  Bull. Chem. Soc. Jpn., 61, 533—537 (1988)

On the Characterization of Fibonacci Numbers as Maximal Independent Sets of Vertices of Certain Trees

Sherif EL-BASIL†
Chemistry Department, University of Georgia, Athens, Georgia 30602, U.S.A.
(Received November 4, 1986)

Fibonacci numbers are identified for the first time as maximal independent sets of vertices of certain caterpillar trees. Their relation to king patterns of certain classes of polyomino graphs as well as polyhex graphs is illustrated.

More than a decade ago Hosoya[1] defined the concept of nonadjacent numbers in chemistry. Thus for a connected nondirected simple graph, G, the quantity $p(G,k)$ is defined to be the number of ways of choosing k disconnected lines from graph G with $p(G,o)$ being taken to be unity. The Z-counting polynomial, $H(G;x)$ is defined as

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

where m is the maximum number of k. The Z-index is the sum of the $p(G,k)$ numbers, i.e.,

$$Z(G)=H(G;1) \tag{2}$$

The above topological index was found to be applicable in many different areas including chemistry, mathematics, dimer statistics, and informatics.[2] The recent revival of interest in graph theory led to a natural extension of the $p(G,k)$ numbers to include other nonadjacent mathematical objects abstracted from molecular graphs. Thus when the concept is applied to benzenoid hydrocarbons[3] $p(G,k)$ becomes $r(B,k)$ i.e. the number of selections of k nonadjacent resonant sextets from the benzenoid graph B. In Clar sextet theory[4] the nonadjacent concept has been extended to sets of nonadjacent vertices $o(G,k)$ chosen from the corresponding Clar graph,[5] C. Further, the latter concept was also recently applied[6] to king polynomials of polyomino graphs.[7] In addition the nonadjacent concept relates to rook theory.[8] Thus, there is a one-to-one correspondence between labelled bipartite graphs with $a+b$ vertices and a chess board, R, with a rows and b columns such that $p(G,k)=\rho(R,k)$ where the latter function counts the number of ways in which one can arrange k non-attacking rooks on R, taking $\rho(R,o)=1$.

Some interesting relations arise for certain types of graphs. Thus the set $\{Z(G_n=L_n)\}$, where L_n is a path on n vertices is the set of Fibonacci numbers,[9] $\{F_n\}$, defined by

$$F_n=\sum_{k=0}^{[n/2]} \binom{n-k}{k} \tag{3}$$

while the set $\{Z(G_n=C_n)\}$, C_n being a cycle on n vertices, generates the Lucas sequence,[9] $\{L_n\}$, where

$$L_n=F_n+F_{n-2};\ n\geqslant 2 \tag{4}$$

The binomial functions of Eq. 3 are coefficients of the Chebyshev polynomials.[10] Because the Fibonacci numbers are well studied any relations to other fields such as chemistry or physics should be interesting. Two classical relations to the Fibonacci numbers are known in chemistry:

(1) The numbers of Kekulé structures, K, of the zigzag nonbranched benzenoid hydrocarbons (phenanthrene, chrysene, picene, fulminene, (benzo[c]picene), ⋯) are defined by[11]

$$K_n=F_{n+1} \tag{5}$$

n, is the number of rings in the polyhex graph.

The analogous relation in statistical physics is[12]

$$K(2\times n)=F_n \tag{6}$$

where $K(2\times n)$ is the number of perfect matchings in a $(2\times n)$ rectangular lattice.

(2) Let $\gamma_{i(n)}$ be the number of permutation integrals[13] involving i rings in a nonbranched zigzag polyacene containing n rings (observe that $\sum\gamma_i=1/2\sum R_i$, where R_i is a conjugated circuit over i rings,[14]) then[15]

$$\gamma_i(n)=\gamma_{i-1}(n-1) \tag{7}$$

$$\gamma_i(n) = \sum_{k=1}^{\theta} F_{\theta-k}F_{k-1}$$

where $\theta=n+1-i$.

Maximal Independent Sets. The vertices of a graph can be partitioned into a finite number of sets. A set of vertices in which no two vertices are adjacent is called an *independent* set of vertices. An independent set of vertices $\{V(r)\}$ in G is said to be *maximal*[16] if every vertex of G $\epsilon\{V(r)\}$ is adjacent to at least one of the r vertices of $\{V(r)\}$. Figure 1 shows three graphs $\mathcal{C}_1$, $\mathcal{C}_2$, and $\mathcal{C}_3$, arbitrarily labelled as shown. There are seven maximal independent sets of vertices in $\mathcal{C}_1$, viz., {1,4},

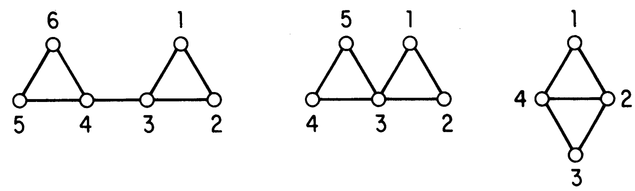


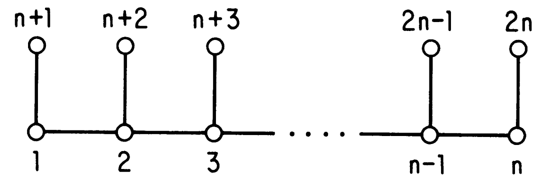
Fig. 1. Three labelled (Clar) graphs.

†Permanent address: Faculty of Pharmacy, Kasr El-Aini Street, Cairo, Egypt.

{1,5}, {1,6}, {2,4}, {2,5}, {2,6}, {3,5}, and {3,6}, while the vertices of $\mathcal{C}_2$, are partitioned into five maximal independent sets: {3}, {1,4}, {1,5}, {2,4}, {2,5}. For $\mathcal{C}_3$ there are only three such sets: {2}, {4}, and {1,4}. Actually $\mathcal{C}_1$ and $\mathcal{C}_2$ are the Clar graphs[5,17] of two nonbranched systems whose ring-annellation[18] sequences are respectively $L^2A^2L^2$ and $L^2A^2L^2$ while $\mathcal{C}_3$ is the Clar graph of pyrene. In fact, quite recently Herndon and Hosoya[17,19,20] identified the number of Clar *structures*[17] of a benzenoid hydrocarbon as the number of maximal independent sets of vertices in the corresponding Clar graphs.

The Comb Tree Graphs

We consider a special type of tree formed by the addition of a single (monovalent) vertex to each of the n vertices of a path, L_n. The resulting caterpillars[21] containing $2n$ vertices are also known as comb trees. The vertices of the original path moiety of such trees will be called *root vertices*. A comb tree will be given the symbol $Tn(1,1,\cdots,1)\equiv T_{n,1}$. An arbitrary labelling of the set of vertices $\{V(r)\}\varepsilon\, T_{n,1}$is shown below



Let us consider the maximal independent sets of vertices of some of the lower members of comb trees.

$V(T_{1,1}) \supset$ {2}; $\{1\}=V_m(T_{1,1})$
$V(T_{2,1}) \supset$ {3,4}; {1,4}, $\{2,3\}=V_m(T_{2,1})$
$V(T_{3,1}) \supset$ {4,5,6}; {1,5,6}; {2,4,6}; {3,4,5}; $\{1,3,5\}=V_m(T_{3,1})$
$V(T_{4,1}) \supset$ {5,6,7,8}; {1,6,7,8}; {2,5,7,8};
{3,5,6,8}; {4,5,6,7}; {1,3,6,8};
{1,4,6,7}; $\{2,4,5,7\}=V_m(T_{4,1})$
$V(T_{5,1}) \supset$ {6,7,8,9,10}; {1,7,8,9,10}; {2,6,8,9,10};
{3,6,7,9,10}; {4,6,7,8,10}; {5,6,7,8,9,10};
{1,7,3,9,10}; {1,4,7,8,10}; {1,5,7,8,9};
{2,4,6,8,10}; {2,5,6,8,9}; {3,5,6,7,9};
$\{1,3,5,7,9\}=V_m(T_{5,1})$.

Where $V(T_{n,1})$ is the total set of vertices of $T_{n,1}$ and $V_m(T_{n,1})$ is a subset of it including all the maximum independent sets in $T_{n,1}$. Let $N(V(T_{n,1}))\equiv\zeta_n$ be the number of such sets. We observe the following results:

$\zeta_1=2,\ \zeta_2=3,\ \zeta_3=5,\ \zeta_4=8,\ \zeta_5=13;\ \zeta_3=\zeta_1+\zeta_2;\ \zeta_4=\zeta_3+\zeta_2;\ \zeta_5=\zeta_4+\zeta_3.$

Which reminds us of the Fibonacci numbers F_2, F_3, F_4, F_5, and F_6 respectively. Actually the above set counts recur in the following general way

$$\zeta_n=\zeta_{n-1}+\zeta_{n-2}, \tag{8}$$

where

$$\zeta_n=F_{n+1}. \tag{9}$$

There are two ways of proving (8) and (9).

A. Graph-Theoretical Reasoning

Define the function f such that f: $V_m(T_{n,1})=\overline{V}_m(T_{n,1})$ where

$$\overline{V}_m(T_{n,1})=\{vi/vi\varepsilon\ V_m(T_{n,1});\ i\varepsilon\ (1,2,\cdots,n);\ \notin (n+1,\ n+2,\cdots,2n)\},$$

where vi is a vertex whose label is i. Therefore the function f maps the set $V_m(T_{n,1})$ into a set of vertices *containing only root type vertices*. The resulting initial sets are:

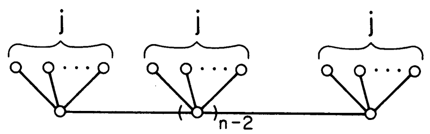
$\overline{V}_m(T_{1,1})=\{\emptyset\}$; {1}
$\overline{V}_m(T_{2,1})=\{\emptyset\}$; {1}; {2}
$\overline{V}_m(T_{3,1})=\{\emptyset\}$; {1}; {2}; {3}; {1,3}
$\overline{V}_m(T_{4,1})=\{\emptyset\}$; {1}; {2}; {3}; {4}; {1,3}; {1,4}; {2,4}
$\overline{V}_m(T_{5,1})=\{\emptyset\}$; {1}; {2}; {3}; {4}; {5};
{1,3}; {1,4}; {1,5}; {2,4};
{2,5}; {3,5}; {1,3,5}.

In general one can then write:

$\overline{V}_m(T_{n,1})=\{\emptyset\}$;
$\{1\}; \{2\}; \cdots; \{n\}$;
$\{1,3\}; \{1,5\}; \cdots; \{2,4\}; \{2,5\}; \cdots; \{i, i+2\}$;
$\{1,3,5\}; \cdots; \{j; j+2; j+4\}; \cdots$,
$\{k, k+2, k+4, k+6, \cdots\}$

The cardinalities of the above sets are nothing else but the independence numbers[5] of paths L_n. Alternatively they are simply the k-matchings of L_{n+1} (observe that L_n is the line graph[22] of L_{n+1}). The latters are indeed the graphical representations of the Fibonacci numbers[9] and since the f function is an injective (i.e. one-to-one) mapping of $V_m(T_{n,1})\rightarrow\overline{V}(T_{n,1})$ relations (8) and (9) become immediate.

The above ideas lead to the more general caterpillar



$T_{n,j}$; $j \geq 1$

Obviously,

$$\zeta(T_{n,j})=\zeta(T_{n,1});\ j\geqslant 1 \tag{10}$$

This is because

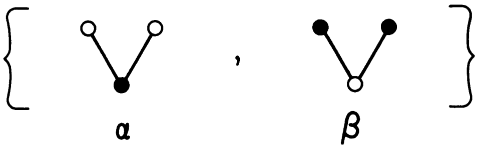
$$\overline{V}_m(T_{n,j})\equiv\overline{V}_m(T_{n,1});\ j\geqslant 1$$

Note, however, that when $j=0$ the Fibonacci recursion is lost.[17,20]

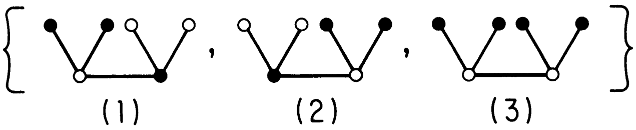
B. Coloring Method

Another method of proving the above result (Eqs. 8 and 9) uses a special coloring scheme. Thus the vertices of a $T_{n,j}$, $(j\geqslant 1)$; are colored in black and white such that (i) no two black vertices are adjacent and (ii) every white vertex is adjacent to at least one black vertex. The resulting colorings then correspond to maximal independent sets of vertices. For simplicity these indices are illustrated using $T_{n,2} \equiv T_n$ but the theory can be generalized to $T_{n,j}$.

Lemma 1. $T_{1,2} \equiv T_1$ generates two colorings, viz., α and β:



The "allowed" colorings of T_2 can be identified from lemma 1 and rules i and ii as:



All colorings of T_3 can be obtained by connecting one of the root vertices of (1)—(3) to the root vertices of α and/or β. However, because of (i), the coloring (1α) is not allowed and thus T_3 has $3\times2-1=5$ colorings. Similarly the colorings of T_n can be obtained from those of T_{n-1} and the set $\{\alpha,\beta\}$.

Theorem 1. Let ζ_n be the number of colorings of T_n. Let the number of colorings in a given set which contains a black root vertex at one (arbitrarily the right) end of the tree be β_n.

Then

$$\zeta_n = \beta_{n+2} \tag{11}$$

Proof. The set $\{\beta_{n+2}\}$ is a subset of the set of colorings $\{\zeta_{n+2}\}$ in which all root vertices at the (right) end are black. Now, because of (i), in any member of $\{\beta_{n+2}\}$ the root vertex adjacent to the one at the right end, i.e. the $(n+1)$th vertex is necessarily *white* and therefore the remaining n vertices must generate the set $\{\zeta_n\}$, i.e. $\{\zeta_n\}\varepsilon\{\beta_{n+2}\}$, and Eq. 11 is proved

Theorem 2.

$$\beta_{n+2} = \beta_{n+1} + \beta_n \tag{12}$$

Proof. Let w_n be the number of colorings in $\{A_n\}$ in which the (right) end root vertex is white. Obviously $\beta_n + w_n = \zeta_n$.

Now from rule (i) and lemma 1:

$$\zeta_{n+1} = 2\zeta_n - \beta_n$$

and

$$w_n = \beta_{n+1} = \zeta_n - \beta_n$$

$$\text{i.e. } \zeta_n = \beta_n + \beta_{n+1} = \beta_{n+2}$$

Eqs. 11 and 12 lead to Eqs. 8 and 9.

Coloring Polynomial. A counting coloring polynomial, $\xi(T_{n,j}; x)$ is conveniently defined by

$$\xi(T_{n,j}; x) = \sum_{r}^{m} \theta(r) x^r, \tag{13}$$

where $\theta(r)$ is the number of colorings of $T_{n,j}$ containing r black vertices and m is the maximum value of r. Then $\xi(T_{n,j}; 1) = \zeta_n$. Inspection of the first few coloring polynomials of any $T_{n,j}$, $j \geqslant 1$, induces Eq. 14, viz.,

$$\xi(T_{n,j}; x) = \sum_{k=0}^{[n/2]} \binom{n-k}{k} x^{mn-(m-1)k} \tag{14}$$

As a corollary when $j=1$ the above function becomes simply a monomial in x.

A Special Class of Benzenoid Hydrocarbons. Figure 2 shows a homologous series of benzenoid hydrocarbons denoted as $B(T_{n,1})$'s. The number of Clar structures in which maximum numbers of hexagons are assigned to have resonant sextets of this series conforms to Eqs. 8 and 9. In principle homologation can be extended infinitely, although the polyhex graph

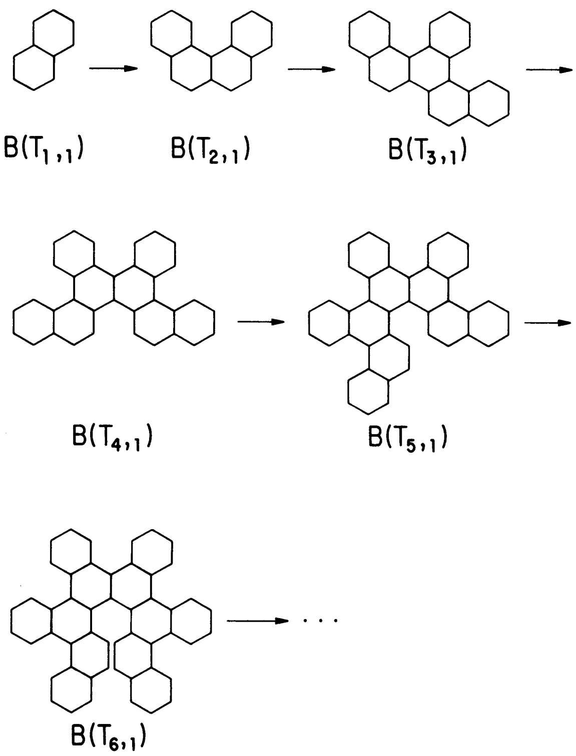


Fig. 2. A homologous series of benzenoid hydrocarbons. The Clar counts, ξ, of the individual members are Fibonacci numbers i.e. $\xi(B(T_{j,1})) = F_{j+1}$.

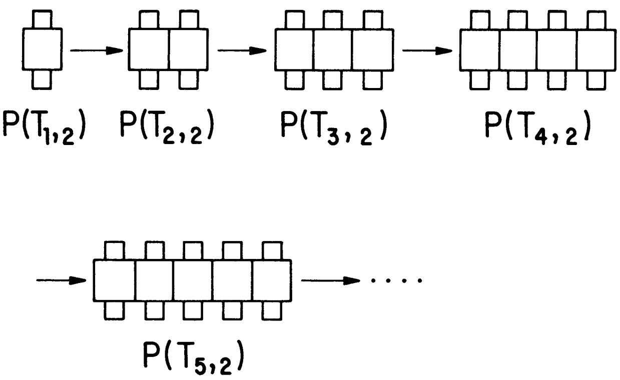


Fig. 3. A homologous series of "bidentate" polyomino graphs. Every graph corresponds to a caterpillar tree $T_{n,2}$, $n=1, 2, 3, 4, 5\cdots$. Relation to other objects is shown in Fig. 4.

above $B(T_{6,1})$ is no long planar. It is interesting to notice that

$$D(B(T_{n,1}))=T_{n,1}$$

where D(G) is the dualist graph[23] of G.

On King Patterns. Motoyama and Hosoya[7] were the first to define king polynomials and king patterns for lattices and polyomino graphs and showed their potential in dimer statistics and the problem of Kekulé count in chemistry. Balasubramanian and Ramaraj[6] demonstrated recently the equivalence between king polynomials and what they called color polynomials[6] of the dualist graphs of the appropriate lattice type. Figure 3 shows a special type of polyomino which corresponds to $T_{n,2}$. But extension to any $T_{n,j}$ is possible. Their king patterns are Fibonacci numbers.

Correspondence with King Pattern,[7] Domino Pattern,[7] and the Matching Pattern.[1,24] A king pattern, {K}, is simply a way of placing kings (circles) on chessboard so that no two kings can take each other. A Kekulé pattern (or dimer pattern), {M}, can be generated by identifying the cells in the chessboard that contain kings as the vertical bonds in the dimer pattern and the empty cells as horizontal bonds (cf. Fig. 4). A "domino pattern," {D}, can also be obtained from the dimer pattern by paving horizontal and vertical rectangles which correspond to horizontal and vertical dimers in the dimer pattern. These relations are depicted in Fig. 4. The set {ζ} is nothing else but the dualist graphs[23] corresponding to the modified polyominos, {P}. Hence one can define two rules of placing kings (circles) in {P} analogous to coloring rules (i), (ii), viz.,

(i′) No two kings are allowed to occupy adjacent cells.

(ii′) Every empty cell is adjacent to at least one occupied cell.

The resulting patterns generate Fibonacci numbers. The last set in Fig. 4, {L}, shows the corresponding matchings in path L_4. The following interesting relation is observed. Let $d\{K_i\}$ be the dualist graph[23] of a

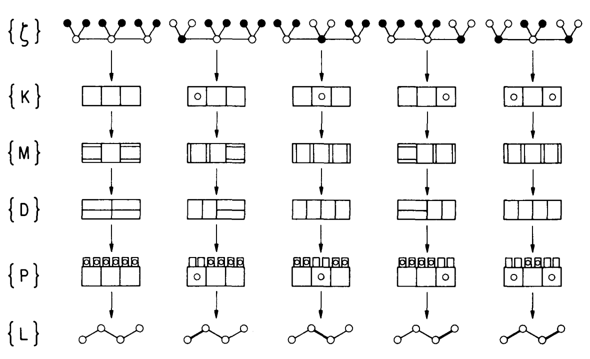


Fig. 4. Fibonacci colorings of $T_{2,2}$ and the corresponding patterns in chemistry and physics. The set {K} is the king pattern, {M} is the dimer pattern, {D} the domino pattern and {P} is a special polyomino pattern. The set {L} is the matchings of L_4.

member K_i from set {K}, and $L\{L_i\}$ be the line graph[25] of the corresponding member L_i, then

$$d\{K_i\}=L\{L_i\}. \tag{15}$$

The last relation is significant since it is well known that the matching polynomials of the paths may be written as Chebyshev polynomials[26] in $(x/2)$.

Fibonacci numbers have been identified for the first time as maximal independence sets of vertices of certain caterpillar trees. Mappings of such sets to well known topological functions such as perfect matchings of a path as well as certain king patterns are discovered.

The author thanks the U.S. Office of Naval Research for partial support of this work. Illuminating remarks of Professor R. B. King are greatly appreciated. Travel assistance from the Fullbright Commission in Cairo is acknowledged.

References

1) H. Hosoya, *Bull. Chem. Soc. Jpn*, **44**, 2332 (1971).

2) H. Hosoya, "Mathematics and Computational Concepts in Chemistry," Ellis Horwood (1986).

3) H. Hosoya and T. Yamaguchi, *Tetrahedron Lett.*, **1975**, 4659.

4) E. Clar, "The Aromatic Sextet," John Wiley, New York (1972). A nice review is found in I. Gutman, *Bull. Soc. Chim. Beograd*, **47**, 453 (1982).

5) I. Gutman, *Z. Naturforsch.*, **37a**, 69 (1982); I. Gutman and S. El-Basil, *ibid.*, **39a**, 276 (1984).

6) K. Balasubramanian and R. Ramaraj, *J. Comput. Chem.*, **6**, 447 (1985).

7) A. Motoyama and H. Hosoya, *J. Math. Phys.*, **18**, 1485 (1977).

8) J. Riordan, "An Introduction to Combinatorial Analysis," Wiley, New York (1958), Chaps. 7 and 8.

9) H. Hosoya, *The Fibonacci Quarterly*, **11**, 255 (1973); **14**, 173 (1974).

10) T. J. Rivlin, "The Chebyshev Polynomials," John Wiley, New York (1974).

11) A. T. Balaban and I. Tomescu, *Croat. Chem. Acta*, **57**, 391 (1984); *Match*, **17**, 91 (1985).

12) H. Hosoya, *Comp. Maths. Appls.*, **12B**, 271 (1986).

13) W. C. Herndon and M. L. Ellzey Jr., *J. Am. Chem. Soc.*, **96**, 6631 (1974).

14) M. Randić, *J. Am. Chem. Soc.*, **99**, 444 (1977); *Tetrahedron*, **33**, 1905 (1977).

15) I. Gutman and S. El-Basil, *Chem. Phys. Lett.*, **115**, 416 (1985).

16) N. Christofides, "Graph Theory, An Algorithmic Approach," Academic Press, New York (1975), Chap. 3.

17) S. El-Basil, *Theor. Chim. Acta*, **70**, 53 (1986).

18) S. El-Basil, *Bull. Chem. Soc. Jpn.*, **56**, 3152 (1983).

19) W. C. Herndon and H. Hosoya, *Tetrahedron*, **40**, 3987 (1984).

20) S. El-Basil, *Disc. Appl. Math.*, (1986) in press.

21) F. Harary and A. J. Schwenk, *Discrete Math.*, **6**, 359 (1973).

22) F. Harary, "Graph Theory," Addison-Wesley, Reading (1969), Chap. 8.

23) C.f., A. T. Balaban and F. Harary, *Tetrahedron*, **24**, 2505 (1968).
24) Actually the first contributions to the theory of matching came from statistical physics: O. J. Heilmann and E. H. Lieb, *Phys. Rev. Lett.*, **24**, 1412 (1970); *Commun. Math. Phys.*, **25**, 190 (1972); H. Kunz, *Phys. Lett.*, **32A**, 311 (1970); C. Gruber and H. Kunz, *Commun. Math. Phys.*, **22**, 133 (1971).
25) Line graphs are defined in: F. Harary, "Graph Theory," Addison-Wesley Publishing Company, Reading, Mass. (1972), p. 71.
26) T. J. Rivilin, "The Chebyshev Polynomials," John Wiley, New York (1974).