

ON THE NUMBER OF KEKULÉ STRUCTURES  
FOR RECTANGLE-SHAPED BENZENOIDS

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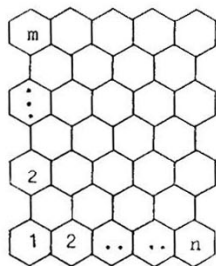
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Abstract

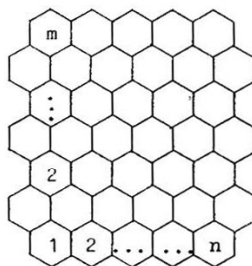
The oblate rectangle-shaped benzenoid with  $2m-1$  tier chains of alternating lengths  $n$  and  $n+1$  (in terms of the number of hexagons) is denoted by  $R_j(m, n)$ . It is known that the algebraic formula for the number ( $K$ ) of Kekulé structures of  $R_j(m, n)$  with fixed value of  $m$  is a polynomial ( $P_m(n)$ ) in powers of  $n$ . Cyvin et al. guessed that this polynomial has factors  $n+1$ ,  $(n+2)^m$  and  $n+3$ . A rigorous proof for the validity of this conjecture is given in the present paper. Also the algebraic formula for  $K\{R_j(6, n)\}$  is obtained by using the fully computerized method.

1. INTRODUCTION

In the present paper we consider the enumeration of Kekulé structures of rectangle-shaped benzenoids. The symbolism and terminology used in this paper is the same as in (1). Hence a rectangle-shaped benzenoid or simply rectangle has both "vertical" sides indented. There are two types of rectangles as shown in Fig.1.



prolate rectangle



oblate rectangle

Fig.1. Definition of the prolate and oblate rectangle.

For a prolate rectangle with  $2m-1$  tier chains of alternating lengths  $n$  and  $n-1$ , the number ( $K$ ) of Kekulé structures is long known (4), viz.  $(n+1)^m$ . In the following we concentrate on oblate rectangles.

We use  $R_j(m,n)$  to denote the oblate rectangle with  $2m-1$  tier chains of alternating lengths  $n$  and  $n+1$ . For oblate rectangles with fixed values of  $n$  ( $n=1,2,3,4$ ), the

algebraic formulas have been derived from recurrence relations [1,5,7-9]. While for oblate rectangles with fixed values of  $m$ , the following results are known nowadays:

$${}^a K\{R_j(2,n)\} = \frac{1}{12} (n+1)(n+2)^2(n+3)$$

$${}^{a-c} K\{R_j(3,n)\} = \frac{1}{120} (n+1)(n+2)^3(n+3)(n^2+4n+5)$$

$${}^d K\{R_j(4,n)\} = \frac{1}{20160} (n+1)(n+2)^4(n+3)(17n^4+136n^3+439n^2+668n+420)$$

$${}^e K\{R_j(5,n)\} = \frac{1}{362880} (n+1)(n+2)^5(n+3)(31n^6+372n^5+1942n^4+5616n^3+9511n^2+8988n+3780)$$

<sup>a</sup>M.Gordon and W.H.T.Davison, *J.Chem.Phys.* 20, 428 (1952).

<sup>b</sup>T.F.Yen, *Theoret.Chim.Acta* 20, 399 (1971).

<sup>c</sup>N.Ohkami and H.Hosoya, *Theoret.Chim.Acta* 64, 153 (1983).

<sup>d</sup>S.J.Cyvin, B.N.Cyvin and J.L.Bergan, *Match* 19, 189 (1986).

<sup>e</sup>S.J.Cyvin, *Match* 19, 213 (1986).

The algebraic formula for  $K\{R_j(4,n)\}$  was achieved by Cyvin et al. by refined applications of some auxiliary benzenoid classes and ingenious employment of new variants of the enumeration techniques [1]. Furthermore, they developed a fully computerized method which was applied to derive for the first time the algebraic formula for the  $K$  number of  $R_j(5,n)$  [2]. This method is based on the important fact that the formula for  $K\{R_j(m,n)\}$  is a polynomial  $(P_m(n))$  in powers of  $n$  with degree  $d_m \leq 3m-2$  [1]. Thus in order to obtain the formula for  $K\{R_j(m,n)\}$  with fixed values of  $m$  a polynomial with indetermined coefficients is

to be assumed and the knowledge of  $d_m+1$ , viz.  $3m-1$  K numbers is required to find the coefficients. The researchers of [1] guessed that the polynomial  $P_m(n)$  ( $m \geq 2$ ) has factors  $n+1, n+3$  and  $(n+2)^m$ . This conjecture coincides with the known polynomials for  $m=2, 3, 4, 5$ . In the present work the validity of the conjecture is established. This will certainly reduce the number of unknowns by  $m+2$  in applying the fully computerized method which leads to the algebraic formulas for  $K\{R_j(m, n)\}$  with fixed values of  $m$ .

## 2. AUXILIARY BENZENOID CLASSES

The auxiliary benzenoid classes  $B(n, 2(m-s), l)$ ,  $s=1, 2, \dots, m-1$ ;  $l=0, 1, \dots, n$ , which are depicted in Fig. 2 play an important role in the present work.

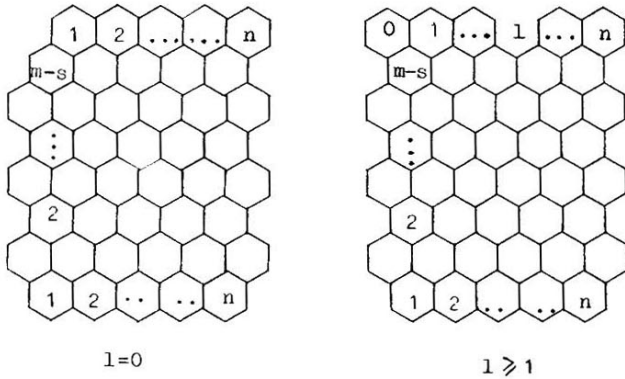


Fig. 2. Auxiliary benzenoid classes  $B(n, 2(m-s), l)$

Consider the bonds of  $B(n, 2(m-s), -1)$  intersected by the straight line X (see Fig.3.). It is not difficult to see that in each of the Kekulé structures of  $B(n, 2(m-s), -1)$  one and only one of those bonds is a double bond. Thus we obtain the following recurrence relations:

$$K\{B(n, 2(m-s), -1)\} = \sum_{i=0}^1 (n+1-i)(i+1)K\{B(n, 2(m-s-1), -i)\} + \sum_{i=1+1}^n (n+1-i)(1+1)K\{B(n, 2(m-s-1), -i)\}$$

$$(1 \leq s \leq m-2; l=0, 1, \dots, n) \tag{1}$$

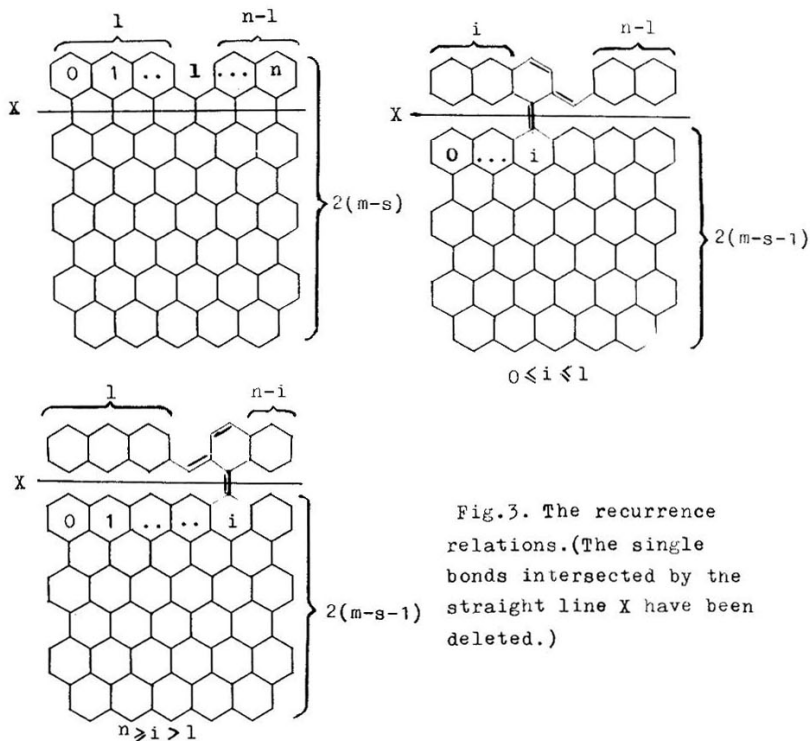


Fig.3. The recurrence relations. (The single bonds intersected by the straight line X have been deleted.)

3. A GENERAL METHOD FOR K NUMBER OF  $R_j(m,n)$ .

Define  $(n+1)$ -dimension vectors  $Y(n,t), t=1,2,\dots,m-1$  as follows:

$$Y(n,t) = (K\{B(n,2t,0)\}, K\{B(n,2t,-1)\}, \dots, K\{B(n,2t,-n)\}).$$

For two  $(n+1)$ -dimension vectors  $Z_1=(a_0, a_1, \dots, a_n)$  and  $Z_2=(b_0, b_1, \dots, b_n)$ , the inner product  $Z_1 * Z_2$  is defined as

$$Z_1 * Z_2 = \sum_{i=0}^n a_i b_i$$

Denote by  $A(n)$  the  $(n+1) \times (n+1)$  matrix whose  $l$ -th row ( $l=0,1,\dots,n$ ) is defined as

$(n+1-l, 2(n+1-l), \dots, (l+1)(n+1-l), (l+1)(n-l), \dots, (l+1)2, l+1)$   
 viz. the  $j$ -th component is  $(j+1)(n+1-l)$  for  $j=0,1,\dots,l$ ; while the  $j$ -th component is  $(l+1)(n+1-j)$  for  $j=l+1, l+2, \dots, n$ .

When  $n=9, A(9)$  is shown in Chart I.

The  $i$ -th ( $i=0,1,\dots,n$ ) column of  $A(n)$  is denoted by  $A(n,i)$ . By the definition of  $A(n)$ , we have

$$A(n,i) = \begin{pmatrix} n+1-i & 0\text{-th} \\ 2(n+1-i) & 1\text{-th} \\ \vdots & \vdots \\ i(n+1-i) & (i-1)\text{-th} \\ (i+1) \cdot (n+1-i) & i\text{-th} \\ (i+1) \cdot (n-i) & (i+1)\text{-th} \\ \vdots & \vdots \\ (i+1)2 & (n-1)\text{-th} \\ (i+1) & n\text{-th} \end{pmatrix} \quad (2)$$

(see Chart I).

$\begin{pmatrix} 10 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\ 9 & 18 & 16 & 14 & 12 & 10 & 8 & 6 & 4 & 2 \\ 8 & 16 & 24 & 21 & 18 & 15 & 12 & 9 & 6 & 3 \\ 7 & 14 & 21 & 28 & 24 & 20 & 16 & 12 & 8 & 4 \\ 6 & 12 & 18 & 24 & 30 & 25 & 20 & 15 & 10 & 5 \\ 5 & 10 & 15 & 20 & 25 & 30 & 24 & 18 & 12 & 6 \\ 4 & 8 & 12 & 16 & 20 & 24 & 28 & 21 & 14 & 7 \\ 3 & 6 & 9 & 12 & 15 & 18 & 21 & 24 & 16 & 8 \\ 2 & 4 & 6 & 8 & 10 & 12 & 14 & 16 & 18 & 9 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 5 \times 11 \\ 9 \times 11 \\ 12 \times 11 \\ 14 \times 11 \\ 15 \times 11 \\ 15 \times 11 \\ 14 \times 11 \\ 12 \times 11 \\ 9 \times 11 \\ 5 \times 11 \end{pmatrix}$	
A(9)	$D^{(1)}(9)$	$D^{(2)}(9)$	
$\begin{pmatrix} 55 \times 121 \\ 105 \times 121 \\ 146 \times 121 \\ 175 \times 121 \\ 190 \times 121 \\ 190 \times 121 \\ 175 \times 121 \\ 146 \times 121 \\ 105 \times 121 \\ 55 \times 121 \end{pmatrix}$	$\begin{pmatrix} 671 \times 1331 \\ 1287 \times 1331 \\ 1798 \times 1331 \\ 2163 \times 1331 \\ 2353 \times 1331 \\ 2353 \times 1331 \\ 2163 \times 1331 \\ 1798 \times 1331 \\ 1287 \times 1331 \\ 671 \times 1331 \end{pmatrix}$	$\begin{pmatrix} 8272 \times 11^4 \\ 15873 \times 11^4 \\ 22187 \times 11^4 \\ 26703 \times 11^4 \\ 29056 \times 11^4 \\ 29056 \times 11^4 \\ 26703 \times 11^4 \\ 22187 \times 11^4 \\ 15873 \times 11^4 \\ 8272 \times 11^4 \end{pmatrix}$	$\begin{pmatrix} 5 \times 11 \\ 9 \times 11 \\ 12 \times 11 \\ 14 \times 11 \\ 15 \times 11 \\ 15 \times 11 \\ 14 \times 11 \\ 12 \times 11 \\ 9 \times 11 \\ 5 \times 11 \end{pmatrix}$
$D^{(3)}(9)$	$D^{(4)}(9)$	$D^{(5)}(9)$	$Y(9, 1)^T$

Chart I. A(n) and  $D^{(i)}(n)$  for n=9 and i=1,2,3,4,5.  
 $Y(n,t)^T$  for n=9, t=1.

The following formula is derived by a similar reasoning as in section 2.

$$K\{R_j(m,n)\} = \sum_{l=0}^n K\{B(n, 2(m-1), -1)\} \quad (3)$$

As an alternative to the above equation we may write

$$K\{R_j(m,n)\} = D^{(1)}(n)^T * Y(n, m-1)$$

where  $D^{(1)}(n)^T$  is the transpose of  $D^{(1)}(n)$ , and  $D^{(1)}(n)$  is a  $(n+1)$ -dimension vector with all components being 1 (see Chart I).

By using the recurrence relation (1), one obtains

$$\begin{aligned} K\{R_j(m,n)\} &= \sum_{l=0}^n \left( \sum_{i=0}^l (n+1-l)(i+1) K\{B[n, 2(m-2), -i]\} \right. \\ &\quad \left. + \sum_{i=l+1}^n (n+1-i)(l+1) K\{B[n, 2(m-2), -i]\} \right) \\ &= \sum_{l=0}^n \left( D^{(1)}(n)^T * A(n, l)^T \right) K\{B[n, 2(m-2), -l]\} \end{aligned}$$

where  $A(n, l)^T$  is the transpose of  $A(n, l)$ .

Denote  $D^{(2)}(n)^T = (d_0^{(2)}, d_1^{(2)}, \dots, d_n^{(2)})$ , where  $d_i^{(2)}$  is defined by  $d_i^{(2)} = D^{(1)}(n)^T * A(n, i)^T$  for  $i=0, 1, \dots, n$ . Thus

we have

$$\begin{aligned} K\{R_j(m,n)\} &= \sum_{l=0}^n d_l^{(2)} \cdot K\{B[n, 2(m-2), -l]\} \\ &= D^{(2)}(n)^T * Y(n, m-2) \end{aligned}$$

Similarly, by the recurrence relation (1) we have

$$\begin{aligned} K\{R_j(m,n)\} &= \sum_{l=0}^n d_l^{(2)} \left( \sum_{i=0}^l (n+1-l)(i+1) K\{B[n, 2(m-3), -i]\} \right. \\ &\quad \left. + \sum_{i=l+1}^n (n+1-i)(l+1) K\{B[n, 2(m-3), -i]\} \right) \\ &= \sum_{l=0}^n d_l^{(3)} \cdot K\{B[n, 2(m-3), -l]\} \\ &= D^{(3)}(n)^T * Y(n, m-3) \end{aligned}$$



where  $d_1^{(3)} = D^{(2)}(n)^T * A(n, 1)^T, l=0, 1, \dots, n$ ; and

$$D^{(3)}(n)^T = (d_0^{(3)}, d_1^{(3)}, \dots, d_n^{(3)}).$$

In general, we have

$$K\{R_j(m, n)\} = \sum_{l=0}^n a_l^{(u)}. K\{B[n, 2(m-u), -1]\} \quad (2 \leq u \leq m-1)$$

$$= D^{(u)}(n)^T * Y(n, m-u)$$

where  $d_1^{(u)} = D^{(u-1)}(n)^T * A(n, 1)^T$  and  $D^{(u)}(n)^T = (d_0^{(u)}, d_1^{(u)}, \dots, d_n^{(u)})$ .

Eventually we reach at

$$K\{R_j(m, n)\} = D^{(m-1)}(n)^T * Y(n, 1) \quad (4)$$

where  $D^{(m-1)}(n)^T = (d_0^{(m-1)}, d_1^{(m-1)}, \dots, d_n^{(m-1)})$  and  $d_1^{(m-1)} = D^{(m-2)}(n)^T * A(n, i)$  for  $i=0, 1, \dots, n$ .

Note that since  $K\{B(n, 2, -1)\} = 1/2 (n+2)(n+1-1)(1+1) [1]$   $Y(n, 1)$  is already known.

#### 4. THE FEATURE OF $d_i^{(t)}$ ( $t=1, 2, \dots, m-1$ )

We claim that  $d_i^{(t)}$  is a polynomial in  $n$  and  $i$  for  $1 \leq t \leq m-1$ . Since  $d_i^{(1)} = 1$ , the conclusion is evident for  $t=1$ . Now suppose that  $d_i^{(s)}$  is a polynomial in  $n$  and  $i$  for  $1 \leq s < m-1$ .

By section 3, we have

$$d_i^{(s+1)} = D^{(s)}(n)^T * A(n, i)^T = \sum_{l=0}^n d_l^{(s)} a_{il}$$

where  $a_{il}$  is the  $l$ -th component of  $A(n, i), l=0, 1, 2, \dots, n$ .

Since  $d_l^{(s)}$  is a polynomial in  $n$  and  $l$ , we may express

it as  $f(n, l)$ . Similarly,  $a_{i, l}$  can be expressed as  $g(n, l, i)$ .

Therefore, the summation

$$d_i^{(s+1)} = \sum_{l=0}^n f(n, l)g(n, l, i)$$

is a polynomial in  $n$  and  $i$ .

By virtue of the inductive principle,  $d_i^{(t)}$  is a polynomial in  $n$  and  $i$  for  $t=1, 2, \dots, m-1$ .

5. THE SUMMATION  $\sum_{w=1}^n w^p$  WITH FIXED VALUES OF  $p (\geq 1)$

For the first five values of  $p$ , we have

$$\sum_{w=1}^n w = 1/2 n(n+1)$$

$$\sum_{w=1}^n w^2 = 1/6 n(n+1)(2n+1)$$

$$\sum_{w=1}^n w^3 = 1/4 n^2(n+1)^2$$

$$\sum_{w=1}^n w^4 = 1/30 n(n+1)(2n+1)(3n^2+3n-1)$$

$$\sum_{w=1}^n w^5 = 1/12 n^2(n+1)^2(2n^2+2n-1)$$

It is reasonable to guess that  $\sum_{w=1}^n w^p$  has the factors  $n$  and  $(n+1)$  for each fixed natural number  $p$ . Indeed, we can prove it by induction on the natural number  $p$ .

Suppose that the summation  $\sum_{w=1}^n w^p$  has the factors  $n$  and  $n+1$  for  $p \leq t-1$  ( $t \geq 2$ ).

Taking  $q=1, 2, \dots, n$  in the following equality

$$(q+1)^{t+1} - q^{t+1} = \sum_{i=0}^t \binom{t+1}{i} q^i$$

one obtains n equalities as follows:

$$\begin{aligned}
 2^{t+1} - 1 &= \sum_{i=0}^t \binom{t+1}{i} \\
 3^{t+1} - 2^{t+1} &= \sum_{i=0}^t \binom{t+1}{i} 2^i \\
 &\vdots \\
 &\vdots \\
 n^{t+1} - (n-1)^{t+1} &= \sum_{i=0}^t \binom{t+1}{i} (n-1)^i \\
 (1+n)^{t+1} - n^{t+1} &= \sum_{i=0}^t \binom{t+1}{i} n^i
 \end{aligned}$$

Taking respectively summation of the right and left hand side of the above n equalities yields

$$(n+1)^t - 1 = \sum_{i=0}^t \left\{ \binom{t+1}{i} \sum_{w=1}^n w^i \right\}$$

It can be reduced to

$$\sum_{w=1}^n w^t = \frac{1}{t+1} \left\{ n(n+1) \sum_{i=1}^{t-1} \binom{t-1}{i} n^i - \sum_{i=1}^{t-1} \left[ \binom{t+1}{i} \sum_{w=1}^n w^i \right] \right\}$$

By the inductive hypothesis, for  $i < t-1$ , the summation  $\sum_{w=1}^n w^i$  has factors n and n+1. Therefore,  $\sum_{w=1}^n w^t$  has factors n and n+1.

#### 6. THE FACTORS $n+1, (n+2)^m$ AND $n+3$ .

We are now in a position to prove that  $n+1, (n+2)^m$  and  $n+3$  are factors in the polynomial  $P_m(n)$  for  $m \geq 2$ .

Investigate the column  $A(n, i)$  of the matrix  $A(n)$

defined in section 3. Denote the  $v$ -th component of  $\Lambda(n, i)$  by  $a_{iv}$ ,  $v=0, 1, \dots, n$ .

From formula (2) in section 3, one obtains:

for  $0 \leq v \leq i, 0 \leq n-v \leq i$

$$a_{iv} + a_{i, n-v} = (v+1)(n+1-i) + (n+1-v)(n+1-i) = (n+2)(n+1-i)$$

for  $0 \leq v \leq i, i < n-v$

$$a_{iv} + a_{i, n-v} = (v+1)(n+1-i) + (i+1)\{n-i+1-(n-v-i)\} = (n+2)(v+1)$$

for  $i < v \leq n, 0 \leq n-v \leq i$

$$a_{iv} + a_{i, n-v} = (i+1)\{n-i+1-(v-i)\} + (n+1-v)(n+1-i) = (n+2)(n+1-v)$$

for  $i < v \leq n, i < n-v$

$$\begin{aligned} a_{iv} + a_{i, n-v} &= (i+1)\{n-i+1-(v-i)\} + (i+1)\{n-i+1-(n-v-i)\} \\ &= (n+2)(i+1) \end{aligned}$$

This means that  $n+2$  is a factor in  $a_{iv} + a_{i, n-v}$  for  $i=0, 1, \dots, n; v=0, 1, \dots, n$ .

In addition, when  $n$  is an even number, the  $(n/2)$ -th component of  $\Lambda(n, i)$  is

$$\frac{1}{2} (n+2)(n+1-i) \quad \frac{n}{2} \leq i$$

$$\text{or} \quad \frac{1}{2} (n+2)(i+1) \quad \frac{n}{2} > i$$

Since

$$D^{(1)}(n)^T = (1, 1, \dots, 1)$$

we have

$$d_i^{(2)} = D^{(1)}(n)^T * \Lambda(n, i)^T = \sum_{h=0}^n a_{ih} = \begin{cases} \sum_{v=0}^{\frac{n-1}{2}} (a_{iv} + a_{i, n-v}) & (n \text{ is odd}) \\ \sum_{v=0}^{\frac{n}{2}-1} (a_{iv} + a_{i, n-v}) + a_{i, n/2} & (n \text{ is even}) \end{cases}$$

By the above discussion we see that  $d_1^{(2)}$  has factor  $(n+2)$ .

Inserting respectively  $i=q$  and  $i=n-q$  into formula (2) gives

$$A(n, q) = \begin{pmatrix} n+1-q \\ 2(n+1-q) \\ \vdots \\ q(n+1-q) \\ (q+1)(n+1-q) \\ (n-q)(q+1) \\ (n-q-1)(q+1) \\ \vdots \\ 2(q+1) \\ q+1 \end{pmatrix} \quad A(n, n-q) = \begin{pmatrix} q+1 \\ 2(q+1) \\ \vdots \\ (n-q-1)(q+1) \\ (n-q)(q+1) \\ (q+1)(n+1-q) \\ q(n+1-q) \\ \vdots \\ 2(n+1-q) \\ n+1-q \end{pmatrix}$$

This shows that  $a_{qv} = a_{n-q, n-v}$  for  $q=0, 1, \dots, n; v=0, 1, \dots, n$ .

Thus

$$\begin{aligned} d_r^{(2)} &= D^{(1)}(n)^T * A(n, r)^T \\ &= \sum_{h=0}^n a_{rh} = \sum_{h=0}^n a_{n-r, n-h} \end{aligned}$$

Denote  $h_* = n-h$ . Then

$$\begin{aligned} d_r^{(2)} &= \sum_{h=0}^n a_{n-r, n-h} = \sum_{h_*=0}^n a_{n-r, h_*} = D^{(1)}(n)^T * A(n, n-r)^T \\ &= d_{n-r}^{(2)} \end{aligned}$$

$(r=0, 1, 2, \dots, n)$

Now suppose that  $d_r^{(u)}$  ( $r=0, 1, \dots, n; 2 \leq u \leq m-2$ ) has factor  $(n+2)^{u-1}$  and  $d_r^{(u)} = d_{n-r}^{(u)}$  for  $r=0, 1, \dots, n$ .

$$\begin{aligned}
 \text{Hence } d_r^{(u+1)} &= D^{(u)}(n)^T * \Lambda(n, r)^T \\
 &= \sum_{i=0}^n d_i^{(u)} a_{ri} \\
 &= \begin{cases} \sum_{i=0}^{\frac{n-1}{2}} d_i^{(u)} (a_{ri} + a_{r, n-i}) & (n \text{ is odd}) \\ \sum_{i=0}^{\frac{n}{2}-1} d_i^{(u)} (a_{ri} + a_{r, n-i}) + d_{\frac{n}{2}}^{(u)} a_{i, \frac{n}{2}} & (n \text{ is even}) \end{cases}
 \end{aligned}$$

Since both  $a_{ri} + a_{r, n-i}$  and  $a_{n/2}$  have factor  $n+2$ , and  $d_i^{(u)}$  has factor  $(n+2)^{u-1}$ ,  $d_r^{(u+1)}$  has factor  $(n+2)^u$ . Moreover

$$\begin{aligned}
 d_r^{(u+1)} &= D^{(u)}(n)^T * \Lambda(n, r)^T \\
 &= \sum_{h=0}^n d_h^{(u)} a_{rh} = \sum_{h=0}^n d_{n-h}^{(u)} a_{n-r, n-h}
 \end{aligned}$$

Denote  $n_* = n-h$ . Then

$$\begin{aligned}
 d_r^{(u+1)} &= \sum_{h_*=r}^n d_{h_*}^{(u)} a_{n-r, n_*} = D^{(u)}(n)^T * \Lambda(n, n-r)^T \\
 &= d_{n-r}^{(u+1)}
 \end{aligned}$$

Repeating the above discussion, we eventually have

$$d_r^{(m-1)} = d_{n-r}^{(m-1)} \text{ and } d_r^{(m-1)} \text{ has factor } (n+2)^{m-2} \text{ for } r=0, 1, \dots, n. \text{ Therefore, we denote } d_r^{(m-1)} = (n+2)^{m-2} \cdot c_r^{(m-1)}.$$

By formula (4) in section 3, we have

$$P_m(n) = K\{R\}(\mathfrak{m}, n) = \sum_{r=0}^n d_r^{(m-1)} K\{B(n, 2, -r)\} \quad (5)$$

Substitution of  $K\{B(n,2,-r)\} = 1/2 (n+2)(n+1-r)(r+1)$  into (5) yields

$$P_m(n) = 1/2 (n+2) \sum_{r=0}^n (n+1-r)(r+1) \cdot d_r^{(m-1)}$$

$$= 1/2 (n+2)^{m-1} \sum_{r=0}^n (n+1-r)(r+1) c_r^{(m-1)}$$

Since  $d_r^{(m-1)}$  is a polynomial in  $n$  and  $r$  (section 4) and hence  $c_r^{(m-1)}$ ,  $(n-r+1)c_r^{(m-1)}$  can be written as

$$\{f_1(n)(r+1)^z + f_2(n)(r+1)^{z-1} + \dots + f_z(n)(r+1) + f_{z+1}(n)\}$$

where  $f_t(n)$  ( $t=1,2,\dots,z+1$ ) is a polynomial in  $n$ . Therefore  $(n+1-r)(r+1)c_r^{(m-1)}$  can be written as

$$\{f_1(n)(r+1)^{z+1} + f_2(n)(r+1)^z + \dots + f_z(n)(r+1)^2 + f_{z+1}(n)(r+1)\}$$

Denote  $r_* = r+1$ . Then we have

$$P_m(n) = 1/2 (n+2)^{m-1} \sum_{r=0}^n \{f_1(n)(r+1)^{z+1} + f_2(n)(r+1)^z + \dots$$

$$+ [f_z(n)(r+1)^2 + f_{z+1}(n)(r+1)]\}$$

$$= 1/2 (n+2)^{m-1} \left\{ f_1(n) \sum_{r_*=1}^{n+1} r_*^{z+1} + f_2(n) \sum_{r_*=1}^{n+1} r_*^z \right.$$

$$\left. + \dots + f_z(n) \sum_{r_*=1}^{n+1} r_*^2 + f_{z+1}(n) \sum_{r_*=1}^{n+1} r_* \right\}$$

By section 5 each of  $\sum_{r_*=1}^{n+1} r_*^{z+1}$ ,  $\sum_{r_*=1}^{n+1} r_*^z$ ,  $\dots$ ,  $\sum_{r_*=1}^{n+1} r_*^2$  and

$\sum_{r_*=1}^{n+1} r_*$  has factors  $(n+1)$  and  $(n+2)$ . Consequently,  $P_m(n)$  has factors  $(n+1)$  and  $(n+2)^m$ . We denote

$$P_m(n) = (n+1)(n+2)^m Q_m^*(n) \tag{6}$$

On the other hand,  $P_m(n)$  can be derived in another way when  $n$  is odd.

It is not difficult to see that

$$K\{B(n, 2, -r)\} = K\{B(n, 2, -(n-r))\} = 1/2 (n+2)(n+1-r)(r+1)$$

Hence when  $n$  is odd

$$\begin{aligned} P_m(n) &= \sum_{r=0}^n d_r^{(m-1)} K\{B(n, 2, -r)\} = 2 \sum_{r=0}^{\frac{n-1}{2}} d_r^{(m-1)} K\{B(n, 2, -r)\} \\ &= (n+2)^{m-1} \sum_{r=0}^{\frac{n-1}{2}} (n+1-r)(r+1) c_r^{(m-1)} \\ &= (n+2)^{m-1} \left\{ f_1(n) \sum_{r_*=1}^{\frac{n+1}{2}} r_*^{z+1} + f_2(n) \sum_{r_*=1}^{\frac{n+1}{2}} r_*^z \right. \\ &\quad \left. + \dots + f_z(n) \sum_{r_*=1}^{\frac{n+1}{2}} r_*^2 + f_{z+1}(n) \sum_{r_*=1}^{\frac{n+1}{2}} r_* \right\} \end{aligned}$$

Again by section 5 each of

$$\sum_{r_*=1}^{\frac{n+1}{2}} r_*^{z+1}, \quad \sum_{r_*=1}^{\frac{n+1}{2}} r_*^z, \quad \dots, \quad \sum_{r_*=1}^{\frac{n+1}{2}} r_*^2 \quad \text{and} \quad \sum_{r_*=1}^{\frac{n+1}{2}} r_* \quad \text{has}$$

factors  $(n+1)/2$  and  $(n+3)/2$ . Therefore, we denote

$$P_m(n) = (n+1)(n+2)^{m-1}(n+3)Q_m^{**}(n) \tag{7}$$

By comparison of (6) and (7), we come to the conclusion that  $P_m(n)$  has factors  $n+1, (n+2)^m$  and  $n+3$ .

7. THE POLYNOMIAL  $P_m(n)$  FOR  $m=6$ .

In this section the algebraic formula for  $K\{R_j(6, n)\}$  is derived for the first time by using the fully computerized method. The result is a polynomial of 16-th degree in  $n$ , viz.



$$P_{\epsilon}(n) = \frac{1}{79833600} (n+1)(n+2)^6(n+3) \{ 691n^8 + 11056n^7 + 79788n^6 + 33820n^5 + 921759n^4 + 1654264n^3 + 1915562n^2 + 1315560n + 415800 \}$$

By section 6,  $P_{\epsilon}(n)$  is partially factorized

$$P_{\epsilon}(n) = (n+1)(n+2)^6(n+3)Q_{\epsilon}(n) \quad (8)$$

where  $Q_{\epsilon}(n)$  is a polynomial of 8-th degree in  $n$ . We write this polynomial as

$$Q_{\epsilon}(n) = A + B \binom{n}{1} + C \binom{n}{2} + D \binom{n}{3} + E \binom{n}{4} + F \binom{n}{5} + G \binom{n}{6} + H \binom{n}{7} + I \binom{n}{8} \quad (9)$$

where  $A, B, \dots, I$  are to be determined.

By the general method described in section 3, nine numerical solutions for  $K[R_j(t, n)]$  are obtained as follows:  $P_{\epsilon}(0)=1; P_{\epsilon}(1)=2 \times 3^5; P_{\epsilon}(2)=1352 \times 2^5; P_{\epsilon}(3)=466 \times 5^5; P_{\epsilon}(4)=107563 \times 3^5; P_{\epsilon}(5)=17994 \times 7^5; P_{\epsilon}(6)=2472352 \times 4^5; P_{\epsilon}(7)=279994 \times 9^5$  and  $P_{\epsilon}(8)=28387789 \times 5^5$ . In particular, we have taken advantage of  $P_{\epsilon}(0)=1$ , which is the trivial case of no rings and consistent with the general formulas (see section 1).

The scheme of computation in the shape of Pascal's triangle is given in Chart II. On inserting into eqns. (8) and (9) we obtain

$$P_{\epsilon}(n) = \frac{1}{79833600} (n+1)(n+2)^6(n+3) \left\{ 415800 + 6237000 \binom{n}{1} + 43326360 \binom{n}{2} + 160914600 \binom{n}{3} + 348868080 \binom{n}{4} + 457023600 \binom{n}{5} + 356954400 \binom{n}{6} + 153236160 \binom{n}{7} + 27861120 \binom{n}{8} \right\} \quad (10)$$

$1/192 =$	$A$	; $A=1/192$
$1/12 =$	$A + B$	; $B=15/192$
$169/240 =$	$A + 2B + C$	; $C=521/960$
$233/60 =$	$A + 3B + 3C + D$	; $D=129/64$
$107563/6720 =$	$A + 4B + 6C + 4D + E$	; $E=14683/3360$
$2999/56 =$	$A + 5B + 10C + 10D + 5E + F$	; $F=3847/672$
$77261/504 =$	$A + 6B + 15C + 20D + 15E + 6F + G$	; $G=4507/1008$
$139997/360 =$	$A + 7B + 21C + 35D + 35E + 21F + 7G + H$	; $H=691/360$
$28387789/31680 =$	$A + 8B + 28C + 56D + 70E + 56F + 28G + 8H + I$	; $I=691/1980$

Chart 11. The scheme of computation in the Pascal's triangle.

The formula (10) can be transferred into the polynomial form given at the beginning of this section.

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