Pell Equation. III. Graph-theoretical meaning of the solutions of the Pell equation through topological index Z

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Abstract For a non-directed graph G composed of vertices and edges the topological index Z_G has been defined by the present author as the total sum of perfect and imperfect matchings. The Z_G values of several typical series of graphs have been known to be equal to Fibonacci, Lucas, and Pell numbers. In this paper the solutions of Pell equation $x^2-Dy^2=\pm N$ for special values of D with N=1 and 4 are shown to give these series of numbers, which means that this is the first graphical or graph-theoretical interpretation of the solutions of Pell equation. In this analysis the Chebyshev polynomials of the first and second kinds, T_n and U_n, together with their modified version, C_n and S_n, are involved. For any D with N=1 and 4, there were found certain series of graphs whose Z_G values just represent the solutions of Pell equation.

1. Introduction

We have been studying the mathematical structure of the solutions of Pell equation of various types, or Pellep-N[1,2)]

$$x^2 - D\,y^2 = \pm N \qquad \text{(Pellep-N)}, \tag{1.1}$$

especially for N=1 and 4. There i) regardless of the chaotic behavior of the solutions of Pell equation a majority of D values can systematically be grouped into several types, and ii) the family of solutions for a given D are explicitly expressed in terms of the Chebyshev polynomials of the first and second kinds.

On the other hand, the present author has proposed the topological index Z_G[3-5)] for characterizing a graph which is composed of sets of vertices and edges, and has recently succeeded in clarifying mathematical structure of various algebras related to elementary mathematics and number theory, such as Fibonacci and Lucas numbers, Pell numbers, Pascal's triangle, Pythagorean and Heronian triangles, *etc.*[6)] Further, It was found that the solutions of Pell equations are closely related to the above-mentioned numbers and mathematical concepts through Z_G, representing some series of relatively simple graphs. For example, the families of solutions of (1.1) with N=4 and D=5 and 8 are nothing else but the Z_G values of the series of path, cycle, and some other graphs, which take Fibonacci, Lucas, Pell, and related numbers. In this paper, the concept and algorithms relevant to the topological index Z_G will be introduced, and newly obtained graph-theoretical interpretation of the solutions of Pell equation will be demonstrated. Further, a novel role of Z_G will be discussed as a new powerful tool for relating algebra and geometry.

However, before introducing the topological index, let us recall several series of numbers, such as Fibonacci, Lucas, Pell, *etc.*, which will play an important role in this paper, together with various series of graphs. Those graphs will also be introduced here.

2. Series of Numbers and Graphs

2.1. Two classes of series of numbers

First define two sets of series of numbers which obey the following recursive relations

$$f_n = (a+1) f_{n-1} + f_{n-2} \qquad (a=0\sim3) \tag{2.1}$$

with the initial conditons as

$$\text{Class A:} \quad f_0 = 1 \quad \text{and} \quad f_1 = a+1 \tag{2.2}$$

$$\text{Class B:} \quad f_0 = 2 \quad \text{and} \quad f_1 = a+1. \tag{2.3}$$

The numbers with a=0 in Classes A and B are, respectively, the Fibonacci (F_n) and Lucas (L_n) numbers. Note, however, that for Class A, different initial conditions are conventionally used as

$$f_0 = 0 \quad \text{and} \quad f_1 = 1 \quad \text{(conventional Fibonacci and Pell numbers).} \tag{2.4}$$

Table 1. Two classes of series of numbers.

a	n	0	1	2	3	4	5	Class
0	F_n	1	1	2	3	5	8	A
	L_n	2	1	3	4	7	11	B
1	P_n	1	2	5	12	29	70	A
	Q_n	2	2	6	14	34	82	B
2	v_n	1	3	10	33	109	360	A
	x_n	2	3	11	36	119	393	B
3	w_n	1	4	17	72	305	1292	A
	y_n	2	4	18	76	322	1364	B

Two series of numbers with a=1, Pell (P_n) and Pell-Lucas (Q_n) numbers,[7,8] respectively, belong to Classes A and B. Also in the case of Pell numbers the initial conditions of (2.4) are conventionally used.[7-11] The merit or advantage of the initial conditions (2.2) for Fibonacci and Pell numbers will gradually be demonstrated. In Table 1 eight series of numbers from a=0 to 3 are given, where two more pairs of series of numbers (v_n, x_n) with a=2 and (w_n, y_n) with a=3 are added.

2.2 Various series of graphs

Path graph S_n is the most fundamental series of graphs, which is composed of consecutively connected n vertices with n–1 edges. By adding a unit edge to each of the vertices of S_n one gets a comb graph U_n. Then by adding a pair and triplet of unit edge to each of the vertices of S_n one gets, respectively, graphs V_n and W_n. These four series of tree graphs are shown in Fig. 1

Although the smallest polygon is triangle, here let us define a series of "monocyle graphs" $\{C_n\}$ beginning from n=1 as shown in Fig. 1. C_2 may be called "digon" composed of a pair of vertices and two edges connecting them. C_1 is not "monogon" without an edge but is equivalent to a vertex. These two graphs do not seem to fit into the category of polygon, but later it will be shown that they smoothly fit into the algebraic structure involved not only in Pell equation but also in other recursive relations treated in this paper through the topological index Z_G. The main bodies of the four series of graphs, C_n, CU_n, CV_n, and CW_n, are non-tree.

In Fig. 1 the topological indices Z_G's of all the eight series of graphs are also given. It is to be noted that all the Z_G's of tree graphs, S_n, U_n, V_n, and W_n, are, respectively, identical to the series of numbers in Class A, F_n, P_n, v_n, and w_n, while the Z_G's of non-tree graphs, C_n, CU_n, CV_n, and CW_n, are, respectively, identical to Class B, L_n, Q_n, x_n, and y_n. No entry for n=0 is defined in non-tree graphs, while in all the tree graphs the entry for n=0 is vacant graph, whose Z_G is unity by definition. The most important conclusion derived from Fig. 1 is that for several well known series of numbers one can find their geometrical counterparts as graphs. It will be shown that this is also the case with other series of numbers if some mathematical condition is satisfied.

Then look at Fig. 2 showing the lower members of the families of solutions of four Pellep-4 with D=5, 8, 13, and 20 (but not 21!). Amazingly, all the non-tree graphs and numbers in Fig. 1 and n=0~4 members of tree graphs therein are appearing. A question arises. Do the solutions of Pellep-4 with any other D value or of general Pellep-N or Pell-N have this kind of graphical or graph-theoretical counterparts? At the present stage of our research the answer is yes at least for N=1 and 4. Now brief explanation of Z_G will be given.

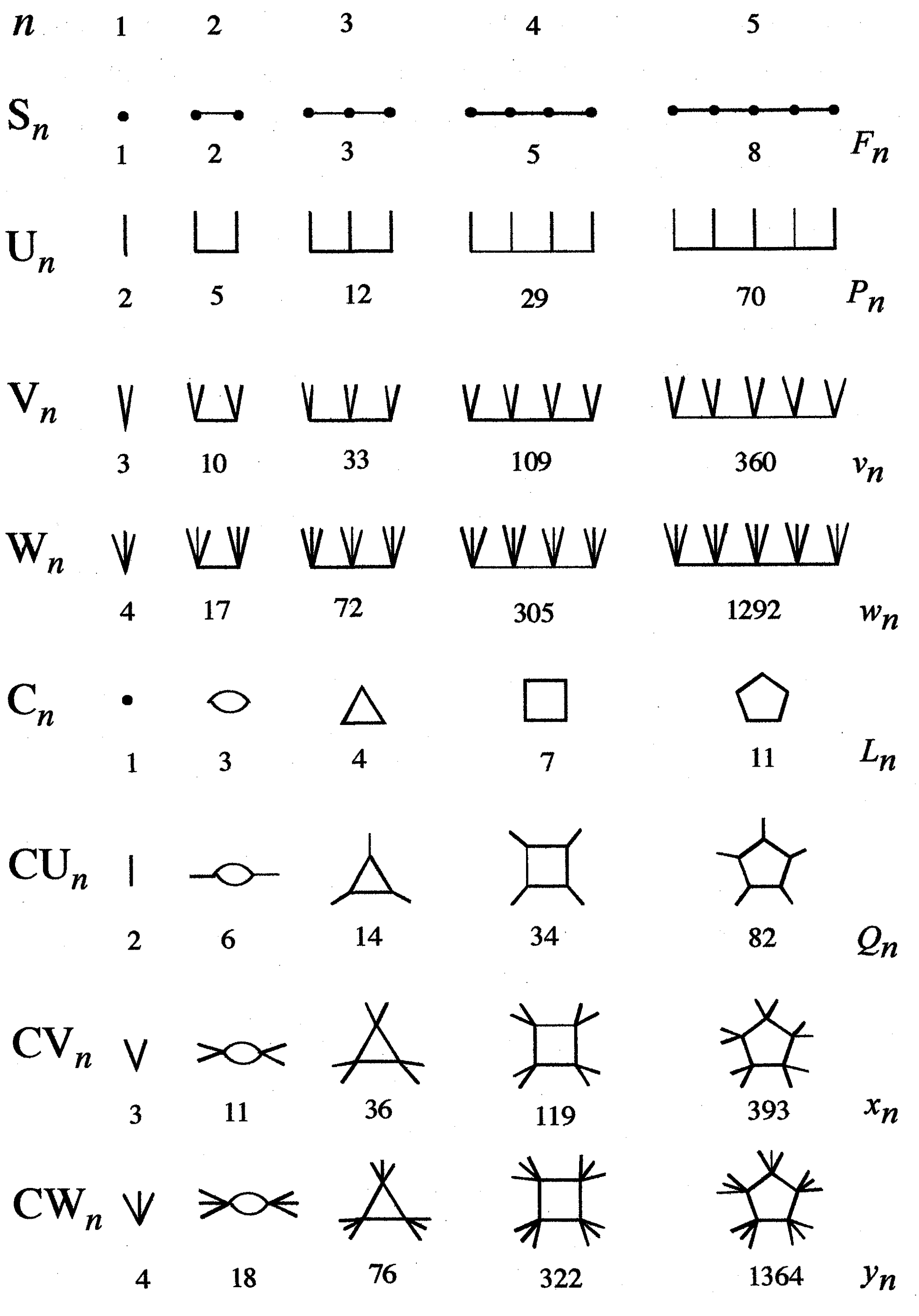


Fig. 1 Various series of graphs derived from path (S_n) and monocycle (C_n) graphs, and their topological indices Z_G corresponding to Fibonacci (F_n), Lucas (L_n), Pell (P_n), Pell-Lucas (Q_n) numbers, *etc.*

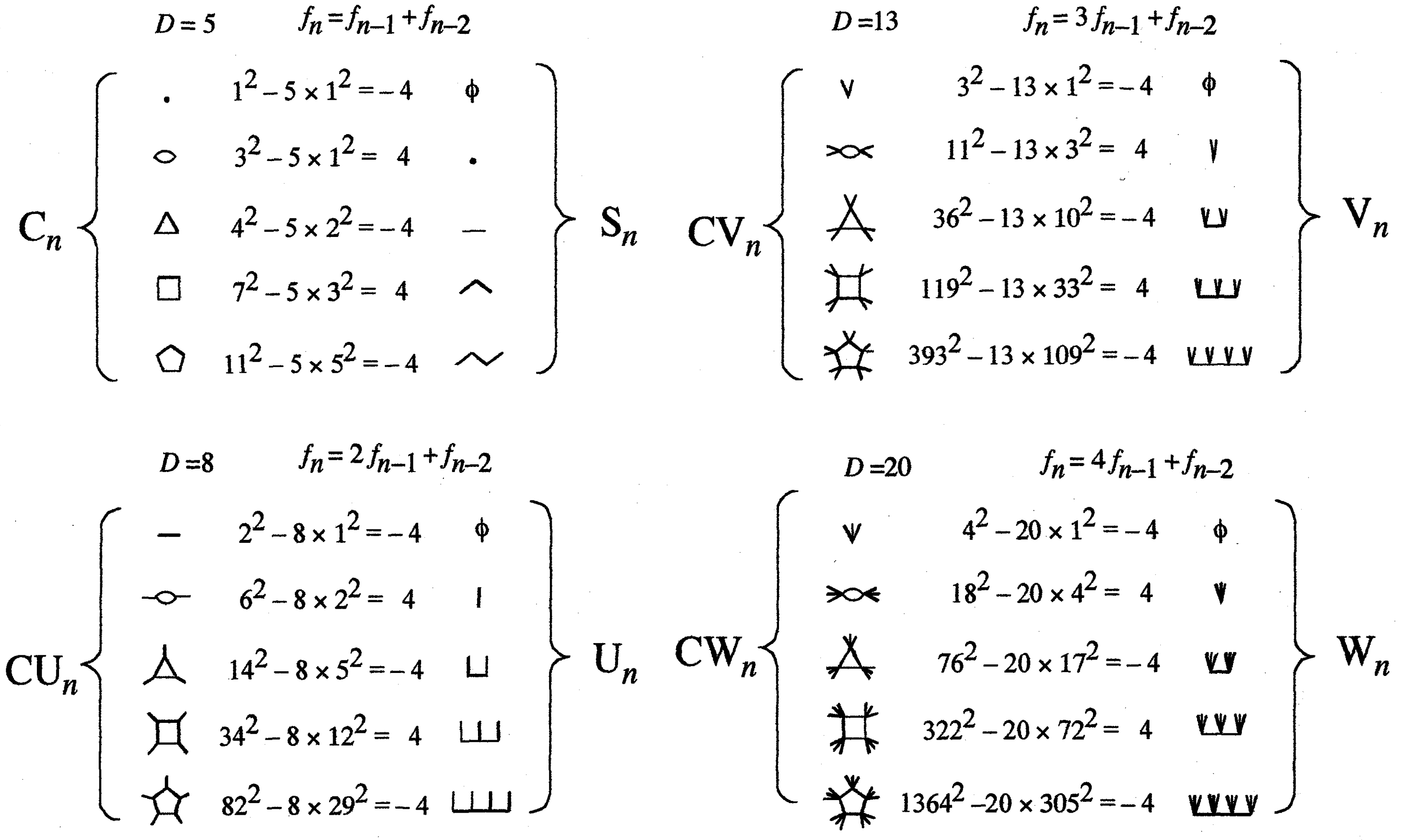


Fig. 2 Solutions of Pellep-4 for D=5, 8, 13, and 20, together with the series of graphs whose Z_G's just correspond to them. *cf.* Fig. 1.

3. Topological Index

Graph-theoretical concepts used here are those which have conventionally been approved.[12-14] All the graphs treated here except for "digon" are non-directed and simply connected. The number of ways for choosing k disjoint edges from a given graph G is defined as the *non-adjacent number* $p(\mathrm{G},k)$.[3,4] Here $p(\mathrm{G},0)$ is defined as unity for any G including vacant graph, and $p(\mathrm{G},1)$ is equal to the number of edges of G.

By using the set of $p(\mathrm{G},k)$'s for G the *Z-counting polynomial* $\mathrm{Q_G}(x)$ is defined as

$$\mathrm{Q}_G(x) = \sum_{k=0}^{m} p(G,k)\, x^k \quad , \tag{3.1}$$

where m is the maximum number of k, or $m = \lfloor N/2 \rfloor$ with N being the number of vertices of G. Total sum of $p(\mathrm{G},k)$'s for a given G is defined as the *topological index* Z_G as

$$Z_\mathrm{G} = \sum_{k=0}^{m} p(G,k) = \mathrm{Q}_G(1) \quad . \tag{3.2}$$

In other words, Z_G is the total sum of perfect and imperfect matchings.

By using the adjacency matrix **A** and unit matrix **I** of the same size the characteristic polynomial for G with N vertices is defined as[12-14]

$$\mathrm{P_G}(x) = (-1)^N \det(\mathbf{A} - x\mathrm{I}) . \tag{3.3}$$

For tree graphs the coefficients of $\mathrm{P_G}(x)$ exactly coincide with the set of $p(\mathrm{G},k)$'s as[3,4]

$$\begin{aligned} \mathrm{P_T}(x) &= \sum_{k=0}^{N} a_k x^{N-k} \\ &= \sum_{k=0}^{m} (-1)^k p(\mathrm{T},k)\, x^{N-2k} \quad (\mathrm{T : tree}) \end{aligned} \tag{3.4}$$

and then we have

$$\begin{aligned} Z_\mathrm{T} &= (-1)^N \mathrm{P_T}(i) \\ &= \sum_{k=0}^{m} |a_k| \quad (\mathrm{T : tree}) \end{aligned} \quad . \tag{3.5}$$

For non-tree graphs $\mathrm{P_G}(x)$ can be expressed by the set of $p(\mathrm{G},k)$'s for G and its subgraphs obtained by deleting the component rings.[15)]

For the series of S_n and C_n the $p(G,k)$'s are given by[3,4)]

$$p(S_n,k) = \binom{n-k}{k} \tag{3.7}$$

$$p(C_n,k) = \frac{n}{n-k}\binom{n-k}{k} . \tag{3.8}$$

These numbers and Z_G's are given in Table 2. The general forms of Z-counting polynomials $Q_G(x)$

Table 2 $p(G,k)$ and Z_G values of (a) path S_n and (b) monocycle C_n graphs

(a)		$p(G,k)$					
n	G	k=0	1	2	3	4	Z_G
1	•	1					1
2		1	1				2
3		1	2				3
4		1	3	1			5
5		1	4	3			8
6		1	5	6	1		13
7		1	6	10	4		21
8		1	7	15	10	1	34

(b)		$p(G,k)$					
n	G	k=0	1	2	3	4	Z_G
2		1	2				3
3		1	3				4
4		1	4	2			7
5		1	5	5			11
6		1	6	9	2		18
7		1	7	14	7		29
8		1	8	20	16	2	47

and Z_G's for these graphs are given by

$$Q_{S_n}(x) = \sum_{k=0}^{m} \binom{n-k}{k} x^k \tag{3.9}$$

$$Q_{C_n}(x) = \sum_{k=0}^{m} \frac{n}{n-k} \binom{n-k}{k} x^k , \tag{3.10}$$

$$Z_{S_n} = Q_{S_n}(1) = \sum_{k=0}^{m} \binom{n-k}{k} \tag{3.11}$$

$$Z_{C_n} = Q_{C_n}(1) = \sum_{k=0}^{m} \frac{n}{n-k} \binom{n-k}{k} . \tag{3.12}$$

That Fibonacci numbers can be obtained by adding the elements of Pascal's triangle has long been known.[10,14] However, its graph-theoretical interpretation including the meaning of each element of Pascal's triangle was first reported by the present author.[4] Rotate Table 2a counterclockwise by 45 degree, and shift each row one by one, then a Pascal's triangle will appear. From Table 2b another triangle, namely, asymmetrical Pascal's triangle will come out, which is obtained by adding a pair of Pascal's triangle.[16] Refer to Ref. 16 for its interesting mathematical properties and features.

Further, for U_n and CU_n graphs, we have

$$Q_{U_n}(x) = \sum_{k=0}^{m} \binom{n-k}{k} (1+x)^{n-2k} x^k \tag{3.13}$$

$$Q_{CU_n}(x) = \sum_{k=0}^{m} \frac{n}{n-k} \binom{n-k}{k} (1+x)^{n-2k} x^k \tag{3.14}$$

$$Z_{U_n} = Q_{U_n}(1) = \sum_{k=0}^{m} 2^{n-2k} \binom{n-k}{k} \tag{3.15}$$

$$Z_{CU_n} = Q_{CU_n}(1) = \sum_{k=0}^{m} 2^{n-2k} \frac{n}{n-k} \binom{n-k}{k} . \tag{3.16}$$

For the pairs of (V_n, CV_n) and (W_n, CW_n) graphs one needs to replace $(1+x)$ in $Q_G(x)$ with $(1+ax)$ and 2 in Z_G with $1+a$. The reason for these tricks comes from the property of the counting polynomial $Q_G(x)$.

Although the definition of $p(G,k)$ is simple, calculation for large graphs will knock against the wall of combinatorial explosion. To overcome this situation several recursive relations have been found and worked out.[3,4] Here only the fundamental recursive relation for $p(\mathrm{G},k)$, $\mathrm{Q_G}(x)$, and Z_G are given.

$$p(\mathrm{G},k) = p(\mathrm{G}-l,k) + p(\mathrm{G}\ominus l,k-1) \tag{3.17}$$

$$\mathrm{Q_G}(x) = \mathrm{Q}_{\mathrm{G}-l}(x) + x\,\mathrm{Q}_{\mathrm{G}\ominus l}(x) \tag{3.18}$$

$$Z_\mathrm{G} = Z_{\mathrm{G}-l} + Z_{\mathrm{G}\ominus l}, \tag{3.19}$$

where G–l is a subgraph of G obtained by deleting edge l from G, and further by deleting all the edges which were incident to l one gets G⊖l. Several examples for using them will be given in Appendix.

4. Analysis of Pellep-4

Already in our analysis it was shown that all the families of solutions of Pell-4 and Pellep-4 can generally be expressed in terms of the modified Chebyshev polynomials of the first and second kinds and their conjugate versions as follows:

Pell-4	Pellep-4
$x_n = C_n(x_1)$	$t_n = C^*_n(t_1)$
$y_n = y_1 S_{n-1}(x_1)$	$u_n = u_1 S^*_{n-1}(t_1)$

(4.1)

Although there have been proposed several different definitions, the following polynomials forms are convenient in this discussion.

Modified Chebyshev polynomials:[17,18]

1st kind
$$C_n(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k \frac{n}{n-k}\binom{n-k}{k} x^{n-2k} \quad (n>0) \tag{4.2}$$

2nd kind
$$S_n(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k \binom{n-k}{k} x^{n-2k} \quad (n\geq 0) \tag{4.3}$$

and their conjugate forms,

1st kind
$$C^*_n(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{n}{n-k}\binom{n-k}{k} x^{n-2k} \quad (n>0) \tag{4.4}$$

2nd kind
$$S^*_n(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n-k}{k} x^{n-2k} \quad (n\geq 0). \tag{4.5}$$

In Table 3 lower members of $C_n(x)$ and $S_n(x)$ are given. Their conjugate forms are obtained just by changing all the negative signs into positive ones.

It has already been shown by the present author that the Lucas L_n and Fibonacci numbers F_n can be obtained from $C_n(x)$ and $S_n(x)$ as follows:[19)]

$$C_n(i) = i^n L_n, \tag{4.6}$$

$$S_n(i) = i^n F_n. \tag{4.7}$$

However, notice that the initial conditions (2.2) of F_n are different from the conventional ones (2.4) but shifted as explained before. These relations are more simply transformed into their conjugates as,

$$C^*_n(1) = L_n, \tag{4.8}$$

$$S^*_n(1) = F_n. \tag{4.9}$$

Further, one can get interesting results by putting x=2, 3, and 4 into S^*_n and C^*_n as

$$S^*_n(2) = P_n, \quad S^*_n(3) = v_n, \quad S^*_n(4) = w_n, \quad (n \geq 0) \tag{4.10}$$

$$C^*_n(2) = Q_n \quad C^*_n(3) = x_n \quad C^*_n(4) = y_n \quad (n>0)\,. \tag{4.11}$$

This means that $S^*_n(x)$ represents the series of graph obtained by joining x–1 unit edges to each vertex of graph S_n. This result is very important for transforming the general algebraic solution of Pellep-4 into the geometric representation. Then try to find the corresponding recipe for the solution of Pell-4.

Table 3. Modified Chebyshev polynomials of the first and second kinds

1st kind	2nd kind
$C_0(x) = 2$	$S_0(x) = 1$
$C_1(x) = x$	$S_1(x) = x$
$C_2(x) = x^2 - 2$	$S_2(x) = x^2 - 1$
$C_3(x) = x^3 - 3x$	$S_3(x) = x^3 - 2x$
$C_4(x) = x^4 - 4x^2 + 2$	$S_4(x) = x^4 - 3x^2 + 1$
$C_5(x) = x^5 - 5x^3 + 5x$	$S_5(x) = x^5 - 4x^3 + 3x$
$C_6(x) = x^6 - 6x^4 + 9x^2 - 2$	$S_6(x) = x^6 - 5x^4 + 6x^2 - 1$

First prepare Table 4 giving the values of $S_n(x)$ and $C_n(x)$ for x=2~6. Both the series of numbers, $S_n(x)$ and $C_n(x)$, with a fixed x value are found to obey the following recursive relation:

$$f_n = x f_{n-1} - f_{n-2}\,. \tag{4.12}$$

By taking into account this relation it was not so difficult to obtain several series of graph whose Z_G values just correspond to the numbers given in Table 4. The results for $S_n(x)$ and $C_n(x)$ with x=3~6 are shown in Fig. 3, which gives us a hint for transforming the solution of Pellep-4 into geometry.

Now one can get the universal recipe for representing the family of solutions of Pell-4 and Pellep-4 both in algebraic and geometric (or graph-theoretical) forms. Once the smallest solution (x_1, y_1) for the case with no Llep-4 solution or the smallest solution (t_1, u_1) for the case of Pellep-4 is obtained, all the family of solutions can systematically be obtained as numbers and/or graphs by using the recipe illustrated as in Fig. 4.

Table 4. The values of $S_n(x)$ and $C_n(x)$ for x=2~6

x =	2	3	4	5	6
$S_1(x)$	2	3	4	5	6
$S_2(x)$	3	8	15	24	35
$S_3(x)$	4	21	56	115	204
$S_4(x)$	5	55	209	551	1189
$C_1(x)$	2	3	4	5	6
$C_2(x)$	2	7	14	23	34
$C_3(x)$	2	18	52	110	198
$C_4(x)$	2	47	194	527	1154

Although two series of non-tree graphs are involved in Fig. 4, they can be replaced by other series of tree graphs, but of less symmetrical shape. Discussion of this problem will be given elsewhere.

5. Analysis of Pellep-1

In the preceding paper of this series[2)] the general expressions for the family solutions of Pell-1 and Pellep-1are also given as

Pell-1	Pellep-1
$x_n = T_n(x_1)$	$t_n = T^*_n(t_1)$
$y_n = y_1 U_{n-1}(x_1)$	$u_n = u_1 U^*_{n-1}(t_1)$,

(5.1)

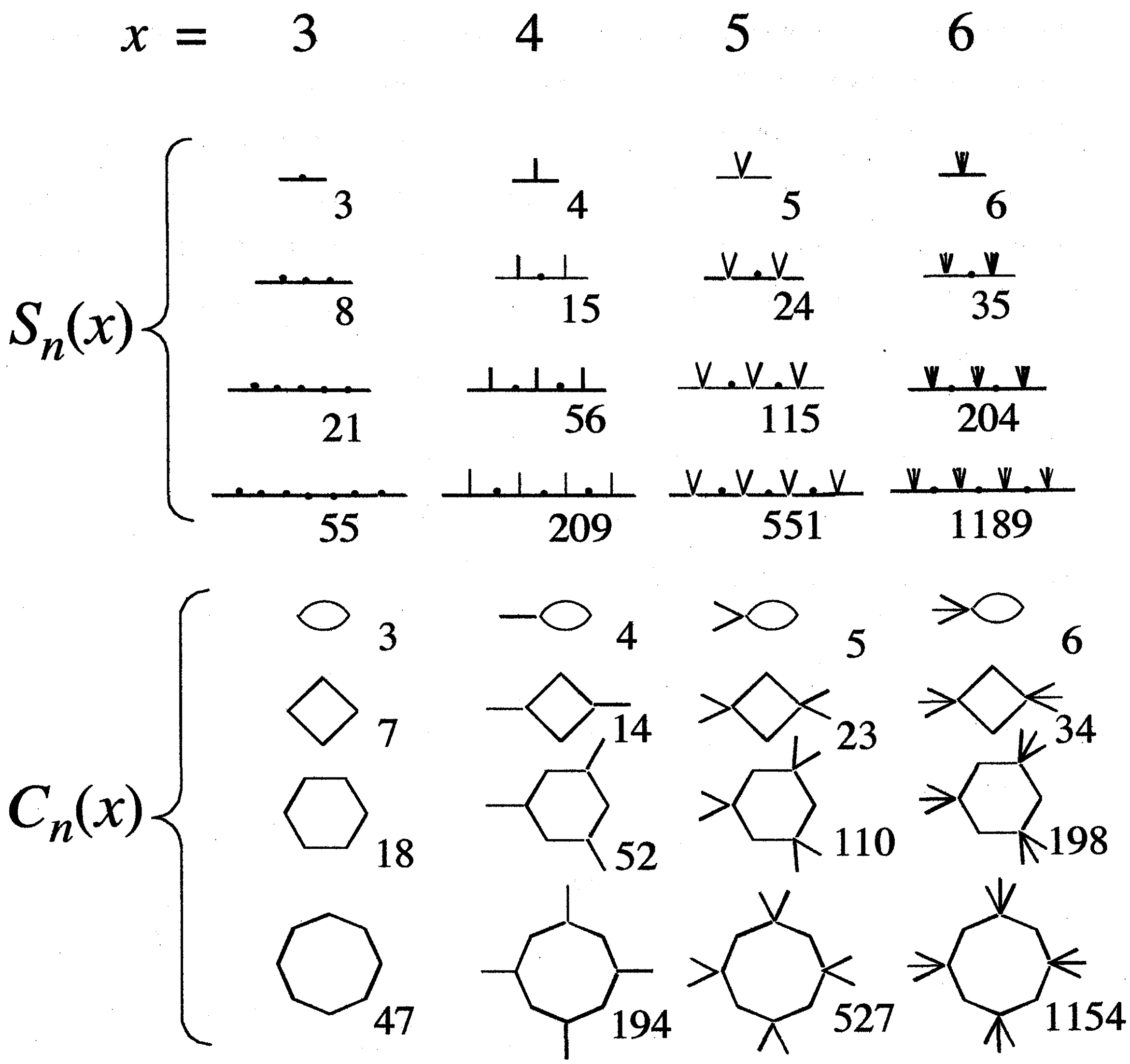


Fig. 3 Eight series of graphs whose Z_G just correspond to the values of modified Chebyshev polynomials of the first ($C_n(x)$) and second ($S_n(x)$) kinds given in Table 4.

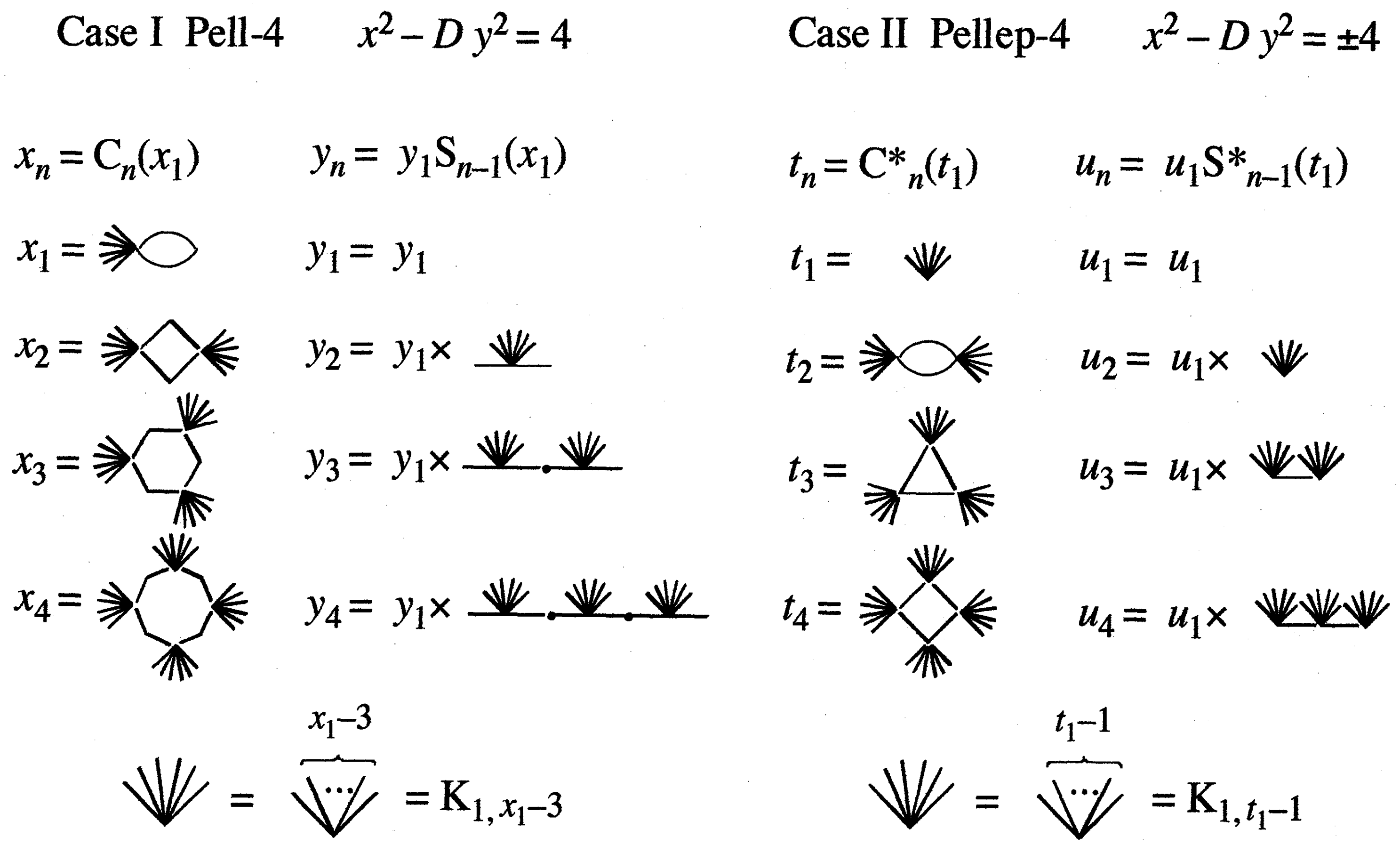


Fig. 4 General recipe for obtaining the series of graphs whose Z_G's just correspond to the family of solutions of Pell-4 and Pellep-4.

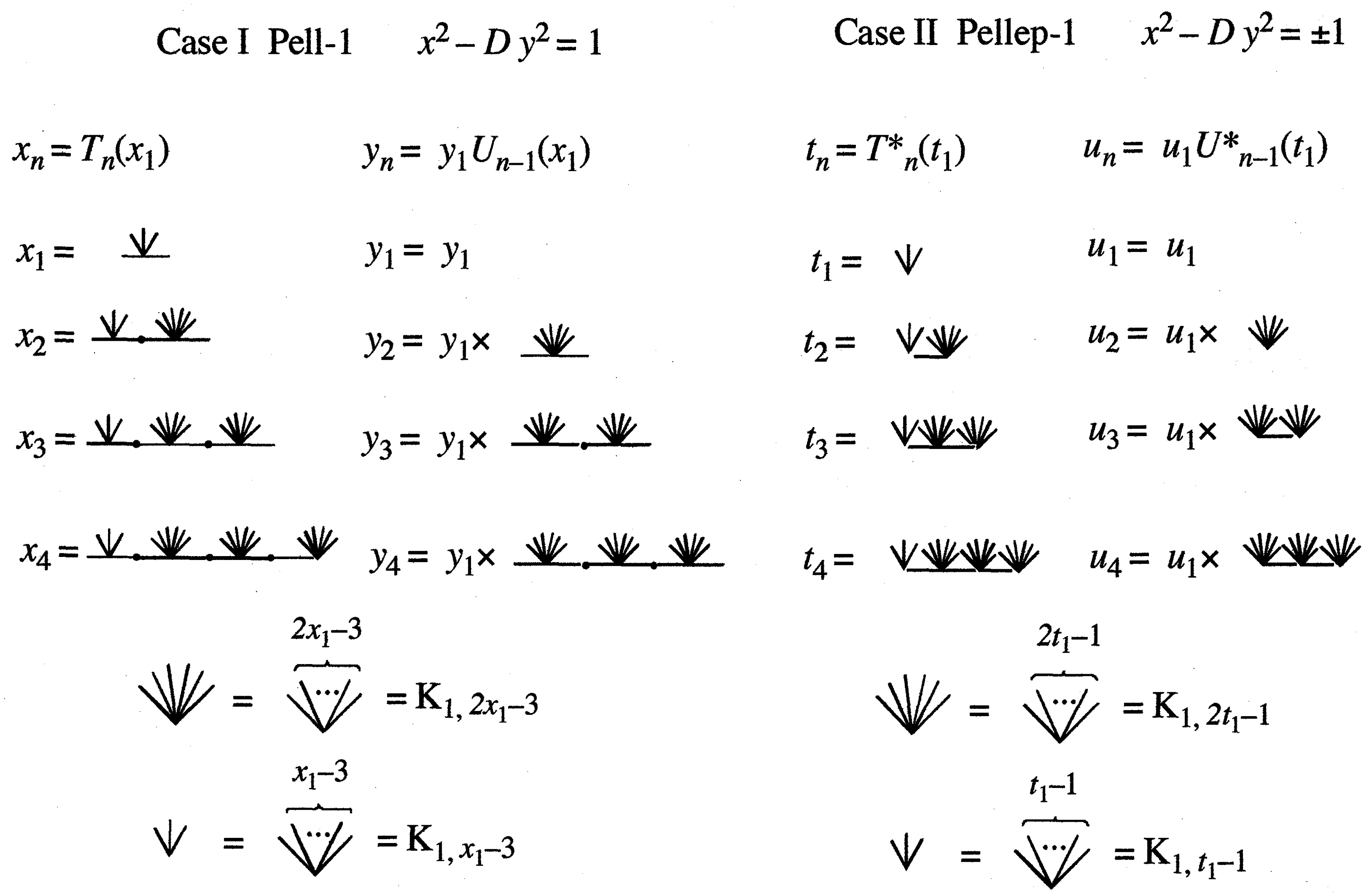


Fig. 5 General recipe for obtaining the series of graphs whose Z_G's just correspond to the family of solutions of Pell-1 and Pellep-1.

where T_n and U_n are the Chebyshev polynomials of the first and second kinds, respectively, and T^*_n and U^*_n are also their conjugate forms. The explicit forms are not given here, because they are easily available.[14,17,18] By doing similar analysis one can obtain the universal recipe for representing the family of solutions of Pell-1 and Pellep-1 both in algebraic and geometrical forms but a little less symmetrical than the case with Pell-4 and Pellep-4 (See Fig. 5). Anyway one can enjoy beautiful mathematics among seemingly chaotic solutions of the Pell equation. Work is in progress toward the general Pellep-N solutions.

Appendix

Fundamental recursive equation

For explaining the recursive relation of $p(\mathrm{G},k)$ numbers two kinds of subgraphs, G–l and GΘl, of G are necessary, which was already introduced in (3.17)-(3.19) as illustrated in Fig. A1. Recall that the $p(\mathrm{G},k)$ number is the number of ways for choosing k disjoint edges from G. This number is the sum of the two sets of counting, the one including a given edge l and the other excluding it. The former number can be obtained by choosing k–1 edges from GΘl, while the latter number is the contribution from graph G–l. The first and second terms of the right-hand-side of (3.17) are, respectively, l-exclusive and l-inclusive contributions. This idea comes from the inclusion-exclusion principle, which is one of the main principles frequently used in the enumeration problems in discrete mathematics, such as graph theory and combinatorics. In the case of $Q_G(x)$ the second term has a factor x meaning that one edge out of k disjoint edges is already reserved.

Let us show two examples for using these recursive relations. See Fig. A2a for comb graph, U_4. Choose the central edge as l, and one gets a pair of U_2=S_4 as G–l and a pair of U_1=S_2 as GΘl. Then we have

$$\begin{aligned} Q_{U4}(x) &= [Q_{S4}(x)]^2 + x\,[Q_{S2}(x)]^2 \\ &= (1 + 3x + x^2)^2 + x\,(1 + x)^2 \\ &= 1 + 7x + 13x^2 + 7x^3 + x^4 \end{aligned}$$

$$Z_{U4} = Z_{S4}^{\;2} + Z_{S2}^{\;2} = 5^2 + 2^2 = 29,$$

which belongs to the Pell numbers.

Next consider gear graph CU_4. By choosing any edge forming a square as l, its G–l and GΘl, respectively, become U_4 and U_2. Then we have

$$\begin{aligned} Q_{CU4}(x) &= Q_{U4}(x) + x\, Q_{U2}(x) \\ &= (1 + 7x + 13x^2 + 7x^3 + x^4) + x(1 + 3x + x^2) \\ &= 1 + 8x + 16x^2 + 8x^3 + x^4 \end{aligned}$$

$$Z_{CU4} = Z_{U4} + Z_{U2} = 29 + 5 = 34.$$

Worked out examples for the solution of Pell-4

See Fig. A3, where four series of graph, A_n, B_n, C_n, and D_n, are shown with their $Q_G(x)$ and Z_G. Among them C_n and D_n have already been introduced in Fig. 3, and actually the solutions of Pell-4 with D=21 ($23^2-21\times5^2=1$ *etc.*). It will be shown here how these four series of graphs are related with each other with the same type of recursive relation.

By applying the fundamental recursive equation of Fig. A1 to $A_n \sim D_n$ one can obtain the following recursive relations:

$$A_n = A_1 B_{n-1} + x A_{n-1} \tag{A.1}$$

$$B_n = B_1 B_{n-1} + x A_{n-1}. \tag{A.2}$$

$$B_n = A_1 C_{n-1} + x B_{n-1}. \tag{A.3}$$

$$C_n = B_1 C_{n-1} + x B_{n-1}. \tag{A.4}$$

$$D_n = B_n + x B_{n-1}.. \tag{A.5}$$

Depending on the choice of edge l in graph G a number of different recursive relations can be obtained. However, it will be shown that the above selection works fairly well for our purpose. By noting $A_1=1+2x$ and $B_1=1+3x$ one can obtain the two sets of matrix representations from the pairs of (A.1) and (A.2), and (A.3) and (A.4) as follows:

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = \begin{pmatrix} x & 1+2x \\ x & 1+3x \end{pmatrix} \begin{pmatrix} A_{n-1} \\ B_{n-1} \end{pmatrix} \tag{A.6}$$

and

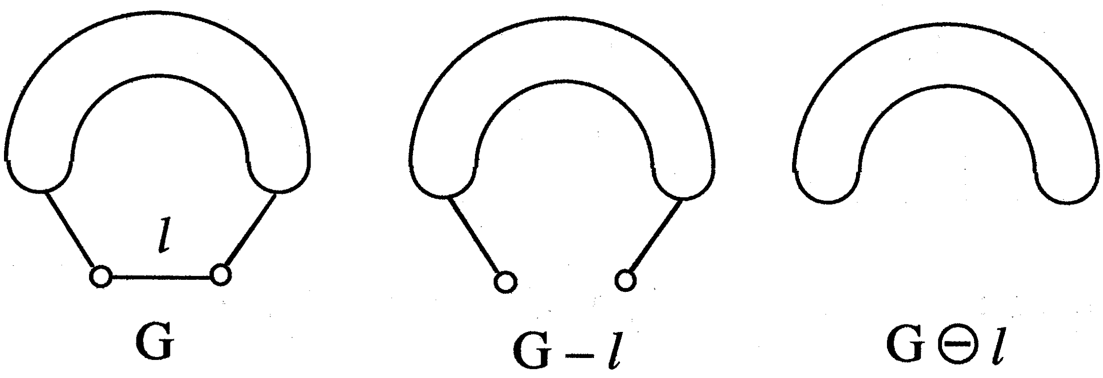
$$\begin{pmatrix} B_n \\ C_n \end{pmatrix} = \begin{pmatrix} x & 1+2x \\ x & 1+3x \end{pmatrix} \begin{pmatrix} B_{n-1} \\ C_{n-1} \end{pmatrix}. \tag{A.7}$$

Note that both the sets of simultaneous recursive equations have the same coefficient matrix.

According to the recipe used in the former paper of this series[2)] one can obtain the following recursive relation equally applied to A_n, B_n, and C_n:

$$f_n = (1 + 4x) f_{n-1} - x^2 f_{n-2}\,. \tag{A.8}$$

The relation (A.5) has a different type from the others. However, as will be shown below D_n also obeys



$$p(G,k) = p(G-l,k) + p(G\ominus l, k\text{-}1)$$

$$Q_G(x) = Q_{G-l}(x) + x\,Q_{G\ominus l}(x)$$

$$Z_G = Z_{G-l} + Z_{G\ominus l}$$

Fig. A1 Fundamental recursive relation for $p(G, k)$, $Q_G(x)$, and Z_G.

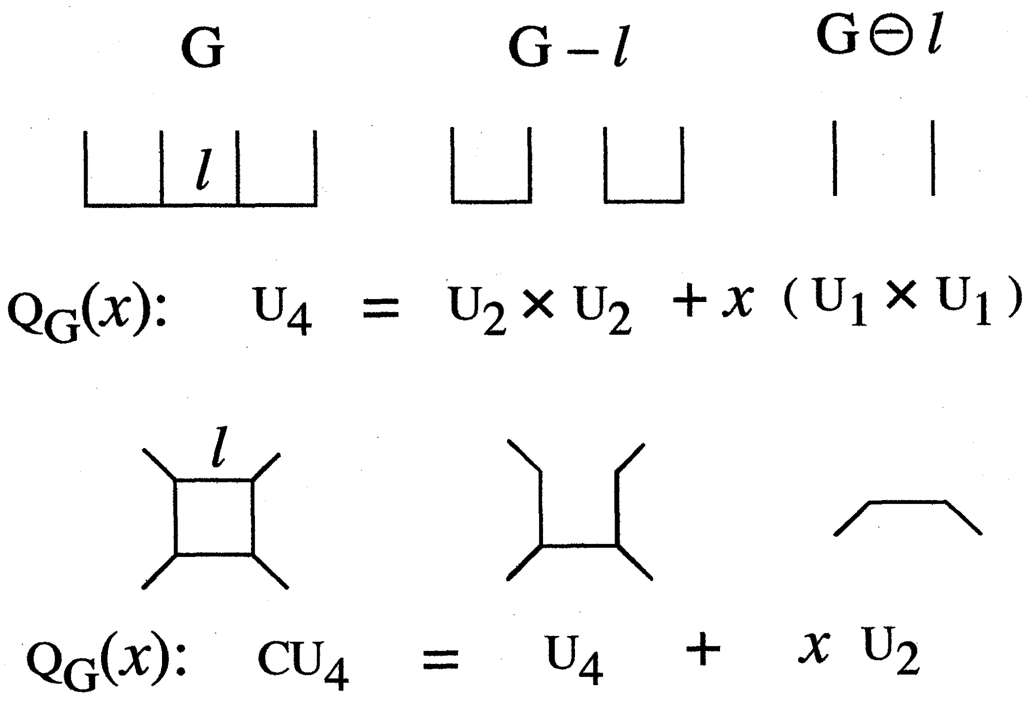
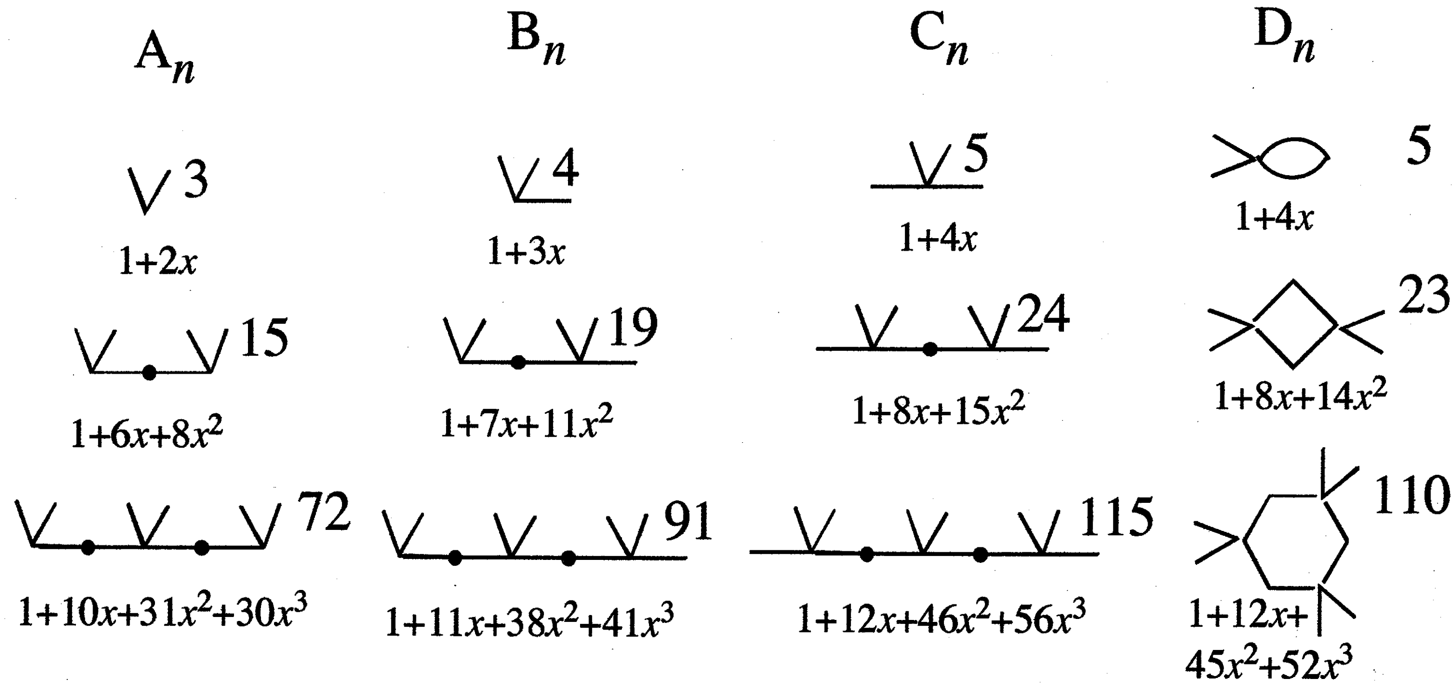


Fig. A2 Examples of applying recursive relation (Fig. A1) to obtain $Q_G(x)$ of comb and gear graphs. Z_G can be obtained by putting x=1 into $Q_G(x)$.



$A_n = A_1 B_{n-1} + x A_{n-1}$ $B_n = B_1 B_{n-1} + x A_{n-1}$

$B_n = A_1 C_{n-1} + x B_{n-1}$ $C_n = B_1 C_{n-1} + x B_{n-1}$

$D_n = B_n + x B_{n-1}$

$f_n = (1 + 4x) f_{n-1} - x^2 f_{n-2}$
f : A, B, C, D

$f_n = 5 f_{n-1} - f_{n-2}$
f : Z_A, Z_B, Z_C, Z_D

Fig. A3 Four series of graphs, Z_G, and recursive relations for their $Q_G(x)$ and Z_G.

the recursive relation (A.8).

(Proof of (A.8) for f=D)

By putting (A.5) into the following formula one obtains:

$$\begin{aligned} &D_n - (1+4x)\,D_{n-1} + x^2 D_{n-2} \\ &= B_n - (1+3x)\,B_{n-1} - x(1+3x)\,B_{n-2} + x^3 B_{n-3} \\ &= B_n - (1+4x)\,B_{n-1} + x^2 B_{n-2} \\ &\quad + x\,[B_{n-1} - (1+4x)\,B_{n-2} + x^2 B_{n-3}], \end{aligned}$$

which is equal to 0 according to (A.8) for f=B. □

Since $Q_G(1)=Z_G$ (3.2), the recursive relation of $Z_n = Z_{Gn}$ for each series of graph can be obtained as

$$Z_n = 5\,Z_{n-1} - Z_{n-2}\,. \tag{A.9}$$

The above results could be obtained by several trial-and-error steps. However, by using the operator technique developed by the present author they can straightforwardly be derived as follows:[20,21]

First define the step-up operator

$$\hat{O} f_n = f_{n+1}\,, \tag{A.10}$$

and assume that this operator commonly functions to A_n~D_n, as has been shown above. Then the set of recursive relations (A.1) and (A.3)-(A.5) can formally be expressed as a set of simultaneous linear equations

$$\begin{cases} (\hat{O}-x)A_n - (1+2x)B_n = 0 \\ (\hat{O}-x)B_n - (1+2x)C_n = 0 \\ -xB_n + [\hat{O}-(1+3x)]C_n = 0 \\ -(\hat{O}+x)B_n + \hat{O}D_n = 0 \end{cases} \tag{A.11}$$

In order for the "variables" A_n~D_n, to have non-trivial solution, the coefficient determinant constructed from the set of simultaneous linear equations (A.11) should be zero as

$$\begin{vmatrix} \hat{O}-x & -(1+2x) & 0 & 0 \\ 0 & \hat{O}-x & -(1+2x) & 0 \\ 0 & -x & \hat{O}-(1+3x) & 0 \\ 0 & -(\hat{O}+x) & 0 & \hat{O} \end{vmatrix} = \hat{O}(\hat{O}-x)\,[\hat{O}^2-(1+4x)\hat{O}+x^2] = 0 \tag{A.12}$$

By applying the third factor of the operator polynomial (A.12) to A_n~D_n one gets (A.8).

Although this operator technique is not mathematically rigorous, a number of useful recursive relations have successfully been obtained in the graph-theoretical analysis of various counting polynomials for large polycyclic networks.[20-22] Anyway the structure of the determinant in (A.12) clearly illustrates the mathematical structure and relations of the set of the series of graphs A_n~D_n.

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