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Sequences of Polyomino and Polyhex Graphs whose Perfect Matching Numbers are Fibonacci or Lucas Numbers: The Golden Family Graphs of a New Category

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Abstract. Several sequences of graphs are introduced whose perfect matching numbers, or Kekulé numbers, K(G), are either Fibonacci or Lucas numbers, or their multiples. Since the ratio of the K(G)s of consecutive members converges to the golden ratio, these sequences of graphs belong to another class of golden family graphs.

1. Introduction

A *graph*, G, is a mathematical object composed of vertices, {V}, and edges {E}, where an edge spans a pair of vertices (HARARY, 1969). A matching of a graph is a set of edges of G such that no two of them share a vertex in common. If a graph with even $n = |V|$ has a matching with $n/2$ edges it is called a *perfect matching graph*. The number of possible perfect matchings of G is the perfect matching number, or *Kekulé number*, K(G). Although a tree graph has at most one Kekulé structure, a number of interesting features have been found for the K(G) numbers of *polycyclic graphs* (HOSOYA, 1986). In chemistry the K(G) of a *polyhex graph*, or hexagonal animal, reflects the stability of the parent polycyclic aromatic hydrocarbon molecule, such as, naphthalene or benzopyrene (CYVIN and GUTMAN, 1988; TRINAJSTIC, 1992). On the other hand, in solid state physics K(G) enumeration for giant polyominoes, or tetragonal animals, is an important subject for discussing the magnetic properties of metals and antiferromagnetic substances (KASTELEYN, 1967: TEMPERLEY, 1981). A variety of useful and interesting methods for enumerating K(G) of polyhex and polyomino graphs are proposed and discussed.

The present author has accumulated data of the K(G) numbers of both polyhexes (YAMAGUCHI *et al.*, 1975; HOSOYA *et al.*, 1986) and polyominoes (MOTOYAMA and HOSOYA, 1976), and he also has proposed several mathematical techniques (HOSOYA and YAMAGUCHI, 1976; MOTOYAMA and HOSOYA, 1977; HOSOYA and OHKAMI, 1983) useful for the study of these problems. Recently the concept of golden family graphs (HOSOYA, 2005) for various sequences of graphs was proposed. Several new sequences of graphs

were found whose topological indices (HOSOYA, 1971, 1973), Z, are equal to either *Fibonacci* or *Lucas numbers*, or their multiples. They are called *golden family graphs*, since the ratio Z-values of their consecutive members converges to the golden mean, τ.

The *topological index Z* is a characteristic quantity obtained by summing the non-adjacent numbers, p(G, k)s, or k-matching numbers, and K(G) is closely related to Z (HOSOYA, 1971, 1973). In this paper it will be shown that the K(G) numbers for several sequences of polyhex and polyomino graphs are Fibonacci or Lucas numbers, or their multiples, and the ratio of K(G)s of their consecutive terms converges to τ.

2. Enumeration Algorithms for K(G)

It is well known that K(G) = 2 for a hexagon corresponding to the pair of the Kekulé structures of the benzene molecule, or hexagon graph (Fig. 1). By fusing hexagons one by one to benzene, linearly and in a zigzag manner one can obtain two sequences of polyhex graphs, I_n, and W_n, as in Fig. 2, where n is the number of hexagons. In chemistry, they correspond, respectively, to the carbon atom skeletons of *linear polyacenes* and *zigzag polyacenes*. Their K(G) values are expressed by $n + 1$ and F_{n+1}, respectively (GORDON and DAVISON, 1952), as

$$I_n = n + 1 \tag{1}$$

and

$$W_n = F_{n+1}, \tag{2}$$

where F_n is the Fibonacci number defined by

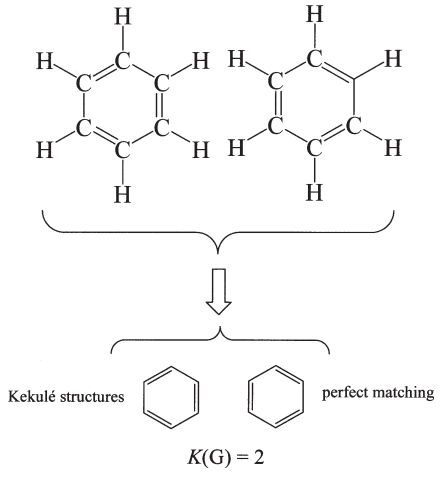

Fig. 1. The Kekulé number, or perfect matching number, of the benzene graph is two.

$$F_n = F_{n-1} + F_{n-2} \ (n \geq 2) \tag{3}$$

with

$$F_0 = F_1 = 1. \tag{4}$$

Note that the initial conditions (4) are different from the conventional ones (see VOROBIEV, 1961; HOGGATT, 1969). The reason is explained elsewhere (HOSOYA, 2005). The K(G) value of the latter increases far more rapidly than the former, reflecting the relative stability of these two sequences of hydrocarbon molecules.

Among a variety of algorithms for enumerating K(G)s of polyhexes, only the one discovered by GORDON and DAVISON (1952) will be explained here because of its ease in

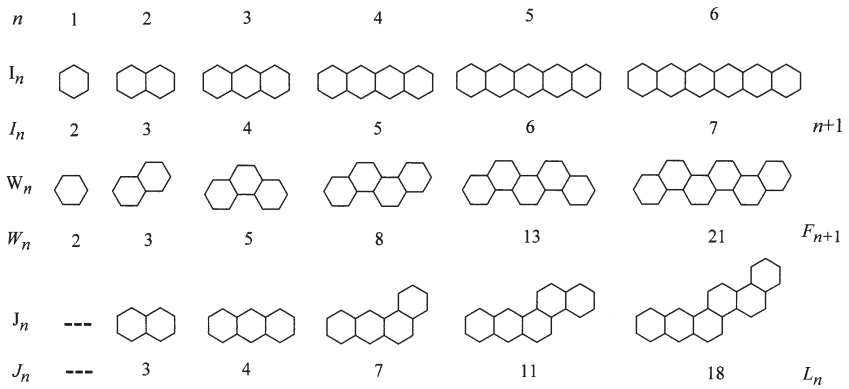

Fig. 2. Three series of polyhex graphs, I_n, W_n, and J_n, and their K(G) values. The latter two are the golden family graphs.

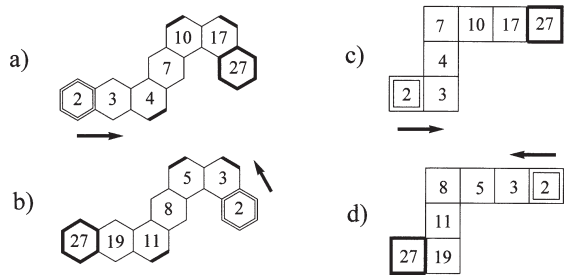

Fig. 3. a) and b): Examples of the algorithm for enumerating the K(G) value of a growing hexagonal animal, or an unbranched catacondensed benzenoid hydrocarbon. Doubly framed and bold hexagons, respectively, indicate the start and goal hexagons. The corner edge drawn with bold line indicates a kink. c) and d): Corresponding diagrams for polyomino graphs.

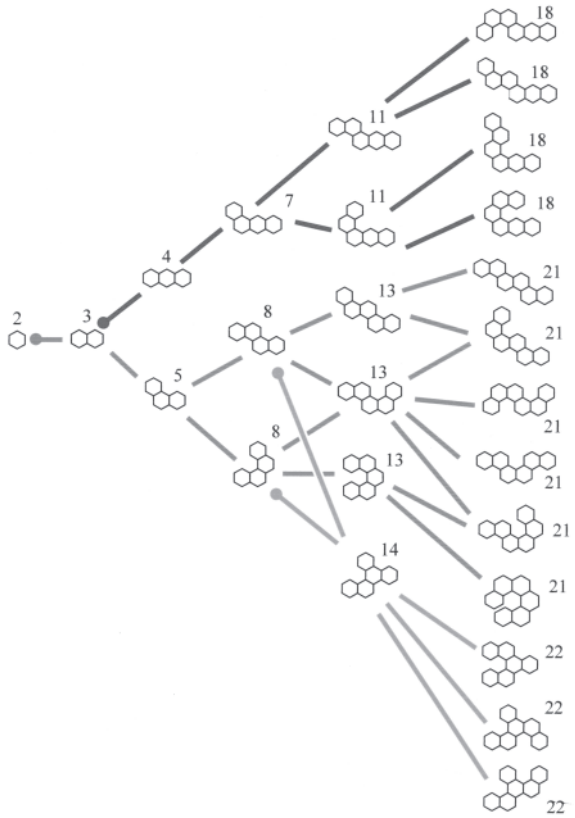

Fig. 4. Smaller catacondensed polyhex series of the golden family graphs, whose K(G) values are either Fibonacci or Lucas numbers, or their multiples. The dots indicate the start of the series.

deriving K(G) for a growing hexagonal animal without branching ("unbranched catacondensed benzenoid hydrocarbon" in chemical terminology. See Fig. 3).

This kind of animal, or benzenoid chain, has two terminal hexagons, irregardless of which is head or tail. For enumerating its K(G) value one can start from either of them. Figures 3a and b, respectively, illustrate the cases where the left- and right-most hexagons are chosen as the starting point. First K(G) = 2 is assigned to the starting hexagon. Then K(G) = 3 is assigned to the adjacent hexagon, because we already know $I_2 = F_2 = 3$. Up to here the procedures in Figs. 3a and b are the same. However, the assignment of K(G) to the third hexagon differs. In Fig. 3a, $I_3 = 4$ is given according to Eq. (1) since the third hexagon adds linearly, while in Fig. 3b, $F_4 = 5$ is given according to Eq. (2) since the third hexagon adds in a zigzag manner. The fourth hexagon in Fig. 3a grows in a zigzag manner after passing a "kink" (bend), and the recursion formula Eq. (3) is applies, i.e., by adding the numbers assigned to the nearest two ancestors one gets 4 + 3 = 7. This is also the case with

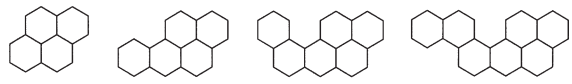

Fig. 5. An example of pericondensed polyhex series of the golden family graphs.

the fourth hexagon in Fig. 3b, and we have 5 + 3 = 8. The fifth hexagon in either Figs. 3a or b grows linearly from their last kink. In this case K(G) is the sum of the numbers assigned to the ancestors of the nearest and the one just before the last kink. That is, 7 + 3 = 10 and 8 + 3 = 11, respectively. By following these two rules of addition one gets the same value K(G) = 27 for this polyhex graph irrespective of the choice of starting hexagon. This algorithm can be proved by using a recursion formula explained in detail elsewhere (HOSOYA, 2005). The inclusion-exclusion principle provides the essence of the proof.

By using this algorithm the perfect matching numbers of the sequences of zigzag polyacene graphs are shown to be the Fibonacci numbers. It is also shown that the K(G)s of the sequences of graphs, J_n, in Fig. 2, are Lucas numbers. Both sequences of graphs may be called golden family graphs since the ratios of consecutive members of the sequence of K(G)s converge to τ.

3. Golden Family of Polyhex Graphs

From the database of the K(G) values for a number of polyhex graphs (HOSOYA and YAMAGUCHI, 1975; HOSOYA *et al*., 1986) one can choose various sequences of golden family graphs. The members of this family rapidly increase as the size of the graphs increases. Thus in Fig. 4 only those smaller members are shown whose K(G) values are either Fibonacci or Lucas numbers, or the multiples of the latter, where a filled circle indicates the start of the sequence. Two sequences of graphs, W_n, and J_n, given in Fig. 2, are included in Fig. 4. All the graphs in Fig. 4 are so-called catahexes (TRINAJSTIC, 1992), in which there is no vertex at which three hexagons meet. In other words a *catahex* is a polyhex whose dual graph is a tree.

As implied by the algorithm in Fig. 3, for the catahexes larger than tetrahexes there arises a possibility for the existence of isomeric members with the same K(G) value as W_n, and the number of these isomers increases quite rapidly with n. Then all the members of the golden family graphs grow by entangling with their isomers (red, blue, and light blue) as seen in Fig. 4.

Those polyhexes where there is more than one vertex at which three hexagons meet are called *perihexes*. Namely, the dual of a perihex is a non-tree. Although a systematic enumeration of them has not yet been performed, a sequence of golden family graphs whose K(G) values are the triple of F_n were found as shown in Fig. 5. Thus it is possible that there exists other golden family members in larger perihexes.

The hydrocarbon molecule corresponding to the second smallest member of this series is benzopyrene notoriously famous for its strong carcinogenic property.

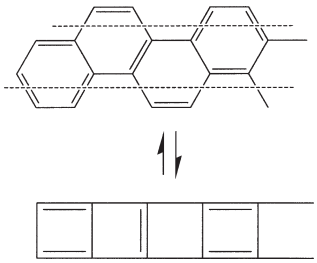

Fig. 6. Diagram showing the equivalency of the parfect marching in polyhex and polyomino graphs.

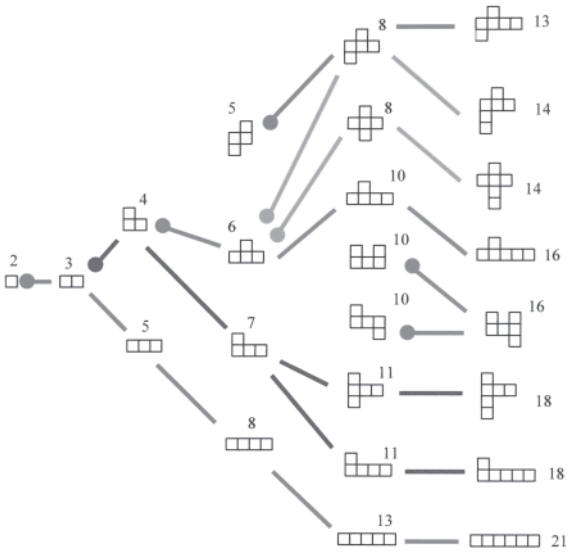

Fig. 7. Smaller catacondensed polyomino series of the golden family graphs, whose K(G) values are either Fibonacci or Lucas numbers, or their multiples. The dots indicate the start of the series.

4. Golden Family of Polyomino Graphs

The K(G) value of the linear polyomino, e.g. L_n, with n squares is known to be equal to that of the zigzag polyacene, W_n, with n hexagons. That these two counting problems are essentially the same is explained diagrammatically by Fig. 6. Namely, a given perfect matching pattern for W_n corresponds to one and only one perfect matching pattern for L_n, and vice versa, meaning that $K(W_n) = K(L_n)$.

Then one can say that the sequence of L_n graphs also belong to the golden family graphs. The correspondence between polyhexes and polyominoes is not limited to the pair,

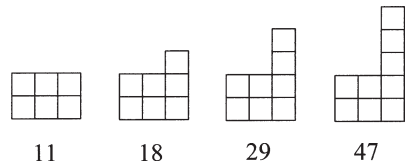

Fig. 8. An example of pericondensed polyomino series of the golden family graphs.

W_n and L_n, but is found in other pairs of growing animals. See Figs. 3c and d, where the Gordon and Davison algorithm for polyhexes is expanded to the corresponding polyomino.

From the compiled database (MOTOYAMA and HOSOYA, 1976) for polyominoes a number of sequences of polyomino graphs were found to belong to the golden family as shown in Fig. 7. They are the so-called *cataominoes*, whose dual graphs are trees.

The linear polyomino graph, L_n, has the largest K(G) value among their isomeric polyomino graphs, while the linear polyacene graphs, I_n, have the smallest value among the isomeric polyacene graphs. This property can be understood by examining the discussion pertinent to Figs. 3a–d.

Although a systematic study has not yet been performed for "periominoes," a sequence of graphs as shown in Fig. 8 were found to belong to the golden family graphs. Either by fusing, branching, or kinking, the K(G) value of polyomino graphs is known to decrease. This property which is opposite to polyhexes can be explained by use of the recursion formulas.

Although the results introduced in this paper have no physico-chemical meaning, these graph-theoretical counterparts of the Fibonacci and Lucas numbers are helpful not only as a proof technique but also for a global understanding of the mathematical structure of the problems where recursive sequences of numbers play an important role.

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