FIBONACCI NUMBERS AND THE NUMBERS OF PERFECT MATCHINGS OF SQUARE, PENTAGONAL, AND HEXAGONAL CHAINS*

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1. Some Preliminaries

Let G be a finite graph. A *perfect matching* in G is a selection of edges in G such that each vertex of G belongs to exactly one selected edge. Therefore, if the number of vertices in G is odd, then there is no perfect matching. We denote by $K(G)$ the number of perfect matchings of G, and refer to it as the *K number* of G.

By a polygonal *chain* $P_{k,s}$ we mean a finite graph obtained by concatenating s k-gons in such a way that any two adjacent k-gons (cells) have exactly one edge in common, and each cell is adjacent to exactly two other cells, except the first and last cells (end cells) which are adjacent to exactly one other cell each. It is clear that different polygonal chains will result, according to the manner in which the cells are concatenated.

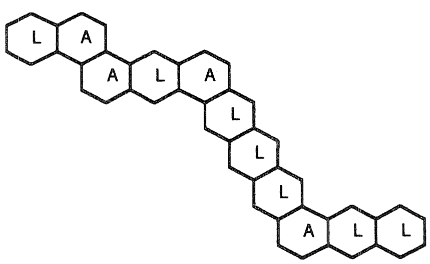

Figure 1

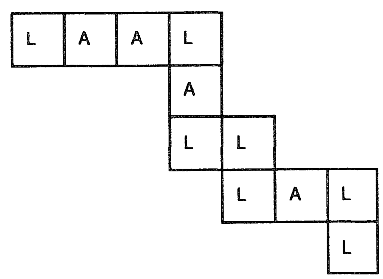

Figure 2

Figure 1 shows a hexagonal chain $P_{6,11}$. The *LA-sequence* of a hexagonal chain is defined in [11] as follows. A hexagonal chain $P_{6,s}$ is represented by a word of the length s over the alphabet $\{A, L\}$. The i^{th} letter is A (and the corresponding hexagon is called a *kink*) iff $1 < i < s$ and the i^{th} hexagon has an edge that does not share a common vertex with any of two neighbors. Otherwise, the i^{th} letter is L. For instance, the hexagonal chain in Figure 1 is represented by a word $LAALALLLALL$, or, in abbreviated form $LA^2LAL^3AL^2$. The LA-sequence of a hexagonal chain may always be written in the form

$$P_6\langle x_1, \ldots, x_n\rangle = L^{x_1}AL^{x_2}A \ldots AL^{x_n},$$

where $x_1 \geq 1$, $x_n \geq 1$, $x_i \geq 0$, for $i = 2, 3, \ldots, n-1$. For instance, the LA-sequence of the hexagonal chain in Figure 1 may be written in the form

$$P_6\langle 1, 0, 1, 3, 2\rangle = LAL^0ALAL^3AL^2.$$

It is well known that the number of a hexagonal chain is entirely determined by its LA-sequence, no matter which way the kinks go ([1], [10], [12]). In [1]

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the term "isoarithmicity" for this phenomenon is coined. Thus,

$$P_6\langle x_1,\ x\ ,\ \ldots,\ x_n\rangle$$

represents a class of isoarithmic hexagonal chains.

Figure 2 above shows a square chain $P_{4,11}$. We introduce a representation of square chains in order to establish a mapping between square and hexagonal chains that will enable us to obtain the K numbers for square chains. A square chain $P_{4,s}$ is represented by a word of the length s over the alphabet $\{A, L\}$, also called its *LA-sequence*. The i^{th} letter is A iff each vertex of the i^{th} square also belongs to an adjacent square. Otherwise, the i^{th} letter is L. For instance, the square chain in Figure 2 above is represented by the word $LAALALLLALL$, or, in abbreviated form $LA^2LAL^3AL^2$. Clearly, the LA-sequence of a square chain may always be written in the form

$$P_4\langle x_1,\ \ldots,\ x_n\rangle = L^{x_1}AL^{x_2}A\ \ldots\ AL^{x_n},$$

where $x_1 \geq 1$, $x_n \geq 1$, $x_i \geq 0$, for $i = 2, 3, \ldots, n - 1$. For example, the LA-sequence of the square chain in Figure 2 may be written in the form

$$P_4\langle 1,\ 0,\ 1,\ 3,\ 2\rangle = LAL^0ALAL^3AL^2.$$

We show below that all square chains of the form

$$P_4\langle x_1,\ \ldots,\ x_n\rangle$$

are isoarithmic.

We will draw pentagonal chains so that each pentagon has two vertical edges and a horizontal one which is adjacent to both vertical edges. The common edge of any two adjacent pentagons is drawn vertical. We shall call such a way of drawing a pentagonal chain the *horizontal representation* of that pentagonal chain. From the horizontal representation of a pentagonal chain one can see that it is composed of a certain number (≥ 1) of segments; namely, two adjacent pentagons belong to the same segment iff their horizontal edges are adjacent. We denote by

$$P_5\langle x_1,\ x_2,\ \ldots,\ x_n\rangle$$

the pentagonal chain consisting of n segments of lengths $x_1, x_2, \ldots, x_n$, where the segments are taken from left to right. Figure 4a below shows

$$P_5\langle 3,\ 2,\ 4,\ 8,\ 5\rangle.$$

Notice that one can assume that $x_1 > 1$ and $x_n > 1$.

Among all polygonal chains, the hexagonal chains were studied the most extensively, since they are of great importance in chemistry, namely, benzenoid hydrocarbon chains. Each perfect matching of a hexagonal chain corresponds to a Kekulé structure of the corresponding benzenoid hydrocarbon. The stability and other properties of these hydrocarbons have been found to correlate with their K numbers. The classical paper [10] contains a general algorithm for the enumeration of Kekulé structures (K numbers) of benzenoid chains and branched catacondensed benzenoids. The algorithm is modified in [6]. An alternative derivation for the case of unbranched chains is described in [4]. In [17] Tosić proposed an algorithm of time complexity $O(n)$ for calculating the number of Kekulé structures of an arbitrary benzenoid chain composed from n linearly condensed segments. The explicit formulas, in terms of the Fibonacci numbers, for the number of Kekulé structures for a zigzag chain were given in [20], [3], and [5]. We will re-derive the formula for K numbers of zigzag chains as a special case of a new general formula. A treatise on three connections between Fibonacci numbers and Kekulé structures is presented in [2] and [15]. A procedure for producing algebraic formulas for the K number of an arbitrary catacondensed benzenoid is elaborated in [1]. Two different explicit formulas for the K number of an arbitrary benzenoid chain are given in [18] and [19]. A whole recent book [7] is devoted to Kekulé structures in benzenoid hydrocarbons. It contains a list of other references on the problem of finding the "Kekulé structure count" for hydrocarbons.

In [14] Gutman & Cyvin investigated the connection between the square and hexagonal chains, and derived the number of a graph $Q_{p,q}$, which is a chain composed of $p + q + 1$ squares, and, in our notation, is denoted by

$$LA^{p-1}LA^{q-1}L\colon\ K(Q_{p,q}) = F_{p+q+2} + F_{p+1}F_{q+1}.$$

In the present paper, we investigate the K number of an arbitrary square chain; the above formula will follow as a special case of a general result.

In [8] and [9] Farrell investigated the K numbers of pentagonal chains of particular forms. The obtained results are special cases of a general formula which will be deduced here.

2. K Numbers of Hexagonal Chains

Recently Tošić and Bodroza [18] proved a recurrence relation and a formula for the K numbers of hexagonal chains using a notation that counts every kink twice. Motivated by the possibility of mapping square and pentagonal chains to hexagonal ones, here we use a different notation that leads to a new recurrence relation and formula. The proofs are omitted because they can be obtained along the same lines as the proofs of Theorems 1 and 2 from [18].

The K formula for a single linear chain (polyacene) of x_1 hexagons, i.e., $P_6\langle x_1\rangle$ is deduced in [10] and [7]. We define $P_6\langle\ \rangle$ as the hexagonal chain with "no hexagons."

Theorem 1: $K(P_6\langle\ \rangle) = 1$, $K(P_6\langle x_1\rangle) = 1 + x_1$,

$$K(P_6\langle x_1, \ldots, x_{n-1}, x_n\rangle) = (x_n + 1)K(P_6\langle x_1, \ldots, x_{n-1}\rangle) + K(P_6\langle x_1, \ldots, x_{n-2}\rangle) \text{ for } n \geq 2.$$

Theorem 2: $K(P_6\langle x_1, \ldots, x_{n-1}, x_n\rangle) =$

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

3. K Number of a Square Chain

Theorem 3: $K(P_4\langle x_1, \ldots, x_{n-1}, x_n\rangle) = K(P_6\langle x_1, \ldots, x_{n-1}, x_n\rangle)$.

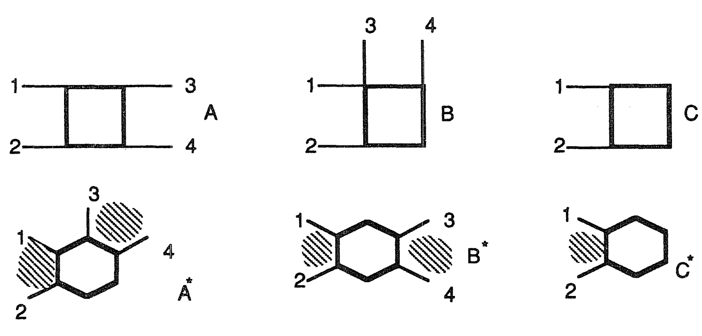

Figure 3

Proof: Referring to Figure 3, it is easy to see that if in a square chain some (or all) structural details of the type A, B, and C are replaced by A*, B*, and C*, respectively, the K number will remain the same. By accomplishing such replacements, each square chain can be transformed into a hexagonal chain with the same LA-sequence. Therefore, a square chain and corresponding hexagonal chain represented by the same LA-sequence have the same K number. For example, the square chain in Figure 2 can be transformed into the hexagonal chain in Figure 1. Note that the corner squares of a square chain correspond to the linear hexagons, and vice versa, in this transformation. □

Thus, the K numbers for square chains are also given by Theorem 2. It is clear that all other properties concerning the K numbers of square chains can be derived from the corresponding results for hexagonal chains and that the investigation of square chains as a separate class from that point of view is of no interest.

Note that the formula

$$K(Q_{p,q}) = F_{p+q+2} + F_{p+1}F_{q+1}$$

of Gutman & Cyvin [14] for the chain $LA^{p-1}LA^{q-1}L$ can be derived from Theorem 2 as a special case. Namely, in the LA-sequence of $Q_{p,q}$, we have

$$n = p + q - 1; \quad x_1 = x_p = x_{p+q-1} = 1; \quad x_i = 0 \text{ for } i \neq 1,\ p,\ p+q-1,$$

and

$$\begin{aligned} K(Q_{p,q}) &= F_{p+q} + F_{p+q-1}F_1 + F_qF_p + F_1F_{p+q-1} + F_qF_{p-1}F_1 + F_1F_{p+q-2}F_1 \\ &\quad + F_1F_{q-1}F_p + F_1F_{q-1}F_{p-1}F_1 \\ &= (F_{p+q} + 2F_{p+q-1} + F_{p+q-2}) + (F_p + F_{p-1})F_q + (F_p + F_{p-1})F_{q-1} \\ &= F_{p+q+2} + F_{p+1}F_q + F_{p+1}F_{q-1} \\ &= F_{p+q+2} + F_{p+1}F_{q+1}. \end{aligned}$$

K Number of a Pentagonal Chain

First, recall a general result concerning matchings of graphs. Let G be a graph and u, x, y, v its distinct vertices, such that ux, xy, yv are edges of G, u and v are not adjacent, and x and y have degree two. Let the graph H be obtained from G by deleting the vertices x and y and by joining u and v. Conversely, G can be considered as obtained from H by inserting two vertices (x and y) into the edge of uv. We say that G can be *reduced* to H, or that G is reducible to H; clearly $K(G) = K(H)$ [13].

Theorem 4: If $x_1 + x_2 + \cdots + x_n$ is odd, then

$$K(P_5\langle x_1, \ldots, x_n\rangle) = 0.$$

Otherwise (i.e., if the sequence $x_1, x_2, \ldots, x_n$ contains an even number of odd integers), let

$$s(j_1),\ s(j_2),\ \ldots,\ s(j_t) \quad (j_1 < j_2 < \cdots < j_t)$$

be the odd numbers in the sequence

$$s(r) = x_1 + \cdots + x_r \quad (r = 1, 2, \ldots, n),$$

and let $s(j_0) = -1$ and $s(j_{t+1}) = s_n + 1$; then

$$K(P_5\langle x_1, \ldots, x_n\rangle)$$

$$= F_{t+2} + \sum_{\substack{0 = i_0 < i_1 < \cdots < i_r \le t+1 \\ 1 \le r \le t+1}} (F_{t+2-i_r})/2^r \prod_{\ell=1}^{r} (s(j_{i_\ell}) - s(j_{i_\ell - 1}) - 2)F_{i_\ell - i_{\ell-1}}.$$

Proof: Clearly a pentagonal chain consisting of p pentagons has $3p+2$ vertices. Hence, a pentagonal chain with an odd number of pentagons has no perfect matching. Therefore, we assume that it has an even number of segments of odd length.

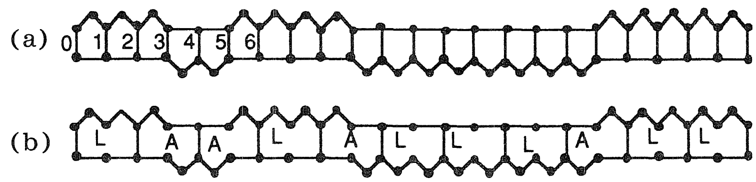

Figure 4

Consider a horizontal representation of $P\langle x_1, x_2, \ldots, x_n\rangle$ (Fig. 4a). Label the vertical edges 0, 1, ..., s_n, from left to right. Clearly no edge labeled by an odd number can be included in any perfect matching of $P_5\langle x_1, x_2, \ldots, x_n\rangle$ since there are an odd number of vertices on each side of such an edge. By removing all edges labeled with odd numbers, we obtain an octagonal chain consisting of $s_n/2$ octagons (Fig. 4b). This octagonal chain can be reduced to a hexagonal chain with $s_n/2$ hexagons (Fig. 1). It is evident that in the process of reduction, each octagon obtained from the two adjacent pentagons of the same segment becomes an L mode hexagon, while each octagon obtained from the two adjacent pentagons of different segments becomes a kink. The number of kinks is t, since each kink corresponds to an odd $s(r)$. It means that this hexagonal chain consists of $t+1$ segments. Let y_i be the number of L mode hexagons in the i^{th} segment. Then

$$y_1 = (s(j_1) - 1)/2 = (s(j_1) - s(j_0) - 2)/2$$

$$y_{t+1} = (s(n) - s(j_t) - 1)/2 = (s(j_{t+1}) - s(j_t) - 2)/2,$$

and, for $2 \le i \le t$,

$$y_i = (s(j_i) - s(j_{i-1}) - 2)/2.$$

Since reducibility preserves K numbers, it follows that

$$K(P_5\langle x_1, x_2, \ldots, x_n\rangle) = K(P_6\langle y_1, y_2, \ldots, y_{t+1}\rangle)$$

$$= F_{t+2} + \sum_{\substack{0 = i_0 < i_1 < \cdots < i_r \le t+1 \\ 1 \le r \le t+1}} F_{t+2-i_r} \prod_{\ell=1}^{r} y_{i_\ell} F_{i_\ell - i_{\ell-1}},$$

which gives, by taking into account the values for y_i, the expression in Theorem 4. □

Now we shall consider some special cases of Theorem 4 in order to derive some useful consequences. As a first specialization, we shall take the regular pentagonal chains, defined as follows. If all segments of a pentagonal chain are of the same length $m(x_1 = x_2 = \cdots = x_n = m)$, we say that it is a *regular pentagonal chain* and denote it by $P_5\langle m^n\rangle$ (similar notation will be used for a regular subchain of a chain).

Theorem 5: Let m and n be positive integers, m odd and n even ≥ 6. Then

$$K(P_5\langle m^n\rangle) = (m+1)^2(F_{n/2} + Q_{(n-2)\ 2}(m-1))/4 + (m+1)(F_{(n-2)/2} + Q_{(n-4)/2}(m-1)) + F_{(n-4)/2} + Q_{(n-6)/2}(m-1),$$

where

$$Q_n(m) = \sum_{\substack{0 = i_0 < i_1 < \cdots < i_r < i_{r+1} \le n+1 \\ 1 \le r \le n}} m^r \prod_{\ell=1}^{r+1} F_{i_\ell - i_{\ell-1}} \quad \text{for } n \ge 1 \text{ and } Q_0(m) = 0.$$

Proof: Let $m = 2k + 1$, $n = 2p$. Then $t = p + 1$ and $y_1 = y_{p+1} = k$, $y_i = 2k$, for $i = 2, 3, \ldots, t$. Hence

$$K(P_5\langle m^n\rangle) = K(P_5\langle k, 2k^{p-1}, k\rangle).$$

Applying Theorem 1 and property $K(P_5\langle x_1, \ldots, x_n\rangle) = K(P_5\langle x_n, \ldots, x_1\rangle)$ we obtain

$$K(P_5\langle k, 2k^{p-1}, k\rangle) = (k + 1)K(P_5\langle 2k^{p-1}, k\rangle) + K(P_5\langle 2k^{p-2}, k\rangle),$$

$$K(P_5\langle 2k^{p-1}, k\rangle) = (k + 1)K(P_5\langle 2k^{p-1}\rangle) + K(P_5\langle 2k^{p-2}\rangle),$$

and

$$K(P_5\langle 2k^{p-2}, k\rangle) = (k + 1)K(P_5\langle 2k^{p-2}\rangle) + K(P_5\langle 2k^{p-3}\rangle).$$

It follows that

$$K(P_5\langle k, 2k^{p-1}, k\rangle) = (k + 1)^2K(P_5\langle 2k^{p-1}\rangle) + 2(k + 1)K(P_5\langle 2k^{p-2}\rangle) + K(P_5\langle 2k^{p-3}\rangle).$$

Thus,

$$K(P_5\langle m^n\rangle) = 1/4(m + 1)^2K(P_5\langle m - 1^{(n-2)/2}\rangle) + (m + 1)K(P_5\langle m - 1^{(n-4)/2}\rangle) + K(P_5\langle m - 1^{(n-6)/2}\rangle).$$

The statement follows by applying Theorem 2. □

We note that all results by Farrell in [9] and other papers concerning the numbers of perfect matchings of pentagonal chains are very special cases of Theorem 5 (which is a special case of Theorem 4).

Corollary 1: $K(P_5\langle 1^{2k}\rangle) = F_{k+2}$.

Proof: Follows as a special case of Theorem 5 when $m = 1$. Then, obviously, $Q_n(1) = 0$ and we have, for $n = 2k$,

$$K(P_5\langle 1^{2k}\rangle) = F_k + 2F_{k-1} + F_{k-2} = F_{k+2}. \quad □$$

Clearly, in this special case, the process of reduction results in a zigzag hexagonal chain, with the LA-sequence $LA^{k-2}L$. This is in accordance with the previously known result for the number of zigzag hexagonal chains derived in [20], [3], and [5].

Corollary 2: Let $x_1, x_2, \ldots, x_n$ be all even positive integers, $n \geq 1$. Then

$$K(P_5\langle x_1, \ldots, x_n\rangle) = (x_1 + \cdots + x_n)/2 + 1.$$

Proof: Since all partial sums $s(r)$ in Theorem 4 are even, no kink is obtained in the process of reduction to a hexagonal chain. Thus, a linear hexagonal chain consisting of $h = (x_1 + x_2 + \cdots + x_n)/2$ hexagons is obtained (i.e., $P_6\langle h\rangle = L^h$). According to [7], we have $K(P_6\langle h\rangle) = h + 1$; hence,

$$K(P_5\langle x_1, \ldots, x_n\rangle) = h + 1. \quad □$$

In the special case of Corollary 2, when $n = 1$, we obtain a *uniform* pentagonal chain, i.e., a pentagonal chain consisting of only one segment. Several results concerning the matchings of the uniform pentagonal chains, including the K number, are deduced in [8] by application of matching polynomials, which, in the case when the perfect matchings are in question, is a very involved technique. Here we generalize the result by deriving the formula for the K number of an arbitrary pentagonal chain, using a much simpler technique.

Corollary 3: Let m be an odd positive integer >1. Then

$$K(P_5\langle m^2\rangle) = (m^2 + 2m + 5)/4; \quad K(P_5\langle m^4\rangle) = (m^3 + 2m^2 + 5m + 4)/4.$$

Proof: Follows as a special case of Theorem 5.

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