graph with the polynomial of a path.

1. Introduction

The recent applications of graph theory and combinatorics to chemistry and physics resulted in several new counting polynomials. Several reference books describe such developments [1,2]. Many of these polynomials have been used to study the topological theory of aromaticity and the thermodynamic stability of benzenoid hydrocarbons. A recent review has been written by Gutman [3]. The coefficients of a graph polynomial are combinatorial descriptions of a certain defined *graph invariant*. The latter is a *count* which is independent of the way of labeling of the graph. Of course, the number of vertices N or the number of edges E in a graph are two more trivial examples. Two other less trivial and more commonly used graph invariants which will be emphasized here are:

+Dedicated to Professor R. Bruce King for his enthusiastic promotion and contributions to Mathematical Chemistry.
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(a) SETS OF INDEPENDENT EDGES IN A GRAPH

The symbol $p(G, k)$ has been introduced by Hosoya [4] to indicate the number of selections of k nonadjacent (i.e. independent) *edges* in a graph G, where $p(G, 0)$ is taken to be 1. Hosoya has shown that the sequence of $p(G, k)$, $0 \leqslant k \leqslant$ max value of k, succeeds in ordering several molecular properties of alkanes [4,5]. A *counting polynomial* $H(G; x)$ is defined according to eq. (1), viz.

$$H(G;x) = \sum_{k=0}^{M} p(G, k)x^k, \tag{1}$$

where M is the maximum value of k. The *matching polynomial* of a graph $M(G, x)$ is given by

$$M(G;x) = \sum_{k=0}^{M} (-1)^k p(G, k)x^{N-2k} . \tag{2}$$

The two polynomials are related as follows [6]:

$$M(G;x) = x^N H(G, -x^{-2}), \tag{3}$$

$$H(G;x) = \mathrm{i}^{-N} x^{N/2} M(G; \mathrm{i}\, x^{-1/2}). \tag{4}$$

The computation of these polynomials becomes very tedious for molecules with average size. The concept of "Fibonacci graphs" reviewed here facilitates such computations.

(b) SETS OF INDEPENDENT VERTICES

In his study of topological properties of benzenoid hydrocarbons, Gutman [7] introduced the symbol $0(G, k)$ to denote the number of ways of selecting k independent *vertices* of G. Accordingly, a polynomial was then called an *independence polynomial* [7], $\omega(G;x)$, defined as

$$\omega(G;x) = \sum_{k=0}^{M} 0(G, k)x^k \tag{5}$$

and used to describe resonance relations among the hexagons of a benzenoid hydrocarbon [7,8].

Subsequently, Balasubramanian and Ramaraj [9] studied the independence polynomial (under the name *color polynomial*) in connection with certain polyominos which have applications in statistical physics, and are related to the so-called *king polynomials* introduced by Motoyama and Hosoya [10].

All the above-mentioned polynomials are essential to the study of the topological theory of aromaticity, and thus their computation is a worthy effort. For this reason, several computer programs and algebraic methods were recently devised for such computations. A review written by Balasubramanian [11] outlines such developments.

Fibonacci Graphs, the objects reviewed in this paper, present a surprisingly easy pencil-and-paper method for calculating many counting graph polynomials of potentially very large graphs.

To illustrate the power of this graphic tool, we quote a statement from Hess, Schaad and Argranant [12] in their study of the topological resonance energy [13] of certain annuleno-annulenes: "The computation of the GT resonance energy of [16]annuleno[16]annulene required 10.5 minutes of CPU time on a DEC 10099 system. [18]annuleno[18]annulene was not completed after approximately 30 minutes." To put this comment into perspective, however, it should be mentioned that programs running on personal computers are now able to give graph-theoretical resonance energies in a few minutes for the size of [18]annuleno[18]annulene.

The aboslute magnitudes of the coefficients of the reference (matching) polynomial of the 18-annuleno – 18-annulene which are its nonadjacent numbers $p(G,0)$, $p(G,1)$, $p(G,2)$, . . . ,$p(G,M = 17)$ can now be *hand-calculated.* They are, respectively:

$$\{1,\ 35,\ 557,\ 5337,\ 34\,361,\ 157\,081,\ 525\,296,\ 1\,304\,426,\ 2\,416\,571,\ 3\,317\,037,\ 3\,362\,528,\ 2\,440\,842,\ 1\,229\,614,\ 407\,814,\ 81\,936,\ 8652,\ 361,\ 3\}.$$

The method of computation of such sequences using the concept of Fibonacci graphs is explained in detail later.

Similarly, we quote another statement made by Randić, Ruščić and Trinajstić [14] concerning the efficiency of computers as the size of the considered graph becomes very large: "The difficulty is, we should emphasize, inherent in a procedure which uses the Sachs theorem for construction, and applied equally to coefficients of the characteristic polynomial as to coefficients of the acyclic polynomial. The explosive growth of combinations limits even the usefulness of computers."

The strategy of this paper is as follows: first we define and illustrate a sequence of Fibonacci graphs, then more involved applications of the concept are given, and thirdly the theory of Fibonacci graphs is presented. Here, the theory is postponed until a later section because it is usually uninteresting to start a topic with closed-form equations! Finally, special types of Fibonacci graphs will be presented.

2. Illustration, definition and construction of Fibonacci graphs

To illustrate the concept [15–18], in fig. 1 we show several graphs and their independence polynomials [eq. (5)]. Similarly, in fig. 2 we show five graphs together with their counting polynomials [top line, eq. (1)] and matching (reference) polynomials [second line, eq. (2)]. In both figures, the relation between the coefficients is illustrated. One can formalize a definition in the following way: Let $\{G_{-1}, G_0, G_1, G_2, \ldots\}$ be a set of graphs (which may be finite or infinite). The above set is called a set of Fibonacci graphs if for any three consecutive members the following relation holds:

$$I(G_{N+2}, k+1) = I(G_{N+1}, k+1) + I(G_N, k), \tag{6}$$

where $I(G_N, k)$ is a graph invariant of an arbitrary graph G on N vertices. In this review, $I(G_N, k)$ is restricted to $p(G, k)$ and/or $0(G, k)$. The graph shown in figs. 1 and 2 thus represent two sets of Fibonacci graphs.

It turns out that it is *not* trivial to characterize members of a set of Fibonacci graphs. For example, T_4 (in fig. 3) may seem to be a member of the Fibonacci sequence $\{T_1, T_2, T_3\}$; however, inspection of their nonadjacent numbers reveals that T_4 does not obey the recursion described by eq. (6). A similar situation is depicted in fig. 4: G_4 is not a member of the Fibonacci family $\{g(1), G(2), G(3)\}$. This is a crucial point because the use of the concept of Fibonacci graphs in the computation of a counting polynomial of a large graph depends on *digression of this graph to much smaller graphs by identifying its leading two members* (i.e. the first two members in the Fibonacci set). It is obvious that the leading two members of T_4 (fig. 3) are *not* T_1 and T_2, and similarly one *cannot* use the counting polynomials of $g(1)$ and $G(2)$ to obtain that of $G(4)$. This is related to the problem of construction of Fibonacci graphs. This problem is treated in refs. [17] and [18], which we review here.

CONSTRUCTION OF FIBONACCI GRAPHS

A set of Fibonacci graphs possesses at least three elements. There are two ways of constructing a set of Fibonacci graphs, viz.:

(a) External subdivisions

This process can be described in the following way. Let G_1 be an arbitrary graph, possessing at least one edge. Its two adjacent vertices are labelled as v_0 and v_1. For all $i \geqslant 1$, the graph G_{i+1} is obtained from G_i by inserting a vertex v_{i+1} on the edge connecting v_{i-1} and v_0. The graph G_0 is obtained from G_1 by identifying the vertices v_0 and v_1, while the graph G_{-1} is obtained from G_1 by deleting the vertices v_0 and v_1. Then the infinite set $\{G_{-1}, G_0, G_1, G_2, \ldots\}$ is a set of Fibonacci graphs. Figure 5 illustrates this mode of construction.

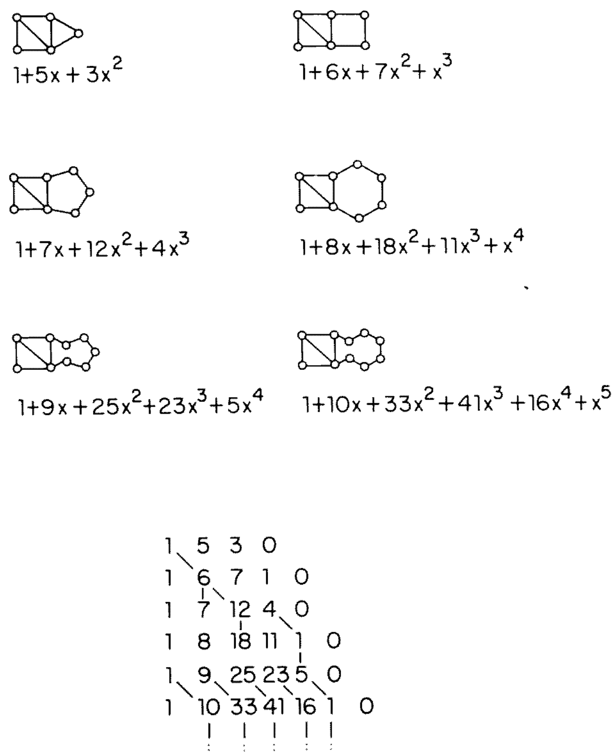


Fig. 1. A sequence of Fibonacci graphs and their corresponding independence (≡ color) polynomials. The lower part of the figure illustrates how the coefficients are related [cf. recursive relation, eq. (6)].

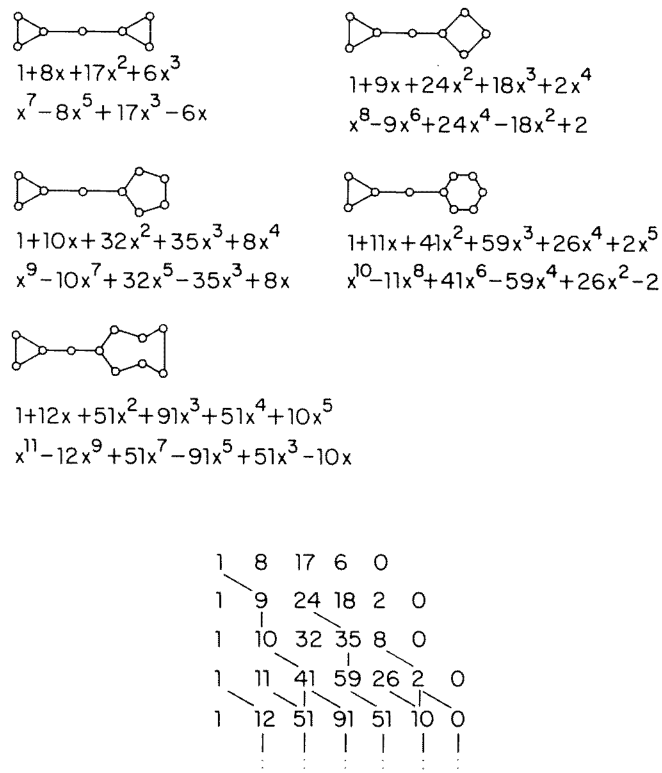


Fig. 2. A sequence of Fibonacci graphs and their counting polynomials (top line) and the corresponding matching polynomials (second line). The recursive relation among the absolute magnitudes of the coefficients is shown below.

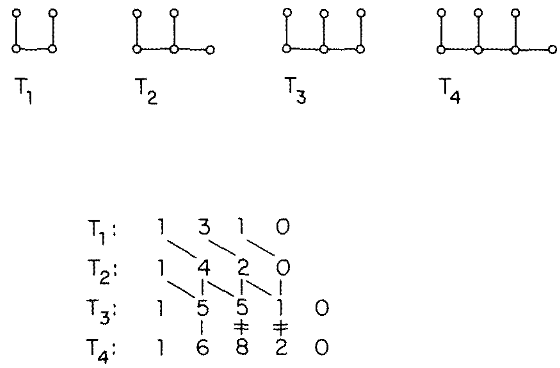


Fig. 3. Four trees and their nonadjacent numbers ordered as $p(T, 0)$, $p(T, 1)$, $p(T, 2)$, ... It can be seen that T_4 is *not* a member of the *finite* set of Fibonacci trees $\{T_1, T_2, T_3\}$.

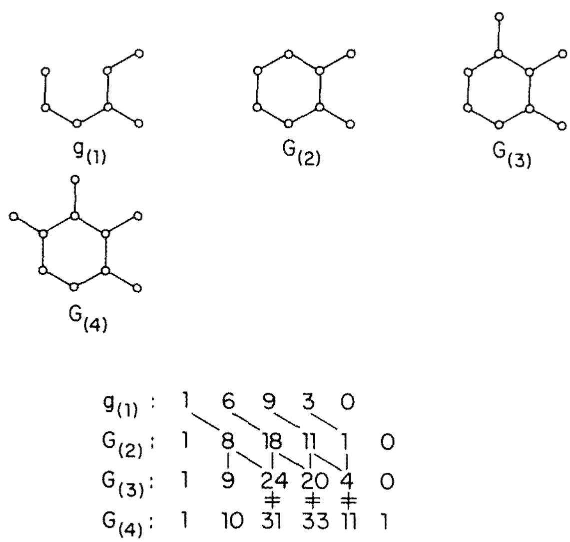


Fig. 4. A set of graphs and their corresponding sequences of nonadjacent numbers listed, respectively, as $p(G, 0)$, $p(G, 1)$, $p(G, 2)$, ... It is observed that $G(4)$ is not a member of the Fibonacci set $\{g(1), G(2), G(3)\}$.

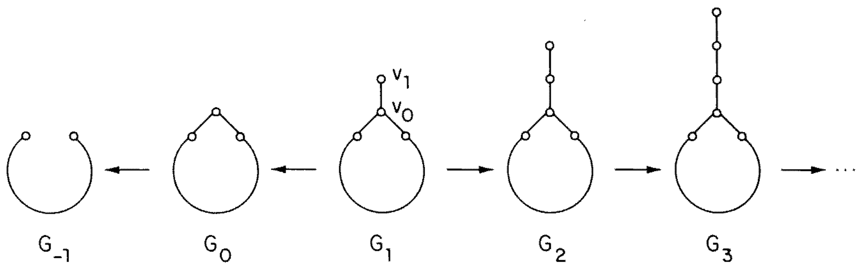


Fig. 5. Construction of Fibonacci graphs via *external subdivision*. The process leads to the *infinite* set $\{G_{-1}, G_0, G_1, G_2, \ldots\}$.

(b) Internal subdivision

This is a process whereby a ring or a path in a graph is enlarged, keeping all other parts of the graph invariant. An illustration is provided in fig. 6.

It is now easy to predict that T_4 is not a member of the Fibonacci set T_1, T_2, T_3 (fig. 3) and similarly for $G(4)$ of fig. 4.

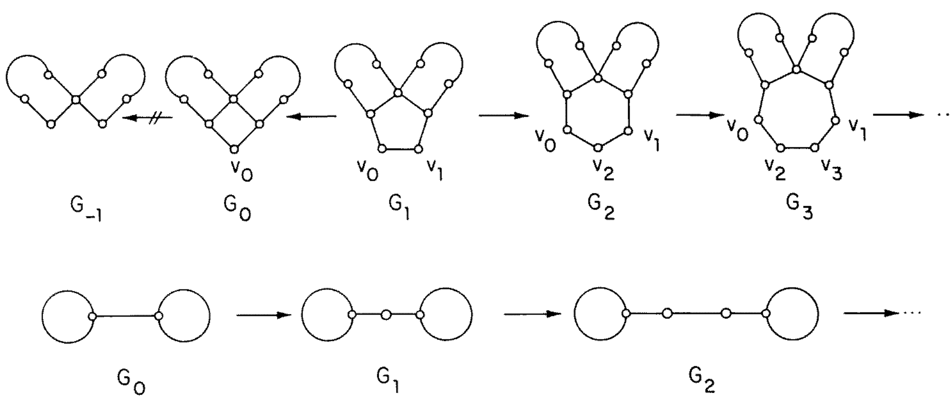


Fig. 6. Illustration of construction of Fibonacci graphs via *internal subdivision*. The infinite set of Fibonacci graphs is $\{G_0, G_1, G_2, \ldots\}$. Observe that G_{-1} is *not* a member of this set. The top set illustrates the subdivision on a ring, while the second set is an internal subdivision along a path.

3. Computational applications of Fibonacci graphs.

We shall briefly review three types of applications, viz., direct applications, more involved applications and, finally, how to use this concept to calculate other polynomials such as the *sextet polynomials* [19], *rook polynomials* and *king polynomials*. This third aspect then links Fibonacci graphs with two important problems: one in chemistry, which is the count of Kekulé structures, an already solved problem since the early fifties [20], but still of interest, and a problem in statistical physics, namely, the distribution of kings on lattice graphs [9,21].

3.1. DIRECT APPLICATIONS

Suppose one wishes to calculate some counting polynomial of a large graph such as the one shown in fig. 7: G_{14}, a graph on 14 vertices. Naturally, it is difficult to calculate all of its nonadjacent numbers by hand. (It is possible, probably, using a

j									
0	1	6	3	0					
1	1	7	8	0					
2	1	8	14	3	0				
3	1	9	21	11	0				
⋮	⋮	⋮	⋮	⋮	⋮				
10	1	17	113	375	654	574	217	23	0

Fig. 7. Graphical synthesis of the nonadjacent numbers $p(G, 0)$, $p(G, 1), \ldots$ of G_{14} by identifying its first two Fibonacci members, viz. $j = 0, j = 1$.

program [22]). This problem can be solved by identifying the first two members of the set of Fibonacci graphs to which G_{14} belongs. The whole computation takes less than 10 minutes using a desk calculator. This example illustrates a case of internal subdivision on a ring. In fig. 8, we illustrate internal subdivision along a path where the nonadjacent numbers of T_{18}, a tree on 18 vertices, are computed from those of T_8 and T_9, i.e. the first two members in the corresponding Fibonacci set.

3.2. MORE INVOLVED APPLICATIONS

3.2a. Characteristic polynomials

Although the spectrum (i.e. eigenvalues) of the characteristic polynomial of fairly large graphs can be obtained routinely using readily available computer programs, the characteristic polynomial itself has been less easy to calculate. Recently, Balasubramanian [23] and Balasubramanian and Randić [24] applied theorems due to Goldsil and McKay [25] and were able to reduce the secular determinant of a graph

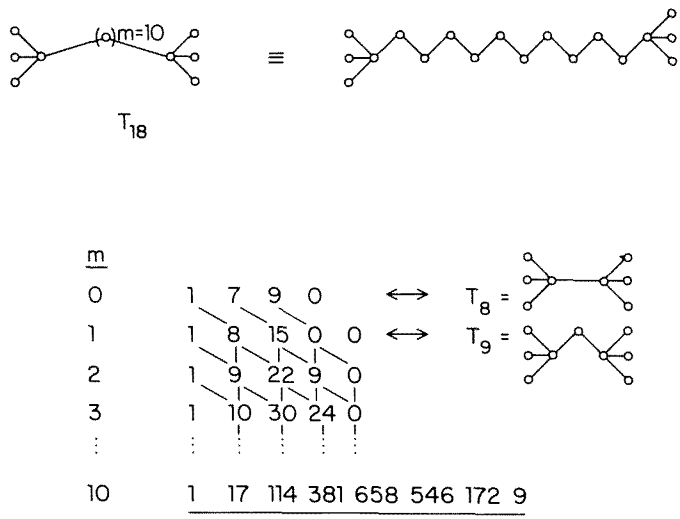


Fig. 8. Graphical induction of the leading Fibonacci tree T_8 to T_{18}. The last line gives $p(T_{18,0}), p(T_{18,1}), \ldots, p(T_{18,7})$ of T_{18}.

adjacency matrix by elegantly pruning the graph at selective points. Their method, however, works mainly for *acyclic graphs and/or graphs with pending bonds* (i.e. a bond with a vertex of degree one).

Here, we demonstrate that using the concept of Fibonacci graphs we can make elegant use of Sachs' theory [26] to calculate the characteristic polynomials of graphs (cyclic or acyclic) of potentially very large size. First, we review the Sachs formula [26]. The characteristic polynomial of a graph containing N vertices is given by

$$P(G;x) = a_0 X^N + a_1 X^{N-1} + a_2 X^{N-2} + \ldots + a_N , \tag{7}$$

where a_m's, $0 \leqslant m \leqslant N$, are coefficients given by the Sachs formula:

$$a_m = \sum_{s \in S_m} (-1)^{c(s)} 2^{r(s)}. \tag{8}$$

$c(s)$ and $r(s)$ are, respectively, the number of components and cycles in S_m, the Sachs graph on m vertices, and the summation is taken over all S_m's, i.e. Sachs graphs on m vertices. A Sachs graph is either a K_2 subgraph, a cycle, and/or a union of both. As an illustration, fig. 9 shows all Sachs graphs for a graph containing two 3-membered rings. Obviously, as the size of the graph grows the number of terms proliferates exponentially and the count of all Sachs graphs by inspection becomes error-prone.

To approach this problem using Fibonacci graphs, we *resolve* the coefficients of the characteristic polynomial into strictly acyclic and cyclic terms; thus:

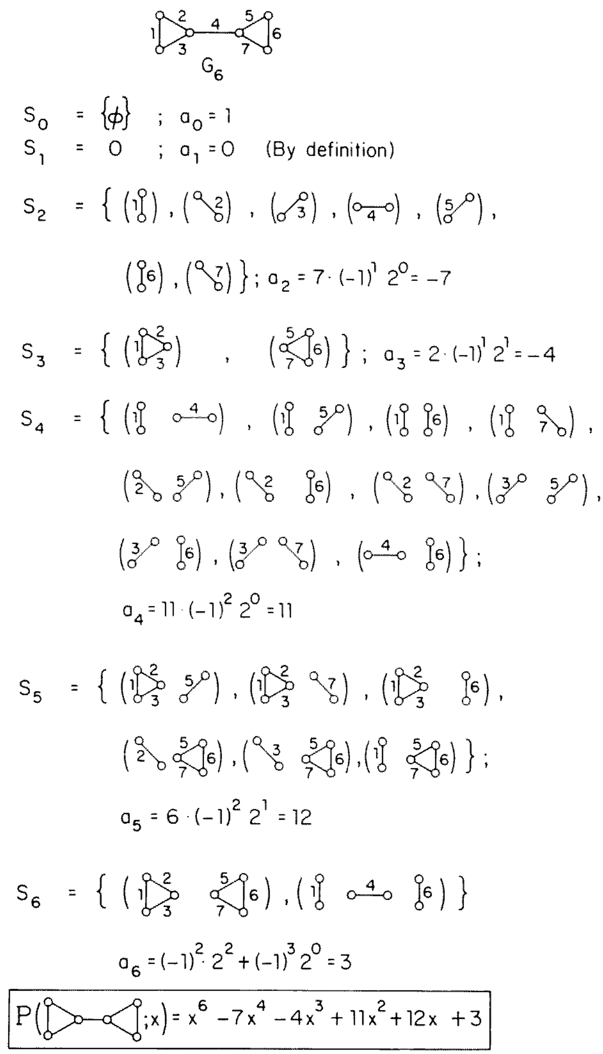


Fig. 9. All sets of Sachs graphs and coefficient of the characteristic polynomial of G_6.

$$a_m^{\mathrm{ac}} = \sum_{s \in S_m^{\mathrm{ac}}} (-1)^{c(s)} \tag{9}$$

$$a_m^{\mathrm{cy}} = \sum_{s \in S_m^{\mathrm{cy}}} (-1)^{c(s)} 2^{r(s)} , \tag{10}$$

where the superscript ac stands for acyclic, while cy means cyclic. S_m^{ac} is an acyclic Sachs graph, i.e. containing *at least* one cycle. The subscript m is the number of its vertices. Therefore, a coefficient in $P(G;x)$ can be expressed as:

$$a_m = a_m^{\text{ac}} + a_m^{\text{cy}} \,. \qquad (11)$$

As an illustration, a_6 of G_6 (fig. 9) can be resolved into two terms, viz.,

$$a_6^{\text{ac}} = (-1)^3\, 2^0 = -1$$

$$a_6^{\text{cy}} = (-1)^2\, 2^2 = 4,$$

whence $a_6 = -1 + 4 = 3$.

Sets of Fibonacci graphs satisfy the following two recursions [16] [which are special cases of eq. (6)]:

$$|a_i^{\text{ac}}(G_N)| + |a_{i+2}^{\text{ac}}(G_{N+1})| = |a_{i+2}^{\text{ac}}(G_{N+2})| \qquad i = 0, 2, 4, \ldots \qquad (13)$$

and

$$|a_i^{\text{cy}}(G_N)| + |a_{i+2}^{\text{cy}}(G_{N+1})| = |a_{i+2}^{\text{cy}}(G_{N+2})| \qquad (14)$$

$$i = 3, 5, 7, \ldots \text{ and/or } i = 0, 2, 4, \ldots (a_1 = 0).$$

Knowing the signs (which is trivial), we can then compute the a_m's. An illustration is depicted in fig. 10. *It is observed that the recurrence holds only for the odd subscripted coefficients of their* $P(G; x)$*'s*. This presents no difficulty, however, since both eqs. (13) and (14) hold (i.e. for the resolved parts). This subtle point is illustrated in fig. 11 for a_6 and a_8 of the Fibonacci graphs shown in fig. 10, namely, it can be seen that contributions of *odd-membered* rings to coefficients with *even subscripts* lead to inequality:

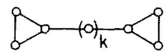
$$|a_i(G_n)| + |a_{i+2}(G_{n+1})| \neq |a_{i+2}(G_{n+2})| \qquad i = 0, 2, 4, \ldots \,. \qquad (15)$$

This is clear from fig. 11. When all rings in G are even-membered, eq. (15) becomes an equality. As an illustration, we consider the characteristic polynomials of the Fibonacci graphs shown in fig. 12.

Evidently, the concept of Fibonacci graphs is quite useful and promising in providing an easy pencil-and-paper approach to the problem of characteristic polynomials of potentially very large graphs. Also, such recursions can be used to facilitate a computer program.

3.2b. Sextet and related polynomials: On the number of Kekulé structures

The several applications of graph-theoretical and combinatorial approaches to problems of organic chemistry (particularly alkanes [4,5] and benzenoid hydro-



Acyclic Coefficients

k	a_0^{ac}	a_2^{ac}	a_4^{ac}	a_6^{ac}	a_8^{ac}
0	1	-7	11	-1	0
1	1	-8	17	-6	0
2	1	-9	24	-17	1
3	1	-10	32	-34	7
⋮	⋮	⋮	⋮	⋮	⋮

Cyclic Coefficients with <u>odd</u> subscripts

k	a_3^{cy}	a_5^{cy}	a_7^{cy}	a_9^{cy}
0	-4	12	0	0
1	-4	16	-4	0
2	-4	20	-16	0
3	-4	24	-32	4
⋮	⋮	⋮	⋮	⋮

Cyclic Coefficients with <u>even</u> subscripts

k	a_6^{cy}	a_8^{cy}
0	4	0
1	4	0
2	4	-4
3	4	-8
⋮	⋮	⋮

Characteristic Polynomial Coefficients

k	a_0	a_2	a_3	a_4	a_5	a_6	a_7	a_8	a_9
0	1	-7	-4	11	12	3	0	0	0
1	1	-8	-4	17	16	-2	-4	0	0
2	1	-9	-4	24	20	-13	-16	-3	0
3	1	-10	-4	32	24	-30	-32	-1	4
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

Fig. 10. Illustration of calculation of the characteristic polynomial of a cyclic graph *containing no pending bonds* using the concept of Fibonacci graphs. Observe that both cyclic and acyclic coefficients obey recursion equation (6), but the *summed* values do not.

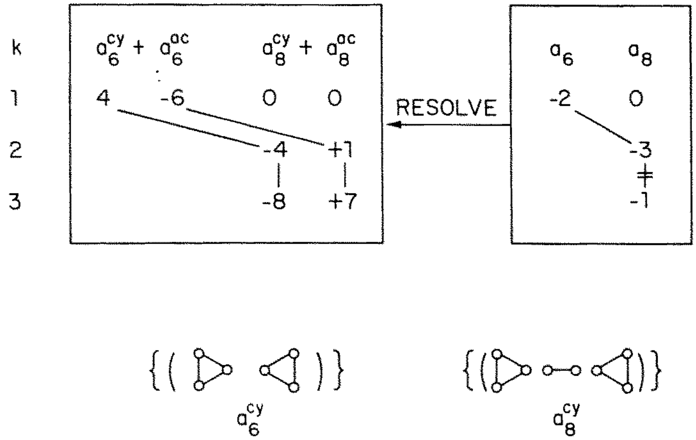
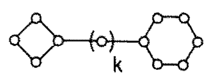


Fig. 11. Illustration of the resolution of the characteristic polynomial coefficients into cyclic and acyclic components.



Cyclic Coefficients

k	a_4^{cy}	a_6^{cy}	a_8^{cy}	a_{10}^{cy}	a_{12}^{cy}
0	-2	10	-10	4	0
1	-2	12	-16	6	0
2	-2	14	-26	16	-4
⋮	⋮	⋮	⋮	⋮	⋮

Acyclic Coefficients

k	a_0^{ac}	a_2^{ac}	a_4^{ac}	a_6^{ac}	a_8^{ac}	a_{10}^{ac}	a_{12}^{ac}
0	1	-11	41	-61	32	-4	0
1	1	-12	51	-92	66	-14	0
2	1	-13	62	-133	127	-46	4
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

Characteristic Polynomial Coefficients

k	a_0	a_2	a_4	a_6	a_8	a_{10}	a_{12}
0	1	-11	39	-51	22	0	0
1	1	-12	49	-80	50	-8	0
2	1	-13	60	-119	101	-30	0
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

Fig. 12. Illustration of the calculation of the characteristic polynomial of a graph containing no odd-membered rings by subduction to lowest Fibonacci member.

carbons [3]) and to statistical physics [20,21] led to the definition of several related counting polynomials, of which the counting polynomial of Hosoya [4] eq. (1) is a special case of a more general definition, namely:

$$F(G;x) = \sum_{k=0}^{M} \theta(G,k) \cdot X^k, \tag{16}$$

where $\theta(G, k)$ is a combinatorial function that enumerates certain defined invariants of G, viz.,

$$\theta(G,k) = \begin{cases} P(G,k) \\ 0(G,k) \\ r(B,k) \\ \rho(r,k) \end{cases} . \tag{17}$$

$p(G, k)$ and $0(G, k)$ are defined by eqs. (1) and (5). The quantity of $r(G, k)$ was first defined by Hosoya and Yamaguchi [27], which they called the kth resonant number. It counts the number of selections of k nonadjacent but mutually resonant hexagons when G is the molecular graph of a benzenoid hydrocarbon. The resulting polynomial is called the *sextet polynomial* $\sigma(B;x)$. It provides a combinatorial analysis of K, the number of Kekulé structures of the benzenoid hydrocarbons, thus:

$$\sigma(B;x) = \sum_{k=0}^{M} r(B;k)x^k. \tag{18}$$

Obviously, for $x = 1$, the value of $\sigma(B;x)$ is simply K; i.e.,

$$\sigma(B;1) = K. \tag{19}$$

The sextet polynomial occupies a central block in the topological theory of benzenoid systems [1–3]. The quantity $\rho(r, k)$ defines the number of ways of selecting r non-attacking rooks on a rook board r. Two rooks are defined to be nonadjacent if they do not share the same row and column. The quantities $\rho(r, k)$'s define the coefficients of the *rook polynomial* given by

$$R(r;x) = \sum_{k=0}^{M} \rho(r,k)x^k. \tag{20}$$

Rook polynomials have a number of chemical [28] and mathematical applications [29]. The above-mentioned polynomials were recently extensively reviewed by this author [30]. The concept of Fibonacci graphs can be used to compute polynomials defined by eqs. (1), (5), (18) and (20) for very large graphs. First, we digress to three types of related graphs which resulted from nearly twenty years of work in mathematical chemistry [1–3,30].

(a) *The caterpillar tree or Gutman tree* [30,31]. This is an acyclic graph formed by the addition of m *monovalent* vertices ($m = 0$ or any other integer) to each of the vertices of a path. These trees play a role in the theory of aromaticity.

(b) *The Clar graph* Λ. When the hexagons of a benzenoid hydrocarbon are replaced by vertices, and then every two vertices corresponding to two nonresonant hexagons are connected, a Clar graph results. If the benzenoid hydrocarbon contains no hexagon surrounded by three other hexagons, i.e. if it is nonbranched, its Clar graph becomes the *line graph* [32] of a certain caterpillar tree whose counting polynomial [eq. (1)] is the sextet polynomial [eq. (18)] of the benzenoid hydrocarbon. This is also the independence polynomial of the Clar graph:

$$\sigma(B;x) = H(T;x) = \omega(\Lambda;x). \tag{21}$$

In such a case, $\{B, T, \Lambda\}$ is called a set of *Equivalent Graphs* [33].

(c) *Rook boards.* Every caterpillar tree (in fact, every bipartite graph) can be associated with a rook board r [28] when the vertices of the tree are replaced by cells such that two cells in r are adjacent only if the corresponding two vertices in T are also adjacent. However, adjacency relations among the cells of r are defined as follows: two cells in r are adjacent if they share the same row and/or column. One can construct a rook board whose rook polynomial is identical to the counting polynomial of T. Thus, the set of equivalent graphs can be expanded to include r, viz., $\{B, T, \Lambda, r\}$. An illustration of a set of equivalent graphs is shown in fig. 13. The main value of a set of equivalent graphs is computational, namely, if one is able to calculate, say $H(T;x)$ other polynomials, viz., $\sigma(B;x)$, $\omega(\Lambda;x)$, $R(r;x)$ become immediately available. Then one can use the concept of Fibonacci graphs to calculate, say, a rook polynomial of a very large rook board by constructing the appropriate set of Fibonacci caterpillar trees. An illustration is shown in fig. 14. Thus, using the idea of equivalent graphs together with the concept of Fibonacci graphs, we have an easy way of hand-calculating many counting polynomials of very large graphs. The sextet polynomial of B_{10} (shown in fig. 14) is $1 + 17x + 114x^2 + 381x^3 + 658x^4 + 546x^5 + 172x^6 + 9x^7$. Whence, $K(B_{10}) = 1898$ (an alternative to the "classic" method of Gordon and Davison [20]). Further, we know from the polynomial that the maximum number of non-attacking rooks is seven and there are only nine ways of placing such seven rooks on the rook board r_{10} drawn in fig. 14. Also, it is trivial to conclude that there are 114 ways of coloring two vertices in Λ_{10} black so that no two black vertices are adjacent, but this number becomes 658 when we choose four nonadjacent vertices.

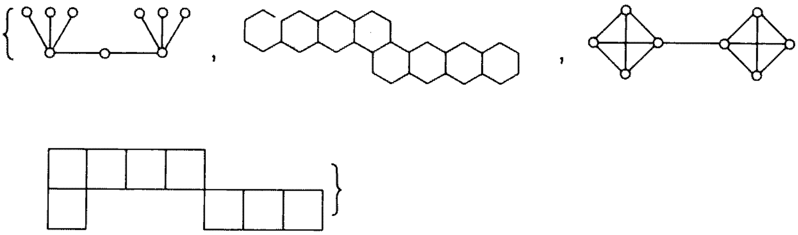
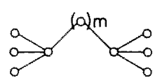


Fig. 13. A set of "equivalent graphs"; respectively, from left to right: a caterpillar tree, a benzenoid graph, a Clar graph, and a rook board. One observes the following interesting identity: $H(T;x) = \sigma(B;x) = \omega(\Lambda;x) = R(r;x) = 1 + 8x + 15x^2$; $K = 24$.



m	Nonadjacent Numbers, p(T,0), p(T,1), ..., p(T,M)							
1	1	8	15					
2	1	9	22	9				
3	1	10	30	24				
⋮	⋮	⋮	⋮	⋮				
10	1	17	114	381	658	546	172	9

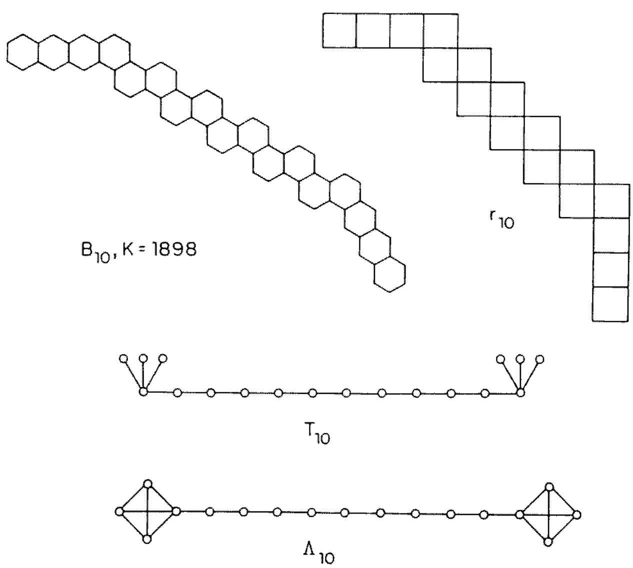


Fig. 14. Induction of the nonadjacent numbers of $m = 1$ to those of $m = 10$ which corresponds to the kth resonant numbers of a non-branched benzenoid hydrocarbon on 17 hexagons. The corresponding Kekulé count is 1898. The Fibonacci approach shown here is an alternative to the combinatorial method of Gordon and Davison [20]. Also shown in the figure is the equivalent Clar and rook graphs.

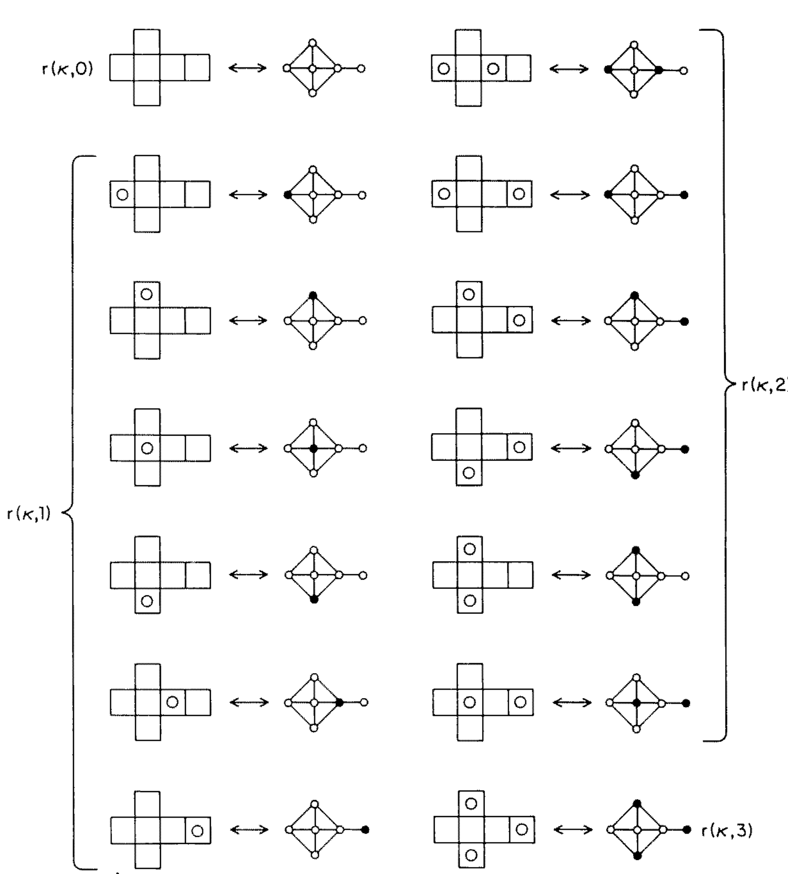


Fig. 15. Colorings of a graph and the corresponding king patterns. The corresponding king polynomial is $1 + 6x + 6x^2 + x^3$.

3.2c. *King polynomino graphs, king polynomials and color polynomials*

Nearly a decade ago, Motoyama and Hosoya [10] generated king polyominos by the stacking of squares of equal sizes, called cells. They defined a king polynomial as follows:

$$K(\kappa;x) = \sum_{k=0}^{M} r(\kappa, k)x^k, \tag{22}$$

where $r(\kappa, k)$ is the number of ways of placing k nontaking kings on the king polyomino κ. Two kings are called nontaking if they occupy nonadjacent cells, i.e. cells sharing no common vertices. Conventionally, $r(\kappa, 0) = 1$. Motoyama and Hosoya's work proved to be useful in treating several enumeration problems of lattice dynamics, namely the partition function of the magnetic properties of transition metal crystals [34], as well as other problems in dimer statistics. In fig. 15, we illustrate various

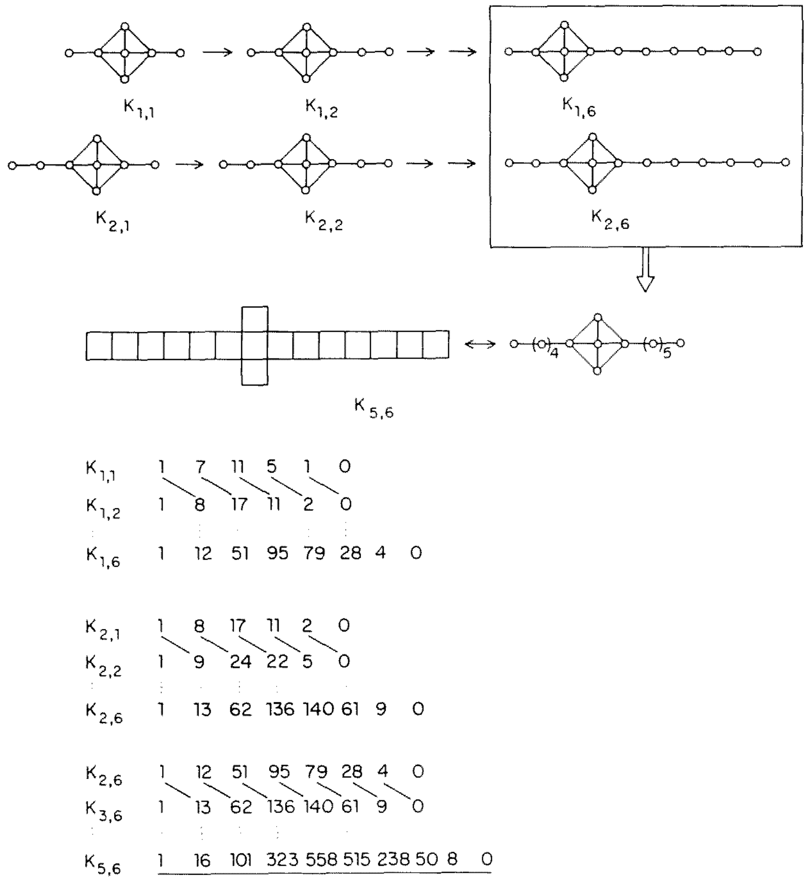


Fig. 16. Fibonacci generation of the king and color polynomials of $K_{5,6}$, a graph on 16 components, by three Fibonacci external subdivisions.

terms of the king polynomial of an arbitrary king polyomino graph. It can be shown that there is a one-to-one correspondence with the colorings of certain graphs, which are the dualist graphs [35] of the king polyominos (fig. 15). Whence, the color and king polynomials can be obtained from one another, which has recently been demonstrated by Balasubramanian and Ramaraj [9]. They computed these polynomials for very large lattices. In a recent paper, the present author [21] demonstrated how to use the concept of Fibonacci graphs to calculate king polynomials of a large lattice. Another example is depicted in fig. 16. The method uses three Fibonacci external subdivisions, viz., $K_{1,1} \to K_{1,6}$; $K_{2,1} \to K_{2,6}$, and finally $K_{1,6}$ and $K_{2,6}$ are used as the first two Fibonacci members leading to the desired $K_{5,6}$, a polyomino on 16 cells. Its king polynomial is $1 + 16x + 101x^2 + 323x^3 + 558x^4 + 515x^5 + 238x^6 + 50x^7 + 8x^8$. Thus, we can immediately see that the maximum number of nontaking kings is eight and that there are exactly eight ways of distributing the eight kings. Similarly, there are exactly 558 ways of arranging four nontaking kings on the king board $K_{5,6}$. The color polynomials of the leading members can be obtained either by inspection or by using a well-known recursion, viz.,

$$\omega(G;x) = (G - v;x) + x\omega(G\theta v;x), \tag{23}$$

where v is any vertex in G and $G - v$ is a subgraph obtained by deleting v from G, while $G\theta v$ is obtained when v and all its adjacent vertices are pruned out of G.

3.2d. Large annuleno – annulenes

In early applications of the topological theory of aromaticity, Hess and Schaad [12] faced a difficulty in computing the matching (reference) polynomials of large annuleno – annulenes, as mentioned in the introduction. The absolute magnitudes of the coefficients of the matching polynomial of a graph are simply its nonadjacent numbers. In fig. 17, we illustrate how to calculate the nonadjacent numbers of 18-annuleno – 18-annulene. Such parameters might be obtained in about three-quarters of an hour using a desk calculator and three steps of internal subdivisions, as depicted in fig. 17.

4. Theory of Fibonacci graphs. Modulation of the polynomial of a graph with the polynomial of a path [18]

4.1. THE MATCHING POLYNOMIAL

Let $M(G_n;x) \equiv M_n$ be the matching polynomial of a graph on n vertices. If G_n, G_{n+1} and G_{n+2} are three Fibonacci graphs, then the following identity is true:

$$M_{n+2} - xM_{n+1} + M_n = 0 . \tag{24}$$

The above equation corresponds to the auxilliary equation:

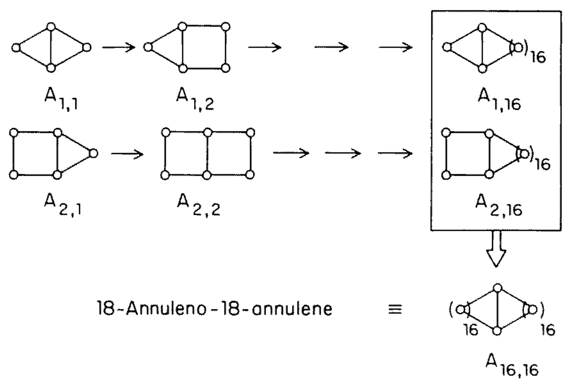
$$\lambda^2 - x\lambda + 1 = 0, \tag{25}$$

with the following solutions:

$$\lambda_{1,2} = \frac{x \pm (x^2 - 4)}{2} . \tag{26}$$

We use the following convenient change of variable

$$x = 2 \cos t . \tag{27}$$



$A_{1,1}$ 1 5 2 0

$A_{1,2}$ 1 6 6 0

⋮

$A_{1,16}$ 1 20 167 756 2015 3212 2970 1464 321 20

$A_{2,1}$ 1 6 6 0

$A_{2,2}$ 1 7 11 3

⋮

$A_{2,16}$ 1 21 186 906 2652 4785 5247 3312 1071 137 3

$A_{1,16}$ 1 20 167 756 2015 3212 2970 1464 321 20

$A_{2,16}$ 1 21 186 906 2652 4785 5247 3312 1071 137 3

⋮

$A_{16,16}$ 1 35 357 5337 34361 157081 525296 1304426 2416571 3327037 3362528 2440842 1229614 407814 81936 8652 361 3

Fig. 17. Generation of the sequence of nonadjacent numbers of 18-annuleno – 18-annulene by starting three Fibonacci internal subdivisions using $A_{1,1}$ and $A_{2,1}$. The last three lines, $A_{16,16}$, were not completed after about 30 minutes on a DEC 1099 system [12]. Using the definition of Fibonacci graphs, we obtained the desired values in less than an hour, using only a desk calculator.

Then,

$$\lambda_{1,2} = \cos t \pm \mathrm{i} \sin t = \mathrm{e}^{\pm \mathrm{i} t}, \tag{28}$$

where $\mathrm{i} = (-1)^{1/2}$.

Now M_n can be expressed by

$$M_n = \alpha\lambda_1^n + \beta\lambda_2^n . \tag{29}$$

Therefore,

$$M_n = \alpha\,\mathrm{e}^{\mathrm{i}nt} + \beta\,\mathrm{e}^{-\mathrm{i}nt}$$

$$= \alpha(\cos nt + \mathrm{i} \sin nt) + \beta(\cos nt - \mathrm{i} \sin nt),$$

i.e.,

$$M_n = (\alpha + \beta) \cos nt + \mathrm{i}(\alpha - \beta) \sin nt. \tag{30}$$

The constants α and β are determined from the initial conditions; thus:

$$M_0 = \alpha + \beta$$

$$M_1 = (\alpha + \beta) \cos t + \mathrm{i}(\alpha - \beta) \sin t, \tag{31}$$

or

$$M_1 = M_0 \cos t + \mathrm{i}(\alpha - \beta) \sin t. \tag{32}$$

Then,

$$\mathrm{i}(\alpha - \beta) = \frac{M_1 - M_0 \cos t}{\sin t} . \tag{33}$$

Now we substitute eqs. (31) and (33) into (30) to obtain:

$$M_n = M_1 \frac{\sin nt}{\sin t} - M_0 \left[\frac{\cos t \sin nt - \cos nt \sin nt}{\sin t}\right] . \tag{34}$$

However,

$$\cos t \sin nt - \cos nt \sin t = \sin (nt - t) = \sin (n - 1) t.$$

Whence,

$$M_n = M_1 \frac{\sin nt}{\sin t} - M_0 \frac{\sin (n - 1) t}{\sin t} . \tag{35}$$

Now, for the *paths* $M_1 = x = 2\cos t$ and $M_0 = 1$, i.e. for the paths $M_n \equiv M(P_n)$, and eq. (35) becomes:

$$M(P_n) = \frac{2\cos t \sin nt - \sin(n-1)t}{\sin t} . \tag{36}$$

However,

$$\sin nt = 2\cos t \sin(n-1)t - \sin(n-2)t,$$

whence eq. (36) becomes

$$M(P_n) = \frac{\sin(n+1)t}{\sin t} . \tag{37}$$

Therefore,

$$\frac{\sin nt}{\sin t} = M(P_{n-1}) \tag{38}$$

and

$$\frac{\sin(n-1)t}{\sin t} = M(P_{n-2}). \tag{39}$$

Using eqs. (38) and (39) into (35), we obtain the desired relation, viz.,

$$M_n = M_1 M(P_{n-1}) - M_0 M(P_{n-2}). \tag{40}$$

Equation (40) described how the matching polynomials of Fibonacci graphs are modulated with the matching polynomials of paths (which are their characteristic polynomials).

We observe that eq. (37) is the *trigonometric representation* of Fibonacci numbers, since they lead to the characteristic polynomials of the paths when the appropriate trigonometric substitutions are made. Thus,

$$M(P_0) = \frac{\sin t}{\sin t} = 1 ,$$

$$M(P_1) = \frac{\sin 2t}{\sin t} = \frac{2\sin t\cos t - \sin(0)t}{\sin t} = 2\cos t = x ,$$

$$M(P_2) = \frac{\sin 3t}{\sin t} = \frac{2\sin 2t\cos t - \sin t}{\sin t} = \frac{(4\sin t\cos^2 t - \sin t)}{\sin t} = x^2 - 1.$$

Higher terms can be similarly generated.

4.2. THE COUNTING AND INDEPENDENCE (COLOR) POLYNOMIALS

Let F_r indicate either the counting or independence polynomials (eqs. (1), (5), respectively) of a graph containing r vertices. For a series of Fibonacci graphs, the following recursion applies:

$$F_{r+2} - F_{r+1} - xF_r = 0, \tag{41}$$

which requires the following auxilliary equation:

$$\lambda^2 - \lambda - x = 0 \tag{42}$$

with the following two solutions:

$$\lambda_{1,2} = \frac{1 \pm (1+4x)^{1/2}}{2} \quad . \tag{43}$$

We use the following change of variable:

$$x = -\left(\frac{1}{2\cos t}\right)^2 . \tag{44}$$

Then,

$$\lambda_{1,2} = \frac{\cos t \pm \mathrm{i}\sin t}{2\cos t} = \frac{\exp(\pm\, \mathrm{i}\, t)}{2\cos t} \quad . \tag{45}$$

The most general solution of F_r is

$$F_r = A\,\lambda_1^r + B\,\lambda_2^r , \tag{46}$$

where A and B are constants to be determined from initial states.

Using (45) and (46), one obtains after straightforward algebraic manipulations:

$$F_r = \left(\frac{1}{2\cos t}\right)^r [(A+B)\cos rt + \mathrm{i}(A-B)\sin rt] \ . \tag{47}$$

Now, to find A and B we proceed as before, namely from (46) and (45):

$$F_0 = A + B \tag{48}$$

$$F_1 = \frac{A(\cos t + \mathrm{i} \sin t)}{2 \cos t} + \frac{B(\cos t - \mathrm{i} \sin t)}{2 \cos t} \tag{49}$$

or

$$F_1 = \frac{F_0}{2} + \mathrm{i}(A - B) \frac{\sin t}{2 \cos t} , \tag{50}$$

whence

$$\mathrm{i}(A - B) = F_1 \frac{2 \cos t}{\sin t} - F_0 \frac{\cos t}{\sin t} . \tag{51}$$

Ussing (48) and (51) into (47), we finally obtain:

$$F_r = \left(\frac{1}{2 \cos t}\right)^r \left[2 \cos t\, F_1 \frac{\sin rt}{\sin t} - F_0 \frac{\sin (r-1)t}{\sin t}\right] . \tag{52}$$

To obtain the function for the paths, we assume the special case:

$$F_0 = F_1 = 1 \tag{53}$$

and use eq. (53) into

$$F_{r+2} = F_{r+1} + xF_r,$$

which, for $r = 0$, leads to:

$$F_2 = F_1 + x,$$

i.e.

$$F_2 = 1 + x. \tag{54}$$

However,

$$1 + x = \omega(P_1; x) = H(P_2; x). \tag{55}$$

Similarly, when $r = 1$, we get

$$F_3 = F_2 + xF_1$$

or

$$\begin{aligned} F_3 &= 1 + 2x \\ &= \omega(P_2;x) \\ &= H(P_3;x) . \end{aligned} \tag{55}$$

So in this special case ($F_0 = F_1 = 1$), we can write

$$F_j = \omega(P_{j-1};x) = H(P_j;x), \qquad (F_0 = F_1 = 1) \tag{56}$$

where P_j is a path on j vertices.

Now, for $F_0 = F_1 = 1$, eq. (52) becomes

$$F_r \equiv f_r = \left(\frac{1}{2\cos t}\right)^r \left[\frac{2\sin rt\cos t - \sin(r-1)t}{\sin t}\right]. \qquad (F_0 = F_1 = 1) \tag{57}$$

However,

$$\sin nt = 2\sin(n-1)t\cos t - \sin(n-2)t .$$

Therefore,

$$f_r = \left(\frac{1}{2\cos t}\right)^r \frac{\sin(r+1)t}{\sin t} \tag{58}$$

and whence

$$f_{r-1} = \left(\frac{1}{2\cos t}\right)^{r-1} \frac{\sin rt}{\sin t} \tag{59}$$

and

$$f_{r-2} = \left(\frac{1}{2\cos t}\right)^{r-2} \frac{\sin(r-1)t}{\sin t} . \tag{60}$$

Now eq. (52) may be rewritten as

$$\begin{aligned} F_r = {} & \left(\frac{1}{2\cos t}\right)^{r-1} \frac{\sin rt}{\sin t} F_1 \\ & - \left(\frac{1}{2\cos t}\right)^r \left[-\left(\frac{1}{2\cos t}\right)^2 \cdot -\left(\frac{1}{2\cos t}\right)^{-2}\right] \frac{\sin(r-1)t}{\sin t} F_0 . \end{aligned} \tag{61}$$

Using (59) and (60) into (67), we obtain:

$$F_r = F_1 f_{r-1} + x F_0 f_{r-2}, \tag{62}$$

and using eq. (56), we obtain the desired relations:

(a) When $F_r = H(G_r; x)$, then

$$H(G_r; x) = H(G_1; x) H(P_{r-1}; x) + x H(G_0; x) H(P_{r-2}; x); \tag{63}$$

(b) When $F_r = \omega(G_r; x)$, then

$$\omega(G_r; x) = \omega(G_1; x) \omega(P_{r-2}; x) + x \omega(G_0; x) \omega(P_{r-3}; x). \tag{64}$$

Equations (63) and (64) describe the moldulation of the counting and color polynomials of Fibonacci graphs with the corresponding path polynomials.

5. A special type of Fibonacci graph: Co-matched Fibonacci graphs [17]

In this final section, we consider an interesting class of Fibonacci graphs possessing identical matching polynomials. The graph $G(q, r{:}s, t)$ is obtained by connecting an isolated vertex v to some of the vertices of a cycle containing $s + t + r + q$ vertices. If we imagine v to be in the center of the cycle, then $r + q$ is the number of vertices to which v is connected, while s and t are sets of vertices not connected to v. An illustration is given in fig. 18. These families of graphs can be genrated by internal subdivisions at either sides of the central vertex. An example is given in fig. 19. The members of such families of such types of Fibonacci graphs are topomers [36], as depicted in fig. 20. These topomers are also called R, S isomers and play a significant role in graph-spectral theory recently developed by Polansky and Zander [36] and others.

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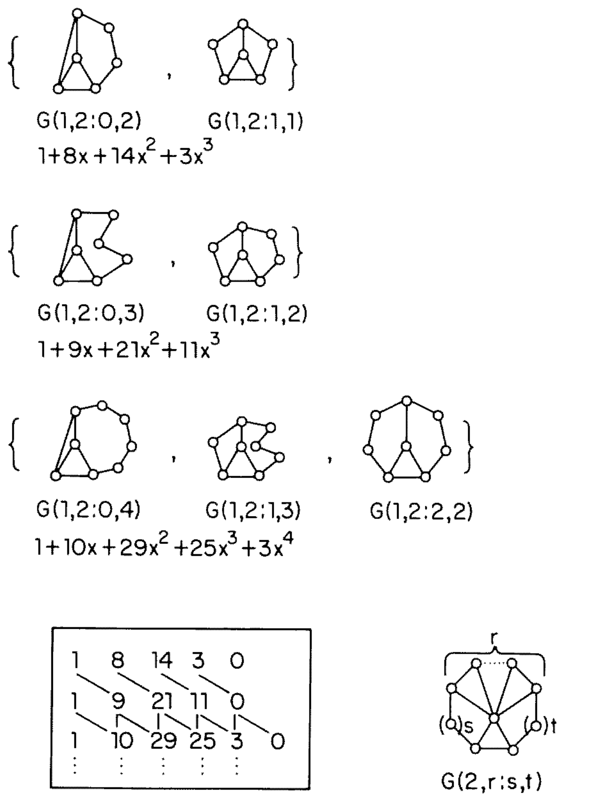

Fig. 18. Sets of Fibonacci graphs possessing identical nonadjacent numbers. Counting polynomials are indicated.

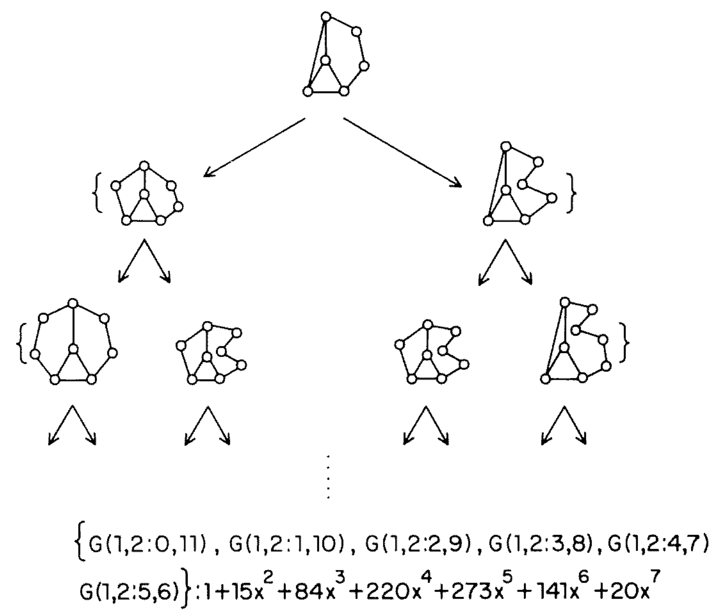

Fig. 19. Systematic generation of sets of co-matched Fibonacci graphs. The last line is the polynomial corresponding to 6 graphs.

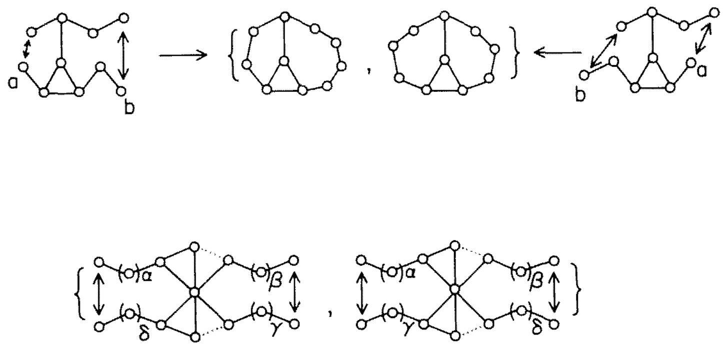

Fig. 20. Depiction of co-matched Fibonacci graphs as pairs of R, S isomers (topomers).

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