Univ. u Novom Sadu
Zb. Rad. Prirod.–Mat. Fak.
Ser. Mat. 25, 2 (1995), 179-195

Review of Research
Faculty of Science
Mathematics Series

CHEMICAL GRAPHS, KEKULE STRUCTURES AND FIBONACCI NUMBERS

Ratko Tošić[1]
Institute of Mathematics, University of Novi Sad
Trg Dositeja Obradovića 4, 21000 Novi Sad, Yugoslavia

Ivan Stojmenović
Computer Science Dept., University of Ottawa
Ontario KIN 9B4, Canada

Abstract

In this paper a new formula for the number of Kekule structures of an arbitrary benzenoid chain is obtained. Combining this formula and some other known formulas, we derive some interesting combinatorial identities (17), (18), (21-24), (27), some of them involving Fibonacci numbers.

AMS Mathematics Subject Classification (1991): 05C
Key words and phrases: Kekule strucures, Fibonacci numbers

1. Some preliminaries

A benzenoid system is a combinatorial geometric object obtained by arranging the regular hexagons in a plane so that two hexagons are either disjoint or have a common edge.

[1]Work supported by Fund for Science of Vojvodina.

There is a fairly obvious correspondence between a benzenoid hydrocarbon and a benzenoid system. One example is given in Fig. 1 in which the structural formula of a benzenoid hidrocarbon (phenantrene) and the corresponding benzenoid system are shown.

In this paper we shall consider benzenoid systems as undirected graphs comprised of 6-cycles.

Let there be a total of h such cycles (hexagons) which we shall denote as $H_1, H_2, ..., H_h$ in each graph of interest. Bacause the problem we treat arises from chemical studies of certain hydrocarbon molecules (benzenoid chains), we impose upon $H_1, H_2, ..., H_h$ the following conditions to reflect the underlying chemistry:

(i) Every H_i and H_{i+1} shall have a common edge denoted by e_i, for all $1 \leq i \leq h-1$.

(ii) The edges e_i and e_j shall have no common vertex for any $1 \leq i < j \leq h-1$.

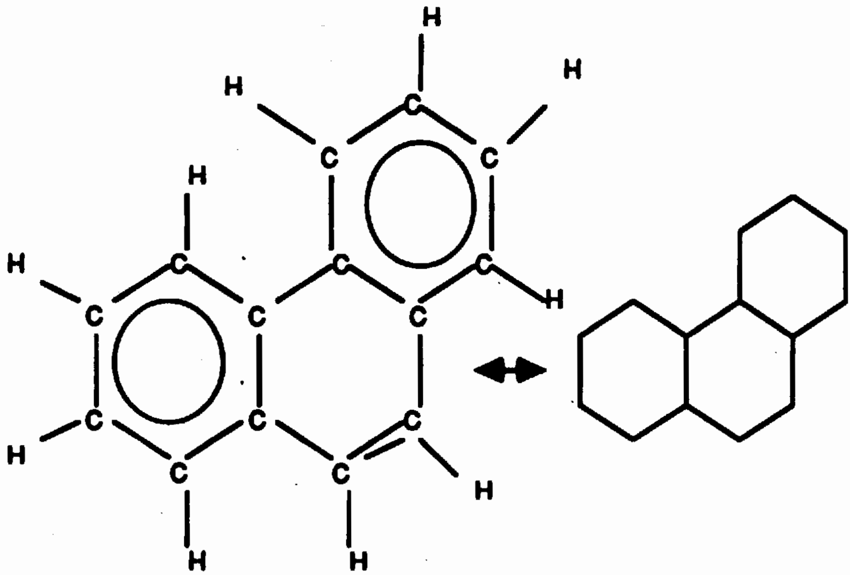

Fig.1

By representing the 6-cycles as regular hexagons in the plane we obtain a planar realization of this graph, as illustrated in Fig. 2. In organic chemistry such graphs correspond to benzenoid chains.

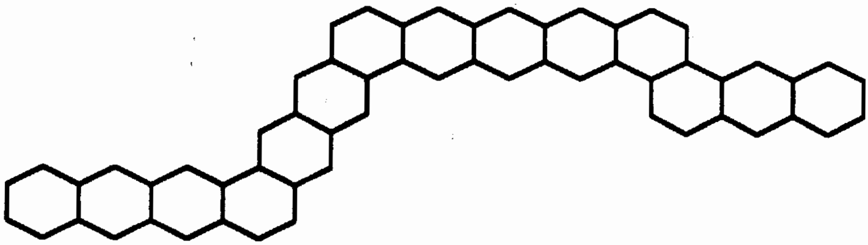

Fig. 2

In connection with the benzenoid chains the LA-sequnce is defined as an ordered h-tuple ($h > 1$) of the symbols L and A (Gutman [13]). The i-th symbol is L if the i-th hexagon is of the mode L_1 or L_2. The i-th symbol is A if the i-th hexagon is of the mode A_2. The definition of L_1, L_2, and A_2 modes of hexagons is clear from Fig.3.

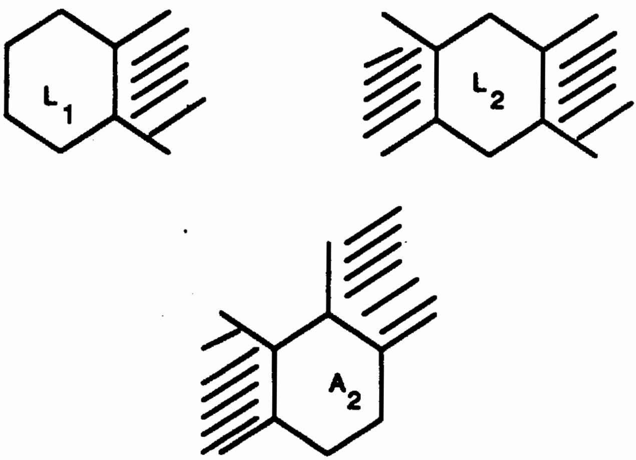

Fig. 3

For instance, the LA-sequence of the benzenoid chain in Fig. 2 is LLLALLALLLAALL or, in the abbreviated form $L^3AL^2AL^3A^2L^2$.

Each perfect matching of a benzenoid system (if any exsists) represents a Kekule structure of the corresponding benzenoid hydrocarbon. The enumeration of Kekule structures of benzenoid hydrocarbons is important because the stability and many other properties of these hydrocarbons have been found to correlate with the number of their Kekule structures (K number).

It is well known that the K number of a benzenoid chain is entirely determined by its LA-sequence, no matter which way the kinks go ([2,12,14]). Balaban and Tomescu [2] coined the term isoarithmicity for this phenomenon. For example, the three benzenoid chains in Fig. 4 are isoarithmic, hence, all three have the same K number.

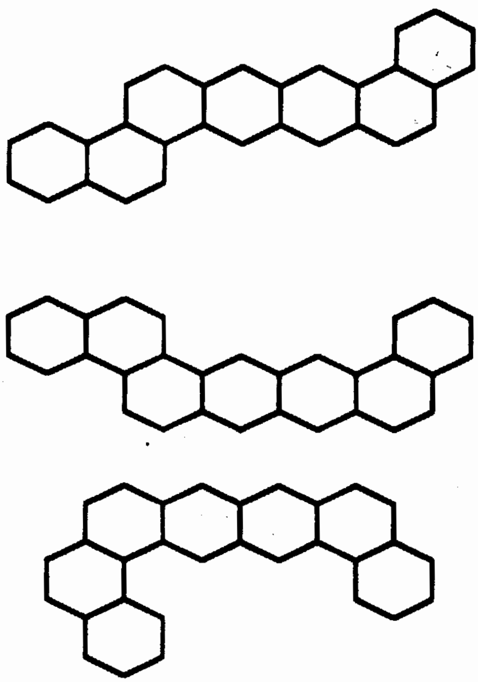

Fig. 4

The classical paper of Gordon and Davison [12] contains a general algorithm for the enumeration of Kekule structures (K numbers) of benzenoid chains and branched catacondensed benzenoids (see also [24]). Cyvin [7] gave an alternative derivation for the case of unbranched chains. This case was revisited by Cyvin and Gutman [9], who produced a useful modification of the Gordon and Davison algorithm. Tošić [20] gave an improved algorithm of time complexity O(n) for calculating the number of Kekule structures of an arbitrary benzenoid chain composed from n linearly condensed segments.

The identification of the number of Kekule structures for a zigzag chain with the Fibonacci numbers was mentioned already by Gordon and Davison [12]. The explicit formula corresponding to Binet's formula was first given by Yen [25] and independently by Cvetkovic and Gutman [6]. Cyvin [8] rederived the connection between Fiboncci numbers and the number of Kekule structures for zigzag chains, and supplemented the treatment by group-theoretical considerations of symmetry. A treatise on three connections betwen Fibonacci numbers and Kekule structures is due to Balaban and Tomescu [4]; see also Hosoya [16].

Balaban and Tomescu [2] elaborated a procedure for producing algebraic formulas for the K number of an arbitrary catacondensed benzenoid. Tošić and Bodroža [21, 22] gave two different explicit formulas for the K number of an arbitrary benzenoid chain.

Many other papers have apperaed on the problem of finding the "Kekule structure count" for hydrocarbons. We must mention here also Trinajstic [24], Hosoya and Yamaguchi [17] and Sachs [19]. A whole recent book [10] is devoted to Kekule structures in benzenoid hydrocarbons.

We denote by $< x_1, x_2, ..., x_n >$ the class of isoarithmic benzenoid chains with the LA-sequence

$$L^{x_1} A L^{x_2} A ... A L^{x_{n-1}} A L_{x_n}, \tag{1}$$

where $n \geq 1$, and $x_1 \geq 1$, $x_n \geq 1$, $x_i \geq 0$, for $i = 2, 3, ..., n-1$.

Figure 2 shows a $< 3, 2, 3, 0, 2 >$.

It is easy to see that each benzenoid chain can be represented in this form.

We see that a benzenoid chain $< x_1, x_2, ... x_n >$ has $n - 1$ A mode hexagons (kinks) each of them separating two linear segments consisting entirely of L mode hexagons.

Clearly, the number of hexagons of benzenoids chains with the LA-sequence (1) is $h = x_1, +x_2, +..., +, x_n +, n-1$.

We denote by $K_n < x_1, x_2, ..., x_n >$ the number of Kekule structures of the chain $< x_1, x_2, ..., x_n >$.

Obviously, $K_n < x_1, ..., x_n > = K_n < x_n, ..., x_1 >$.

Let F_i be the i-th Fibonacci number, defined as follows:

$F_0 = 0,\ F_1 = 1\ ; F_k = F_{k-1} + F_{k-2}$, for $k \geq 2$.

$\lfloor x \rfloor$ denotes the greates integer $\geq x$.

For all other definitions see [10] .

2. Recurence relation and algebraic exspression for $K_n < x_1, ..., x_n >$

It is easy to deduce the K formula for a single linear chain (polyacene) of x_1 hexagons, say $< x_1 >$ (see [12] and [10]):

$$K_1 < x_1 > = 1 + x_1. \tag{2}$$

We define

$$K_0 = 1. \tag{3}$$

It may be interpreted as the number of Kekule structures for "no hexagons".

Theorem 1. *If $n \geq 2$ then for arbitrary $x_1 \geq 1,\ x_n \geq 1,\ x_i \geq 0, (i = 2, ..., n-1)$, the following recurrence relation holds:*

$$\begin{aligned} &K_n < x_1, ..., x_{n-1}, x_n > \\ &= (x_n + 1) K_{n-1} < x_1, ..., x_{n-1} > + K_{n-2} < x_1, ..., x_{n-2} > . \end{aligned} \tag{4}$$

Proof. Let H be the last kink (A mode hexagon) of $< x_1, ..., x_n >$ and u and v be the vertices belonging only to hexagon H (Fig. 5). We apply the method of fragmentation [18,10] by attacking the bond uv (Fig. 5).

Every perfect matching (Kekule structure) containing the double bond uv does not contain any other edge belonging only to H. The rest of such a perfect matching will be the perfect matching of the graph consisting of two components: $< x_n >$ and $< x_1, ..., x_{n-1} >$ (Fig. 5a). The number of such perfect matchings is $K_1 < x_n > K_{n-1} < x_1, ..., x_{n-1} >$, i.e., according to (2),

$$(x_n + 1)K_{n-1} < x_1, ..., x_{n-1} > . \tag{5}$$

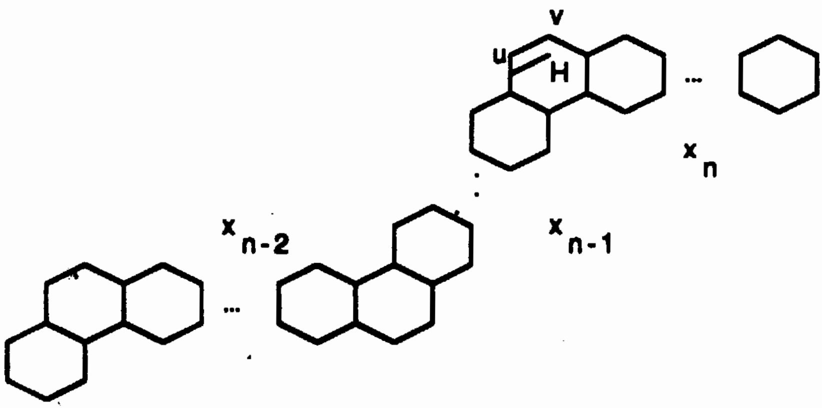

Fig. 5*a*

On the other hand, each perfect matching not containing uv (uv is a single bond in the corresponding Kekule structure) must contain all the double bonds indicated in Fig. 5*b*. The rest of such a perfect matching will be a perfect matching of $< x_1,\ x_2, ..., x_{n-2} >$ and the number of such perfect matchings is

$$K_{n-2} < x_1, ..., x_{n-2} > . \tag{6}$$

The recurrence relation (4) follows from (5) and (6).

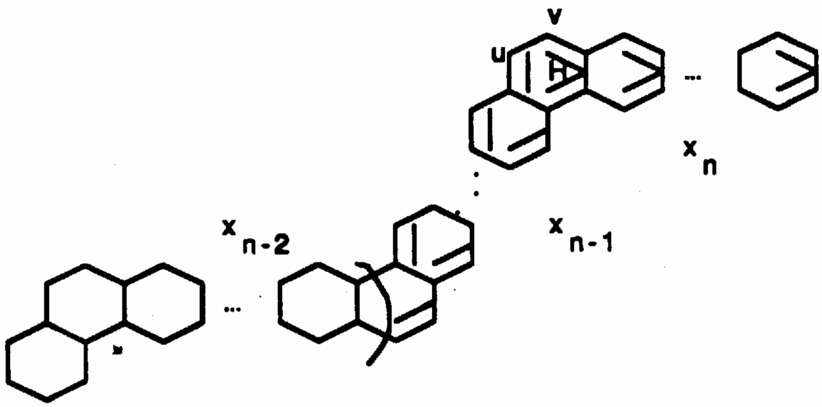

Fig. 5*b*

Theorem 2. *Let* $x_1 \geq 1$, $x_n \geq 1$; $x_i \geq 0$ *for* $i = 2, ..., n-1$. *Then*

$$K_n < x_1, ..., x_{n-1}, x_n >= F_{n+1} +$$

$$+ \sum_{\substack{0<i_1<...<i_k\leq n, \\ 1\leq k\leq n}} F_{n+1-i_k} F_{i_k-i_{k-1}} ... F_{i_2-i_1} F_{i_1} x_{i_1} x_{i_2} ... x_{i_k}. \tag{7}$$

Proof. According to (2), (3) and (4), $K_n < x_1, ..., x_n >$ is, obviously, a polynomal of the form

$$K_n < x_1, ..., x_n >= c_n^0 + \sum_{\substack{0<i_1<...<i_k\leq n, \\ 1\leq k\leq n}} c_n(i_1, ..., i_k) x_{i_1} ... x_{i_k}.$$

Theorem 2 follows from the following two lemmas.

Lemma 3.

$$c_n^0 = F_{n+1}. \tag{8}$$

Lemma 4.

$$c_n(i_1, ..., i_k) = F_{n+1-i_k} F_{i_k-i_{k-1}} ... F_{i_2-i_1} F_{i_1}. \tag{9}$$

Both lemmas can be proved by induction.

Proof of Lemma 3. According to (3) and (2), $c_0^0 = 1 = F_1$, and $c_1^0 = 1 = F_2$. Suppose that $c_{n-2}^0 = F_{n-1}$ and $c_{n-1}^0 = F_n$. Then, according to (4), $c_n^0 = c_{n-1}^0 + c_{n-2}^0 = F_n + F_{n-1} = F_{n+1}$.

Proof of Lemma 4. The statement can be easyly checked for $K_0 = 1, K_1 < x_1 >= 1 + x_1$, and also for $K_2 < x_1, x_2 >= (x_2 + 1)(1 + x_1) + 1 = 2 + x_1 + x_2 + x_1 x_2$. Suppose that

$$c_{n-1}(i_1, ..., i_k) = F_{n-i_k} F_{i_k - i_{k-1}} ... F_{i_2 - i_1} F_{i_1},$$

for

$$0 < i_1 < ... < i_k \leq n-1,\ 1 \leq k \leq n-1,$$

and

$$c_{n-2}(i_1, ... i_k) = F_{n-1-i_k} F_{i_k - i_{k-1}} ... F_{i_2 - i_1} F_{i_1},$$

for

$$0 < i_1 < ... < i_k \leq n-2,\ 1 \leq k \leq n-2.$$

Consider now $c_n(i_1, ..., i_k)$, where $0 < i_1 < ... < i_k \leq n$ and $1 \leq k \leq n$.

If $i_k = n$, then, according to (4), $c_n(i_1, ..., i_{k-1}, n) = c_{n-1}(i_1, ..., i_{k-1})$, i.e., by induction hypothesis,

$$c_n(i_1, ..., i_{k-1}, i_k) = F_{n-i_{k-1}} F_{i_{k-1} - i_{k-2}} ... F_{i_2 - i_1} F_{i_1} =$$

$$= F_{n+1-n} F_{n-i_{k-1}} F_{i_{k-1} - i_{k-2}} ... F_{i_2 - i_1} F_{i_1}.$$

(We used the fact that $F_{n+1-n} = F_1 = 1$).

If $i_k = n-1$ then, according to (4),

$$c_n(i_1, ..., i_{k-1}, n-1) = c_{n-1}(i_1, ..., i_{k-1}, n-1),$$

i.e., by induction hypothesis,

$$c_n(i_1, ..., i_{k-1}, n-1) = F_{n-(n-1)} F_{n-1-i_{k-1}} ... F_{i_2 - i_1} F_{i_1} =$$

$$= F_1 F_{n-1-i_{k-1}} ... F_{i_2 - i_1} F_{i_1} = F_2 F_{n-1-i_{k-1}} ... F_{i_2 - i_1} F_{i_1} =$$

$$= F_{(n+1)-(n-1)} F_{n-1-i_{k-1}} ... F_{i_2 - i_1} F_{i_1}.$$

(We used the fact that $F_{(n+1)-(n-1)} = F_2 = F_1 = F_{n-(n-1)} = 1$.)

If $i_k < n-1$, then, according to (4)

$$c_n(i_1,...,i_{k-1},i_k) = c_{n-1}(i_1,...,i_{k-1},i_k) + c_{n-2}(i_1,...,i_{k-1},i_k),$$

i.e., by induction hypothesis,

$$c_n(i_1,...,i_k) =$$

$$= F_{n-i_k}F_{i_k-i_{k-1}}...F_{i_2-i_1}F_{i_1} + F_{n-1-i_k}F_{i_k-i_{k-1}}...F_{i_2-i_1}F_{i_1} =$$

$$= (F_{n-i_k} + F_{n-1-i_k})F_{i_k-i_{k-1}}...F_{i_2-i_1}F_{i_1} = F_{n+1-i_k}F_{i_k-i_{k-1}}...F_{i_2-i_1}F_{i_1}.$$

So, in each case, we obtain (9). Now, the proof of Theorem 2 follows from (8) and (9).

3. Some relations involving different formulas of K numbers

In [21] a benzenoid chain $L(x_1,...,x_n)$ is defined as the chain with the LA-sequence

$$L^{x_1-1}AL^{x_2-2}A...AL^{x_{n-1}-2}AL^{x_n-1},$$

where $x_i \geq 2$, for $i = 1,2,...,n$.

In this case, each of $n-1$ kinks is considered as belonging to two adjacent segments. So, the total number of hexagons in $L(x_1,...,x_n)$ is $h = x_1 + x_2 + ... + x_n - n + 1$.

In [21] it is proved that the number of Kekule structures of $L(x_1,...,x_n)$ is

$$K_n(x_1,...,x_{n-1},x_n) = (-1)^n F_{n-3} +$$

$$(10)\quad + \sum_{\substack{0<i_1<...<i_k\leq n,\\ 1\leq k\leq n}} (-1)^{n-k} F_{n-1-i_k} Fi_k - i_{k-1}...F_{i_2-i_1}F_{i_1-2}x_{i_1}...x_{i_k}.$$

Here, $F_{-1} = 1$. The formula (10) was proved by using a recurrence relation similar to (4), which also was derived in [21].

In [22] a benzenoid chain $[x_1,x_2,...,x_n]$ is defined as the chain with the LA-sequence

$$L^{x_1}AL^{x_1-1}A...AL^{x_{n-1}-1}AL^{x_n-1},$$

where $x_i \geq 1$ for $i = 1, 2, ..., n-1$ and $x_n \geq 2$. Sometimes, however, we permit $x_n = 1$, taking $[x_1, ..., x_{n-1}, 1]$ to be the same chain as $[x_1, ..., x_{n-1} + 1]$. In this case, each kink is considered as belonging to exactly one segment. It means that the first segment does not contain any kinks while each of $n-1$ remaining segments has exactly one kink which is the first hexagon of that segment. So, the total number of hexagons in $[x_1, ..., x_n]$ is $h = x_1 + x_2 + ... + x_n$

In [22] it is proved that the number of Kekule structures of $[x_1, ..., x_n]$ is

$$K_n[x_1, ..., x_n] = 1 + \sum x_{i_1} x_{i_2} ... x_{i_k}, \tag{11}$$

where the sum is taken over all subsets $\{i_1, ..., i_k\}$ of $\{1, 2, ..., n\}$ $1 \leq k \leq n$, such that $n - i_k = 0 \pmod 2$ and $i_{j+1} - i_j = 1 \pmod 2$, for $j = 1, 2, ..., k-1$ $(i_1 < i_2 < ... < i_k)$.

It is easy to see that the number of terms in the polynomial (11) is F_{n+2}, where F_i is the i-th member of Fibonacci sequence.

All the three polynomials (7), (10) and (11) possess some symmetry properties, i.e., the following statements ar true.

Theorem 3. (a) $K_n(x_1, ..., x_n) = K_n(x_n, x_{n-1}, ... x_1)$;
(b) $K_n[x_1 - 1, x_2, ..., x_n] = K_n[x_n - 1, x_{n-1}, ..., x_1]$;
(c) $K_n < x_1, ..., x_n >= K_n < x_n, ..., x_1 >$.

Proof. Follows from the fact that in each of the three cases, both the left-hand and the right-hand exspressions are equal to the number of perfect matchings of the seme graph. Namely, the order of the segments of a chain can be taken in two ways.

Having in mind the definitions of $L(x_1, ..., x_n)$, $[x_1, ..., x_n]$ and $< x_1, ..., x_n >$, it is easy to establish the following relationship for the polynomials (7), (10) and (11).

Theorem 4. *Let* $n \geq 2$. *Then*

(12) (a) $K_n(x_1, x_2, ..., x_{n-1}, x_n) = K_n[x_1 - 1, x_2 - 1, ..., x_{n-1} - 1, x_n]$,

for $x_i \geq 2$; $i = 1, 2, ..., n$;

(13)(b) $K_n(x_1, x_2, ..., x_{n-1}, x_n) = K_n' < x_1 - 1, x_2 - 2, ..., x_{n-1} - 2, x_{n-1} >$

for $x_i \geq 2;\ i = 1, 2, ..., n;$

(14)(c) $K_n[x_1, x_2, ..., x_{n-1}, x_n] = K_n < x_1, x_2 - 1, ..., x_{n-1} - 2, x_n - 1 >$

for $x_n \geq 2;\ x_i \geq 1;\ i = 1, 2, ..., n-1.$

4. Some identities involving Fibonacci numbers

Now we are going to derive some identities involving Fibonacci numbers, using the formulae (7), (10), (11), the relations (12), (13), (14) and some previously known results.

Consider first the benzenoid chain with n segments of the same lenght m. We shall denote it by $< m, m, ..., m >_n$. According to the notation adopted in [10], this chain is denoted by $W"(m+2, n+1)$. It was proved by Bergan et all [5] that the number of Kekule structures of $W"(m+2, n+1)$ is

$$K_n < m, ..., m >=$$

$$\frac{(m+1+\sqrt{(m+1)^2+4})^{n+1} - (m+1-\sqrt{(m+1)^2+4})^{n+1}}{2^{n+1}\sqrt{(m+1)^2+4}}$$

The right-hand side of the last formula can be transformed so that the last equation can be written in the form

$$K_n < m, ..., m >= \frac{2}{m+1}\sum_{k=0}^{\lfloor n/2 \rfloor} C(n,\ 2k+1)(1+\frac{4}{(m+1)^2})^k. \tag{15}$$

Here, $C(i,j) = i!/(i!(i-j)!)$ is a binomail coefficient.

On the other hand, taking $x_1 = x_2 = ... = x_n = m$, we obtain from (7) as a special case, that the number of Kekule structures of $W"(m+2, n+1)$ is

$$K_n < m, ..., m >= F_{n+1} +$$

$$+ \sum_{\substack{0 < i_1 < \ldots < i_k \leq n, \\ 1 \leq k \leq n}} m_k * F_{n+1-i_k} F_{i_k - i_{k-1}} ... F_{i_2 - i_1} F_{i_1}. \tag{16}$$

From (15) and (16) we can obtain the following identity involving Fibonacci numbers.

$$F_{n+1} + \sum_{\substack{0<i_1<\ldots<i_k\leq n,\\ 1\leq k\leq n}} m_k * F_{n+1-i_k} F_{i_k-i_{k-1}} \ldots F_{i_2-i_1} F_{i_1} = \tag{17}$$

$$= \tfrac{2}{m+1} \sum_{k=0}^{\lfloor n/2\rfloor} C(n,\ 2k+1)(1+\tfrac{4}{(m+1)^2})^k.$$

By further specialization, taking $m = 1$, from (15) and (16) we derive the following identity

$$F_{n+1} + \sum_{\substack{0<i_1<\ldots<i_k\leq n,\\ 1\leq k\leq n}} F_{n+1-i_k} F_{i_k-i_{k-1}} \ldots F_{i_2-i_1} F_{i_1} \tag{18}$$

$$= \sum_{k=0}^{\lfloor (n-1/2)\rfloor} C(n,\ 2k+1)2^k.$$

According to notation adopted in [10], $W'(m+1,\ n+1)$ denotes the benzenoid chain $[m, m, ..., m]$ with n segments. We shall denote it by $[m, ..., m]_n$. It was proved [2,3,4,10] that, for $m \geq 1$,

(19) $K(W'(m+1, n+1)) = K(W"(m+1,\ n+1)) + K(W"(m+1,\ n))$.

Having in mind (15), one can obtain by summing

$$K_n[m, ..., m] = \frac{2}{m} \sum_{k=0}^{\lfloor n/2\rfloor} \frac{2n-2k-1}{2k+1} C(n-1, 2k)(1+\frac{4}{m^2})^k. \tag{20}$$

Now, if in (11) we put $x_1 = x_2 = ... = x_n = m$, we obtain

$$1 + \sum m^k = \frac{2}{m} \sum_{k=0}^{\lfloor n/2\rfloor} \frac{2n-2k-1}{2k+1} C(n-1,\ 2k)\,(1+\frac{4}{m^2})^k, \tag{21}$$

where the sumation in the left-hand sum of (21) is taken over all subsets $\{i_1, ..., i_k\}$ of $\{1, 2, ..., n\}$, $1 \leq k \leq n$, such that $n - i_k = 0 \pmod 2$ and $i_{j+1} - i_j = 1 \pmod 2$, for $j = 1, 2, ..., k-1$ $(i_1 < i_2 < ..., < i_k)$.

Let us determine the number of subsets $\{i_1,,...,i_k\}$ of $\{1,2,...n\}$ satisfying these conditions, for given k. We map the subset $\{i_1,...,i_k\}$ into a binary sequence of lenght n such that j-th member of the sequence is equal to 1 if and only if there exist an r such that $i_r = j$. For example, $\{3,6,7\}$ is maped onto 00100110 (for $n = 8$).

The requested number of subsets is then equal to the number of sequences of 0's and 1's of the lenght n such that there are exactly k 1's and the total number of 0's following each 1 is an even number. We say such sequence to be an acceptable sequence of the lenght n with k 1's. For instance, 0001001100 is an acceptable sequence of the lenght 10.

An acceptable sequence can be produced in the following way. We partition $n-k$ 0's, in blocks, each block consisting of two adjacent 0's, only the first block is permitted to consist of one 0. Now, k 1's can be distributed among blocks (excluding the begining of the sequence if the first block consists of one 0) in $C(k+\lfloor\frac{n-k}{2}\rfloor, k)$ ways. Namely, we have combinations of k 1's out of $k+\lfloor\frac{n-k}{2}\rfloor$ elements, where $\lfloor\frac{n-2}{2}\rfloor$ is the number of blocks (i.e. pairs of 0's).

So, there are $C(0+\lfloor\frac{n-k}{2}\rfloor,\ k)$ subsets $\{i_1,...,i_k\}$ satisfying the conditions reqested in (21).

Taking into account that $C(0+\lfloor\frac{n-0}{2}\rfloor,\ 0) = 1$, (21) can be written in the form

$$(22)\sum_{k=0}^{n} C(k+\lfloor\frac{n-k}{2}\rfloor, k)m^k = \frac{2}{m}\sum_{k=0}^{\lfloor n/2\rfloor}\frac{2n-2k+1}{2k+1}C(n,\ 2k)(1+\frac{4}{m^2})^k,$$

for $m \geq 2$.

Specialy, for $m = 2$, we obtain

$$(23)\qquad \sum_{k=0}^{n} C(k+\lfloor(n-k)/2\rfloor, k)2^k = \sum_{k=0}^{\lfloor n/2\rfloor}\frac{2n-2k+1}{2k+1}C(n,\ 2k)2^k.$$

Note also the following identity:

$$(24)\qquad \sum_{k=0}^{n} C(k+\lfloor(n-2)/k\rfloor, k) = F_{n+2}.$$

It follows easily by proving that total number of acceptable sequences of the length n is F_{n+2}.

Indeed, if we denote by $f(n)$ the number of acceptable sequences of the lenght n, then, obviously, $f(1) = 2$, $(0,1)$, $f(2) = 3$ (00, 01, 11). We can take that $f(0) = 1$. Now, the number of acceptable sequences of the lenght n with the last digit 1 is $f(n-1)$, and the number of those with the last digit 0 is $f(n-2)$ (since, in that case the sequence must end with at least two 0's). It follows that $f(n) = f(n-1) + f(n-2)$, for $n \geq 3$. Taking into account that the initial terms are $f(1) = 2 = F_3$, $f(2) = 3 = F_4$, it follows that $f(n) = F_{n+2}$.

Consider now the benzenoid chain denoted by $W(m+1, n+1)$, $m \geq 1$, according to the notation adopted in [10]. In our notation (see also [4]) it is denoted by $L_n(m+1, ..., m+1)$ It means that it consists of n segments. Its LA-sequence is $L^m AL^{m-1}A...AL^{m-1}AL^m)$ and the total number of hexagons is $h = nm + 1$.

For this class, Balaban and Tomescu [8] found that

$$K(B) = \frac{1}{\sqrt{m^2+4}}(\sqrt{m^2+4}+2)(\frac{m+\sqrt{m^2+4}}{2})^n + (\sqrt{m^2+4}-2)(\frac{m-\sqrt{m^2+4}}{2})^n). \tag{25}$$

Our general formula (10) (see also [12]), in the special case, $x_1 = x_2 = ... = x_n = m + 1$, gives, for the same benzenoid system B

$$K(B) = (-1)^n F_{n-3} + \sum_{\substack{0<i_1<...<i_k \leq n, \\ 1 \leq k \leq n}} (-1)^{n-k} F_{n-1-i_k} F_{i_k - i_{k-1}} ... F_{i_2-i_1} F_{i_1-2} (m+1)^k. \tag{26}$$

We shall write exsplicitly only an identity which can be derived from (25) and (26) in a special case. When $m = 1$, the formula (25) for $K(B)$ reduces to F_{n+3}. If we put in (26) $m = 1$, then we have the following interesting identity

$$\sum_{\substack{0<i_1<...<i_k \leq n, \\ 1 \leq k \leq n}} (-1)^{n-k} 2^k F_{n-1-i_k} F_{i_k-i_{k-1}} ... F_{i_2-i_1} F_{i_1-2} = F_{n+3} + (-1)^{n+1} F_{n-3}. \tag{27}$$

References

[1] Balaban, A.T., Artemi, C., Tomescu, I., Algebraic exspresions for Kekule structure counts of non-branched regularly cata-condensed benzenoid hydrocarbons, MATCH 22 (1987), 77-100.

[2] Balaban, A.T., Tomescu, I., Algebraic expressions for the number of Kekule structure of isoarithmic cotacondensed benzenoid polycyclic hydrocarbons, MATCH 14 (1983), 155-182.

[3] Balaban, A.T., Tomescu, I., Chemical graphs - XLI - Numbers of conjugated circuitis and Kekule structures for zigzag catafusenes and (j, k)-hexes- generalized Fibonacci Numbers, MATCH 17 (1985), 91-120.

[4] Balaban, A.T., Tomescu, I., Chemical graphs - XL - Three relations between the Fibonacci sequence and the numbers of Kekule structures for non- branched catacondensed polycyclic aromatic hydrocarbons, Croat. Chem. Acta 57 (3) (1984), 391-404.

[5] Bergen, J.L., Cyvin, B.N., Cyvin, S.J., The Fibonacci numbers and Kekule structures of some corona-condensed benzenoids (corannulens), Acta Chim. Hung. 124 (1987), 299.

[6] Cvetkovic, D., Gutman, I., Kekule structures and topology - II - Cotacondensed systems, Croat. Chem. Acta 46 (1974), 15.

[7] Cyvin, S.J., Numbers of Kekule structures of single-chain aromatics, Monatsh. Chem. 114 (1983), 13-20.

[8] Cyvin, S.J., Kekule structures and the Fibonacci series, Acta Chim. Hung. 112 (1983), 281.

[9] Cyvin, S.J., Gutman, I., Topological properties of benzenoid systems - Part XXXVI - Algorithm for the number of Kekule structures in some pericondensed benzenoids, MATCH 19 (1986), 229-242.

[10] Cyvin, S.J., Gutman, I., Kekule structures in benzenoid hydrocarbons, Lecture Notes in Chemistry 46, Springer-Verlag, Berlin, 1988.

[11] Farell, E.J., Wahid, S.A., Matchings in pentagonal chains, Discr. Apll. Match. 7 (1984), 31-40.

[12] Gordon, M., Davison, W.H.T., Resonance topology of fully aromatic hydrocarbons, J. Chem. Phys. 20 (1952), 428-435.

[13] Gutman, I., Topological properties of benzenoid systems - An identity for the sextet polynomal, Theor. Chim. Acta 45 (1977), 309.

[14] Gutman, I., Topological properties of benzenoid systems - XXI - Theorems, conjectures, unsolved problems, Croat. Chem. Acta 56 (3) (1983), 365-374.

[15] Herndon, W.C., Resonance theory and the enumeration of Kekule structures, J. Chem. Educ. 51 (1974), 10-15.

[16] Hosoya, H., Topological index and Fibonacci numbers with relation to chemistry, Fibonacci Quarterly 11 (1973), 255-269.

[17] Hosoya, H., Yamaguchi, T., Sextet polynomal, a new enumeration and proof techiniques for the resonance theory applied to the aromatic hydrocarbons, Tetrahedron Letters 52 (1975), 4659-4662.

[18] Lovacz, L., Plummer, M.D., Matching theory Akademiai Kiado, Budapest, 1986.

[19] Sachs, H., Perfect matchings in hexagonal systems, Combinatorica 4 (1) (1984), 89-99.

[20] Tosic, R., A fast algorithm for calculating the number of Kekule structures of unbranched benzenoid chains, (submitted for publication).

[21] Tosic, R., Bodroza, O., An algebraic expression for the number of Kekule structures of benzenoid chains, Fib. Quartely, (to appear).

[22] Tosic, R., Bodroza, O., On the number of Kekule structures of unbranched benzenoid chains, (accepted in MATCH).

[23] Tosic, R., Stojmenovic, I., Some combinatorial consequence of Clars resonant sextet theory, (submitted for publication).

[24] Trinajstic, N., Chemical graph theory, CRC Press, Boca Raton, FL, 1983.

[25] Yen, T.F., Resonance topology of polynuclear aromatic hydrocarbons, Theor. Chim. Acta 20 (1971), 399.

Received by the editors April 15, 1991