

# The Structure of Lucas Cubes and Maximal Resonant Sets of Cyclic Fibonacenes

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## Abstract

Fibonacenes are well known benzenoid graphs and their resonance graphs are isomorphic to Fibonacci cubes. In this paper we introduce so called cyclic fibonacenes and it turns out that their resonance graphs are isomorphic to Lucas cubes (together with two isolated vertices in even case). Further we establish a bijective correspondence between the maximal resonant sets of a cyclic fibonacene and the maximal hypercubes of its resonance graph t.i. Lucas cube, what gives us the insight into the structure of the latter.

## 1 Introduction

Lucas cubes and before them Fibonacci cubes were introduced in 1993 [11, 12] as models for interconnection networks, see for instance a survey paper [14] on Fibonacci cubes and papers [21, 15] on some properties of Lucas cubes.

Fibonacenes form a subclass of benzenoid graphs, t.i. 2-connected bipartite plane graphs where every inner face is a hexagon (for details see the survey [10]). By joining the terminal hexagons of a fibonacene via edges with ends of degree two we obtain a cyclic structure called the cyclic fibonacene. One class of cyclic fibonacenes are cyclic polyphenantrenes which belong to very interesting structures chemically known as carbon nanotubes. We are interested in the resonance graphs of cyclic fibonacenes. The resonance

graphs of a bipartite graph  $G$  reflects the structure of perfect matchings of  $G$  or we can say that it models the interaction between Kekulé structures of the corresponding chemical molecule.

The main result from [30] is that the nontrivial connected component of the resonance graph of a cyclic polyphenantrene with  $2n$  hexagons is isomorphic to the Lucas cube  $\Lambda_{2n}$ . In this paper we extend this result to any cyclic fibonacene, what brings us to the main result about the one-to-one correspondence between maximal resonant sets of a cyclic fibonacene and the maximal hypercubes of its resonance graph t.i. Lucas cube. Similar result was proved in [26] for (non-cyclic) benzenoid graphs with no coronene as a nice subgraph. Our main result together with one of the results from [20] enables an insight into the structure of Lucas cubes.

In the next section we give some basic definitions followed by known results about resonant sets in connection to the hypercubes of their resonance graphs and the extension of those results to cyclic fibonacenes. The fourth section covers new results and in the last section we give two interesting corollaries; one referring to the number of maximal resonant sets and the other to the Clar number of cyclic fibonacenes.

## 2 Preliminaries

*Benzenoid graphs* are 2-connected plane graphs such that every inner face is encircled by a 6-cycle (hexagon). Benzenoid graphs are a generalization of benzenoid systems, also called hexagonal systems, which can be defined as benzenoid graphs that are also subgraphs of a hexagonal lattice. If all vertices of a benzenoid graph  $G$  lie on its perimeter, then  $G$  is said to be catacondensed; otherwise it is pericondensed. We refer to [8, 9] for more information about these graphs, especially for their chemical meaning as representation of benzenoid hydrocarbons.

If two hexagons of a benzenoid graph share an edge, then they are *adjacent*. If every hexagon of a catacondensed benzenoid graph  $G$  has at most two adjacent hexagons, then  $G$  is a *chain*. Note that a hexagon  $h$  of a chain that is adjacent to two other hexagons contains two vertices of degree two. We say that  $h$  is *angularly annelated* if its two vertices of degree two are adjacent otherwise  $h$  is *linearly annelated*. Now, a chain is called a *fibonacene*\* if all of its hexagons, apart from the two terminal ones, are angularly

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\*We will use the term fibonacene as introduced by Balaban in [3].

annulated. Note that fibonacenes are not necessarily embeddable in the hexagonal lattice, but if so, they are called *simple* and otherwise they are *jammed* ([16]). An important class of fibonacenes are *polyphenantrenes*; if embedded in the hexagonal lattice, their inner dual is a zig-zag path.

If we embed polyphenantrenes on a surface of a cylindrical hexagonal lattice and join the terminal hexagons via an edge, we obtain cyclic polyphenantrenes (note that this can be done only with phenantrenes with even number of hexagons). They belong to very interesting structures chemically known as carbon nanotubes, discovered in 1991 [13]. Since then, carbon nanotubes have attracted great deal of attention due to their almost alien property of electrical conductivity and super-steel strength, for the details see [5, 6]. Carbon nanotubes are formally defined via hexagonal lattice and two chiral vectors. Since they are not of the main interest of our research, we will omit the formal definition and thereby refer the reader to [29] or [30].

The idea of getting the cyclic polyphenantrene from a polyphenantrene can be generalized to any fibonacene. Let  $F_n$  be a fibonacene with  $n$  hexagons where  $h_1$  and  $h_n$  are terminal hexagons,  $n \geq 2$ . Further, let  $e = uv$  be an edge of  $h_1$  with end vertices of degree 2. Then  $e' = u'v'$  is an edge of  $h_n$  with end vertices of degree 2, where  $u'$  and  $v'$  satisfy the condition  $d_p(u, u') < d_p(u, v')$  (or  $d_p(v, v') < d_p(v, u')$ ), where  $d_p(x, y)$  is the shortest distance between vertices  $x$  and  $y$  on the perimeter. Note that for the edge  $e$  of  $h_1$  there are two possible choices for the edge  $e'$  of  $h_n$  (see Figure 1 (a) where the other possible edge is denoted  $e'' = u''v''$ ). Edges  $e$  and  $e'$  are *tessellation* edges of  $F_n$ . By identifying edges  $e$  and  $e'$  via vertices  $u$  with  $u'$  and  $v$  with  $v'$ , we obtain a cyclic structure called *cyclic fibonacene*  $F_n^c$ . Note that every hexagon of the cyclic fibonacene  $F_n^c$  is angularly annulated. In [28] authors introduced the concept of a *cyclic chain* of a nanotube which consists of some cyclically concatenated hexagons with each hexagons adjacent to exactly two other hexagons. If a cyclic fibonacene is the cyclic polyphenantrene with even number of hexagons, then it is also a cyclic chain of a nanotube.

A cyclic fibonacene  $F_n^c$  can be drawn on a plane with all the perimeter edges of  $F_n$ , except the tessellation edges, divided into two disjoint cycles  $C_1$  and  $C_2$ , see Figure 1 (a), called the *inner* and the *outer* cycle of  $F_n^c$ . If an edge of  $F_n^c$  is neither in  $C_1$  nor in  $C_2$ , then it is a *transversal* edge of  $F_n^c$ . Note that the tessellation edge of a fibonacene is always a transversal edge of a cyclic fibonacene. It is not difficult to see that in the case of even  $n$

cycles  $C_1$  and  $C_2$  are of even length; and if  $n$  is odd, so is the length of both cycles.

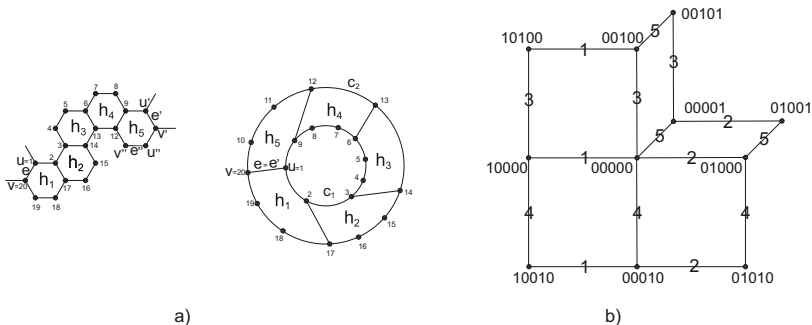


Figure 1: a) Two drawings of  $F_5^c$  with the tessellation edges  $e$  and  $e'$  (or  $e''$ ), b) the resonance graph  $R(F_5^c) \simeq \Lambda_5$ .

A *1-factor* or a *perfect matching* of a benzenoid graph  $G$  is a spanning subgraph with every vertex having degree one (in the chemical literature these are known as Kekulé structures); ([9]). Let  $M$  be a perfect matching of a benzenoid graph  $G$ . A cycle  $C$  of  $G$  is  *$M$ -alternating* if the edges of  $C$  appear alternately in and off the perfect matching  $M$ .

Let  $P$  be a set of hexagons of a benzenoid graph  $G$ . The subgraph of  $G$  obtained by deleting from  $G$  the vertices of the hexagons in  $P$  is denoted by  $G - P$ . It is clear that  $G - P$  can be the empty graph.

Let  $P$  be a set of hexagons of a benzenoid graph  $G$  with a perfect matching. Then the set  $P$  is called a *resonant set* of  $G$  if the hexagons in  $P$  are pair-wise disjoint and there exists such a perfect matching of  $G$  that contains a perfect matching of each hexagon in  $P$  ([1, 2]). It is easy to see that if  $P$  is a resonant set of a benzenoid graph  $G$ , then  $G - P$  is empty or has a perfect matching [22, 25]. A resonant set is *maximal* if it is not contained in another resonant set. A resonant set  $P$  such that  $G - P$  is empty or has a unique perfect matching is called a *canonical resonant set*. The maximum of the cardinalities of all resonant sets is called the *Clar number* and is denoted by  $Cl(G)$ . A *maximum cardinality resonant set* or a *Clar formula* is a resonant set whose cardinality is the Clar number.

The *resonance graph*  $R(G)$  of a benzenoid graph  $G$  is the graph whose vertices are the perfect matchings of  $G$ , and two perfect matchings are adjacent whenever their symmetric difference is the edge set of a hexagon of  $G$ . The concept is quite natural and has a chemical

meaning, therefore it is not surprising that it has been independently introduced in the chemical literature [4, 7] as well as in the mathematical literature [28] under the name *Z-transformation graph*.

The vertex set of the  $n$ -dimensional *hypercube*  $Q$ ,  $n \geq 1$ , consists of all binary strings of length  $n$ , two vertices being adjacent if the corresponding strings differ in precisely one place.

The *Fibonacci cubes* are for  $n \geq 1$  defined as follows. The vertex set of  $\Gamma_n$  is the set of all binary strings  $b_1b_2 \dots b_n$  containing no two consecutive 1's. Two vertices are adjacent in  $\Gamma_n$  if they differ in precisely one bit. A *Lucas cube*  $\Lambda_n$  is very similar to the Fibonacci cube  $\Gamma_n$ . The vertex set of  $\Lambda_n$  is the set of all binary strings of length  $n$  without consecutive 1's and also without 1 in the first and the last bit. The edges are defined analogously as for the Fibonacci cube. On Figure 2 we see first four Lucas cubes. Both, Fibonacci and Lucas cubes are subgraphs of hypercubes.

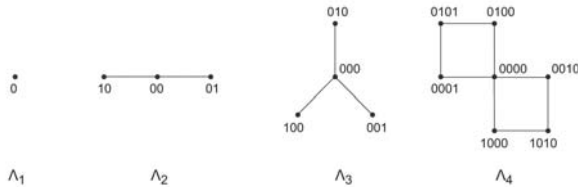


Figure 2: First four Lucas cubes.

### 3 Known results and cyclic fibonaccienes

Recently quite a few results concerning resonant sets of benzenoid graphs in connection to the hypercubes of their resonance graphs were established ([23, 24, 17]). In order to list some of them we need the following notations first.

For a benzenoid graph  $G$  let  $\mathcal{H}(R(G))$  be the set of all hypercubes of its resonance graph  $R(G)$  and let  $\mathcal{RS}(G)$  be the set of all resonant sets of  $G$ . The main result from [23] states that there exists a surjective mapping  $f : \mathcal{H}(R(G)) \rightarrow \mathcal{RS}(G)$  such that a  $k$ -dimensional hypercube is mapped onto a resonant set of cardinality  $k$ . Therefore we say that  $\mathcal{R}_Q \in \mathcal{RS}(G)$  is a resonant set (of cardinality  $k$ ) associated to a hypercube  $Q \in \mathcal{H}(R(G))$  (of dimension  $k$ ).

This line of research was then continued in [24] with the following result:

**Theorem 3.1** [24] *Let  $G$  be a benzenoid graph possessing at least one perfect matching and let  $f : \mathcal{H}(R(G)) \rightarrow \mathcal{RS}(G)$  be a mapping defined with  $f(Q) = \mathcal{R}_Q$  for  $Q \in \mathcal{H}(R(G))$ . Then the inverse image of a nonempty resonant set  $P$  under the mapping  $f$  is  $\mathcal{H}_P$ .*

Here  $\mathcal{H}_P \subseteq \mathcal{H}(R(G))$  is a set of hypercubes associated to a resonant set  $P$  from  $\mathcal{RS}(G)$ . More precisely, given a resonant set  $P$  of  $G$  of cardinality  $k$  for some positive integer  $k$ , we can associate a unique subgraph of  $R(G)$  isomorphic to the  $k$ -dimensional hypercube if  $P$  is a canonical set, otherwise we can associate as many (vertex-disjoint) subgraphs of  $R(G)$  isomorphic to the  $k$ -dimensional hypercube as the number of perfect matchings of  $G - P$ .

Just mentioned results can be easily extended to cyclic fibonacenes, since cyclicity does not affect the proofs, which are thereby identical and we will omit them. The reader is referred to the origin papers for more details (see Theorem 2 in [23] and Theorem 3.1 in [24]).

## 4 New results

The resonance graphs or  $Z$ -transformation graphs of bipartite planar graphs are well investigated, see for example [28, 27]. Recently the concept of a resonance graph was extended to cyclic benzenoid systems, more precisely to cyclic polyphenantrenes. It was shown in [30] that the resonance graph of a cyclic polyphenantrene with  $2n$  hexagons,  $n \geq 1$ , is isomorphic to the Lucas cube  $\Lambda_{2n}$  together with two isolated vertices. "Cyclic polyphenantrenes" with odd number of hexagons were not considered then since they are not nanotubes. Although, they are interesting from the mathematical point of view, since a bit altered main result from [30] can be easily applied to them as well. Even more, the result can be extended to the family of cyclic fibonacenes.

Because of the clarity we will give the detailed proof of Theorem 4.2 despite its similarity to the proof of the main result from [30]. The proof is based on the following result from [19] regarding the non-cyclic case t.i. fibonacenes.

**Theorem 4.1** [19] *Let  $G$  be an arbitrary fibonacene with  $n$  hexagons. Then  $R(G)$  is isomorphic to the Fibonacci cube  $\Gamma_n$ .*

Let us first define the labeling function  $\ell$  on fibonacenes (introduced first in [18] for any catacondensed benzenoid graph), since it is essential in the proof of Theorem 4.1 and

also for the proof of our new result.

Let  $h$  and  $h'$  be adjacent hexagons of a fibonacene  $F_n$  and  $M$  a perfect matching of  $F$ . Then the two edges of  $M$  in  $h$  that have exactly one vertex in  $h'$  are called the *link* from  $h$  to  $h'$ . Let  $h_1, h_2, \dots, h_n$  be the hexagons of  $F_n$ , where  $h_1$  and  $h_n$  are terminal hexagons. Let  $\mathcal{M}(F_n)$  be the set of all perfect matchings of  $F_n$  and let us define a labeling function

$$\ell : \mathcal{M}(F_n) \rightarrow \{0, 1\}^n$$

as follows. Let  $M$  be an arbitrary perfect matching of  $F_n$  and let  $e$  be the edge of  $h_1$  with ends of degree two such that  $e$  is not the opposite edge of the common edge of  $h_1$  and  $h_2$ . Then for  $i = 1$  we set

$$(\ell(M))_1 = \begin{cases} 0; & e \in M, \\ 1; & e \notin M, \end{cases}$$

while for  $i = 2, 3, \dots, n$  we define

$$(\ell(M))_i = \begin{cases} 1; & M \text{ contains the link from } h_i \text{ to } h_{i-1}, \\ 0; & \text{otherwise.} \end{cases}$$

Note that the labeling  $\ell$  produces the vertices of  $\Gamma_n$  (for more details see [19]).

Now we can proceed with the new result regarding the resonance graph of cyclic fibonacenes.

**Theorem 4.2** *Let  $F_n^c$  be a cyclic fibonacene,  $n \geq 2$ . Then the resonance graph of  $F_n^c$  is isomorphic to the union of  $\Lambda_n$  and two isolated vertices if  $n$  is even, and is isomorphic to  $\Lambda_n$  if  $n$  is odd.*

**Proof.** Let  $F_n$  be a fibonacene with  $n$  hexagons,  $n \geq 2$ , where hexagons are numbered consecutively with  $h_1, h_2, \dots, h_n$  and let  $e \in h_1, e' \in h_n$  be its tessellation edges. Further, let  $F_n^c$  be the corresponding cyclic fibonacene.

By Theorem 4.1 the perfect matchings of  $F_n$  can be labeled with the binary strings of length  $n$  without consecutive 1's, obtained by the labeling function  $\ell$ , as described above. Then the corresponding resonance graph  $R(F_n)$  is isomorphic to the Fibonacci cube  $\Gamma_n$ .

Let  $\mathcal{M}(F_n)$  be the set of perfect matchings of the fibonacene  $F_n$  and  $\mathcal{M}(F_n^c)$  be the set of perfect matchings of the cyclic fibonacene  $F_n^c$ . Further, let  $\mathcal{M}_1(F_n)$  be the set of perfect matchings of  $F_n$  that contain at least one of the edges  $e$  or  $e'$  and let  $M_1$  be a perfect matching from  $\mathcal{M}_1(F_n)$ . It is straightforward to see, that with removal of either

an edge  $e$  or  $e'$ , the perfect matching  $M_1$  can be contracted onto the perfect matching  $M'_1$  of  $F_n^c$ . Let  $\mathcal{M}_1(F_n^c)$  be the set of all such perfect matchings of the cyclic fibonacene  $F_n^c$ .

Now, let  $M_2$  be a perfect matching from  $\mathcal{M}(F_n) - \mathcal{M}_1(F_n)$ . Then  $M_2$  does not contain neither edge  $e$  nor  $e'$  and it can not be contracted to a perfect matching of  $F_n^c$ . Note that  $(\ell(M_2))_1 = (\ell(M_2))_n = 1$ .

Therefore the subgraph of the resonance graph of  $F_n$  (t.i. of a Fibonacci cube  $\Gamma_n$ ), induced with the vertex set  $\mathcal{M}_1(F_n)$  is isomorphic to the Lucas cube  $\Lambda_n$ . Since any  $M \in \mathcal{M}_1(F_n)$  can be contracted to the perfect matching  $M' \in \mathcal{M}_1(F_n^c)$ , the subgraph of the resonance graph of the cyclic fibonacene  $F_n^c$ , induced with the vertex set  $\mathcal{M}_1(F_n^c)$ , is also isomorphic to  $\Lambda_n$  (see Figure 3 (a)).

Next, let us consider perfect matchings of  $F_n^c$  that are not in  $\mathcal{M}_1(F_n^c)$ , so let  $M''$  be a perfect matching from  $\mathcal{M}(F_n^c) - \mathcal{M}_1(F_n^c)$ . Tessellation edges  $e = uv$  and  $e' = u'v'$  of  $F_n^c$  coincide where the identified vertices are  $u = u'$  and  $v = v'$ . Suppose  $u$  lies on the inner cycle and  $v$  on the outer cycle of  $F_n^c$ . Further, let  $u_1, u_n$  be neighbors of  $u$  on the inner cycle and let  $v_1, v_n$  be neighbors of  $v$  on the outer cycle such that  $u_i, v_i \in h_i, i = 1, n$  (see Figure 3 (b)). Since perfect matching  $M''$  is not induced by perfect matchings of a fibonacene  $F_n$ , either edges  $uu_n$  and  $vv_1$  must be in  $M''$  or vice versa, t.i. edges  $uu_1$  and  $vv_n$ . Then non of the transversal edges of  $F_n^c$  is in  $M''$ . Therefore both inner and outer cycle of  $F_n^c$  must be  $M''$ -alternating cycles. If  $n$  is odd number, there is no such perfect matching  $M''$  and if  $n$  is even there are two such perfect matchings, one with edges  $uu_n$  and  $vv_1$  and the other with edges  $uu_1$  and  $vv_n$ .

To conclude the proof we observe, the both new perfect matchings are not adjacent to any other perfect matching of  $F_n^c$ . □

Let us mention that results from Section 3 applied to cyclic fibonacenes assert the following observation. Let  $MM'$  be an edge of a resonance graph  $F_n^c$  such that binary labels of  $M$  and  $M'$  differ at the  $j$ -th place for some  $j = 1, 2, \dots, n$ . Then the symmetric difference of perfect matchings  $M$  and  $M'$  is the hexagon  $h_j$  and the label  $j$  is assigned to the edge  $MM'$ , see Figures 1, 4 or 5.

On Figure 1 (b) we see the resonance graphs of  $F_5^c$  t.i. Lucas cube  $\Lambda_5$  and on Figure 4 (b) the nontrivial connected component of the resonance graph of  $F_6^c$ , t.i.  $\Lambda_6$ . For example, the inverse image of the resonant set  $P = \{h_3, h_5\}$  of a cyclic fibonacene  $F_5^c$  (see Figure 1) under the mapping  $f$  is a 2-dimensional hypercube  $Q$  induced with edges



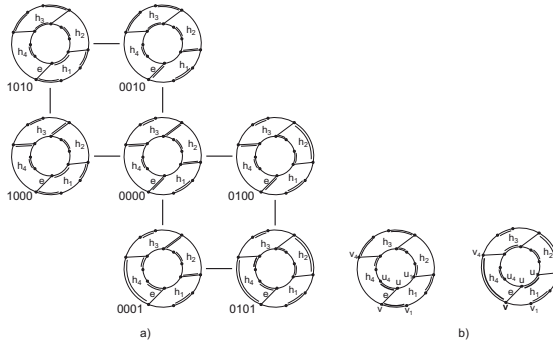


Figure 3: a) Perfect matchings from  $\mathcal{M}_1(F_4^c)$  and the induced resonance graph, b) perfect matchings from  $\mathcal{M}(F_4^c) - \mathcal{M}_1(F_4^c)$  t.i. isolated vertices of  $R(F_4^c)$ .

labeled with 3 and 5. On the other side for the resonant set  $P' = \{h_2, h_4\}$  of  $F_6^c$  (see Figure 4) the inverse image under  $f$  is the set  $\mathcal{H}_{P'} = \{Q'_1, Q'_2\}$ , where both hypercubes are 2-dimensional and induced with edges labeled 2 and 4. Note, that  $P$  is a canonical resonant set and  $P'$  not, what brings us to Lemma 4.3.

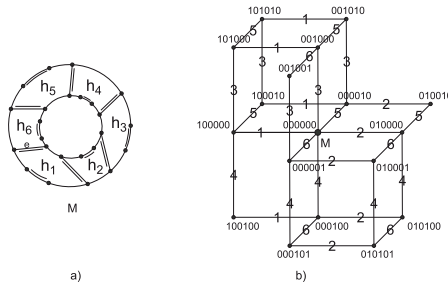


Figure 4: a) A perfect matching  $M$  of  $F_6^c$  with  $\ell(M) = 000000$ , b) the nontrivial connected component of  $R(F_6^c)$  t.i.  $\Lambda_6$ .

**Lemma 4.3** For  $n \geq 2$  let  $F_n^c$  be a cyclic fibonacene. Then  $P$  is a maximal resonant set of  $F_n^c$  if and only if  $P$  is a canonical resonant set.

**Proof.** The only if part is proved as in [17](Proposition 7.1) where instead of resonant sets of a benzenoid graph we are interested in the resonant sets of a cyclic fibonacene and the proof is therefore omitted.

For the if part let  $P$  be a maximal resonant set of  $F_n^c$  and suppose  $P$  is not canonical. Then  $F_n^c - P$  allows at least two different perfect matchings. Therefore  $F_n^c - P$  contains a cycle  $C$  which is an alternating cycle in both perfect matchings. Since  $C$  is an alternating cycle of a cyclic fibonacene, in which every hexagon is angularly annelated,  $C$  must be either of length six or contains an alternating cycle of length six, what is a contradiction with the maximality of  $P$ .  $\square$

The main result of this paper is:

**Theorem 4.4** *For  $n \geq 2$  let  $F_n^c$  be a cyclic fibonacene. Then there exists a bijective mapping from the set of subgraphs of  $R(F_n^c)$  that are maximal hypercubes into the family of maximal resonant sets of  $F_n^c$ .*

**Proof.** The proof is similar to the proof of Theorem 4.3 from [26]. Let  $Q$  be a maximal hypercube of dimension  $k$  of the resonance graph  $R(F_n^c)$ . Then the image of  $Q$  under the mapping  $f$  from Theorem 3.1 is a resonant set  $P$  of cardinality  $k$ .  $P$  must be a maximal resonant set, otherwise the inverse image of  $P$  under the mapping  $f$  is  $\mathcal{H}_P$ , where the hypercubes in  $\mathcal{H}_P$  are of dimension greater than  $k$ , which is a contradiction, since  $Q \in \mathcal{H}_P$ .

By Lemma 4.3 a maximal resonant set  $P$  of  $F_n^c$  is also a canonical resonant set. Hence, by Theorem 3.1 the inverse image of a maximum cardinality set under the mapping  $f$  defined therein, is a singleton set containing a subgraph of  $R(F_n^c)$  isomorphic to the  $k$ -dimensional hypercube.  $\square$

**Corollary 4.5** *The vertex of a Lucas cube  $\Lambda_n$  with a binary label  $0^n$  is contained in any maximal hypercube of  $\Lambda_n$ .*

**Proof.** Let  $F_n^c$  be a cyclic fibonacene,  $n \geq 2$ . By Theorem 4.2 (the nontrivial connected component of) the resonance graph of  $F_n^c$  is isomorphic to the Lucas cube  $\Lambda_n$ . Let  $\ell$  be a binary labeling of the vertices of  $R(F_n^c)$  as described in Section 4 and let  $M$  be a vertex of  $R(F_n^c)$  such that  $\ell(M) = 0^n$  (see Figure 4 (a)). Since neighbors of  $M$  are vertices whose labels have exactly one bit equal to 1 and another  $n - 1$  bits are 0, all  $n$  hexagons of  $F_n^c$  are  $M$ -alternating hexagons.

Further, let  $P$  be a maximal resonant set of  $F_n^c$ . By Theorem 4.4 there exists a unique subgraph of  $R(F_n^c)$ , isomorphic to a hypercube, associated to  $P$  and let it be denoted

with  $Q_P$  (note that  $Q_P$  is a maximal hypercube). Since every hexagon from  $F_n^c$  is  $M$ -alternating, so are hexagons from  $P$   $M$ -alternating and therefore  $M$  belongs to the vertex set of  $Q_P$ .  $\square$

Suppose we can list all maximal resonant sets of a cyclic fibonacene  $F_n^c$ . Next proposition gives the relation between the corresponding maximal hypercubes of the resonance graph of  $F_n^c$  t.i. Lucas cube.

**Proposition 4.6** *Let  $P'$  and  $P''$  be maximal resonant sets of a cyclic fibonacene  $F_n^c$  ( $n \geq 2$ ) and let  $Q_{P'}$  and  $Q_{P''}$  be the associated hypercubes in the resonance graph  $R(F_n^c)$ . If  $P' \cap P'' = P$ , where  $|P| = k \geq 1$ , then  $Q_{P'} \cap Q_{P''}$  is a subgraph of  $R(F_n^c)$  isomorphic to a  $k$ -dimensional hypercube and belongs to the inverse image of the resonant set  $P$  under the mapping  $f$ .*

**Proof.** Let  $P'$  and  $P''$  be maximal resonant sets of a cyclic fibonacene  $F_n^c$  and let their intersection be a nonempty resonant set  $P = \{h_{i_1}, h_{i_2}, \dots, h_{i_k}\}$  (otherwise the assertion is trivial). By Theorem 3.1 the inverse image under the mapping  $f$  is  $\mathcal{H}_P$ . The elements of  $\mathcal{H}_P$  are isomorphic to a hypercube of dimension  $k$  and are induced by edges of  $R(F_n^c)$  with labels  $i_1, i_2, \dots, i_k$ . Since  $Q_{P'}$  and  $Q_{P''}$  are hypercubes associated to maximal resonant sets  $P'$  and  $P''$  respectively, both of them are induced with edges with common labels  $i_1, i_2, \dots, i_k$  and some other distinctively labeled edges, what completes the proof.  $\square$

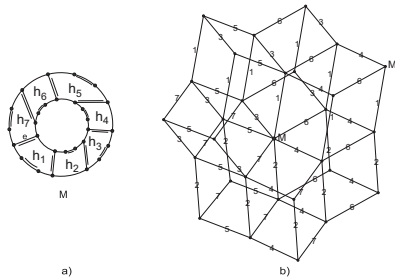


Figure 5: a) A perfect matching  $M$  of  $F_7^c$  with  $\ell(M) = 0000000$ , b) the resonance graph  $R(F_7^c) \simeq \Lambda_7$ .

For example, in the case of the resonance graph of a cyclic fibonacenes  $F_7^c$  we have 7 (follows from [20]) 3-dimensional maximal hypercubes. They are induced by edge

triples with labels 1, 3, 5; 1, 3, 6; 1, 4, 6; 2, 4, 6; 2, 4, 7; 2, 5, 7 and 3, 5, 7, since the corresponding hexagons are maximal resonant sets of  $F_7^c$ , see Figure 5 (a). On Figure 5 (b) we have then the resonance graph of  $F_7^c$  t.i. a Lucas cube  $\Lambda_7$ . The binary codes of vertices of  $\Lambda_7$  are easily constructed. For example the binary code for a vertex  $M'$  on Figure 5 (b) is  $\ell(M') = 1001010$ , since the shortest path between vertex  $M$  (with  $\ell(M) = 0000000$ ) and  $M'$  consists of edges with labels 1, 4 and 6.

## 5 Corollaries

Just recently Mollard ([20]) found some interesting properties of Fibonacci and Lucas cubes. One of them is the following:

**Theorem 5.1** [20] *Let  $1 \leq k \leq n$  and  $g_{n,k}$  be the number of maximal hypercubes of dimension  $k$  in  $\Lambda_n$ . Then:*

$$g_{n,k} = \frac{n}{k} \binom{k}{n-2k}.$$

From Theorems 4.4 and 5.1 directly follows the next corollary.

**Corollary 5.2** *For  $n \geq 2$  let  $F_n^c$  be a cyclic fibonacene and  $1 \leq k \leq n$ . Then the number of maximal resonant sets of size  $k$  in  $F_n^c$  equals*

$$\frac{n}{k} \binom{k}{n-2k}.$$

And we will conclude with one more corollary about the Clar number and the number of Clar formulas of a cyclic fibonacene.

**Corollary 5.3** *For  $n \geq 2$  let  $F_n^c$  be a cyclic fibonacene. Then*

$$Cl(F_n^c) = \left\lfloor \frac{n}{2} \right\rfloor.$$

*Further, the number of Clar formulas of  $F_n^c$  is*

$$\begin{cases} 2 & ; n = 2k, \\ n & ; n = 2k + 1. \end{cases}$$

**Proof.** The first claim follows from [20] as we know that the maximum dimension of a maximal induced hypercube in  $\Lambda_n$  is less or equal to  $\lfloor \frac{n}{2} \rfloor$  and the second claim is a straightforward calculation from Corollary 5.2. □

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## References

- [1] H. Abeledo, G. Atkinson, The Clar and Fries problems for benzenoid hydrocarbons are linear programs, in: P. Hansen, P. Fowler, M. Zheng (Eds.), *Discrete Mathematical Chemistry*, Am. Math. Soc., Providence, 2000, pp. 1–8.
- [2] H. Abeledo, G. Atkinson, Unimodularity of the Clar number problem, *Lin. Algebra Appl.* **420** (2007) 441–448.
- [3] A. T. Balaban, Chemical graphs. L. Symmetry and enumeration of fibonacenes (unbranched catacondensed benzenoids isoarithmic with helicenes and zigzag catafusenes), *MATCH Commun. Math. Comput. Chem.* **24** (1989) 29–38.
- [4] S. El-Basil, Generation of lattice graphs. An equivalence relation on Kekulé counts of catacondensed benzenoid hydrocarbons, *J. Mol. Struct. (Theochem)* **288** (1993) 67–84.
- [5] M. S. Dresselhaus, G. Dresselhaus, P. C. Eklund, *Science of Fullerenes and Carbon Nanotubes*, Academic Press, New York, 1996.
- [6] M. S. Dresselhaus, G. Dresselhaus, P. Avonris, *Carbon Nanotubes Synthesis, Structure, Properties and Applications*, Springer-Verlag, Berlin, 2001.
- [7] W. Gründler, Signifikante Elektronenstrukturen für benzenoide Kohlenwasserstoffe, *Wiss. Z. Univ. Halle* **31** (1982) 97–116.
- [8] I. Gutman, Topological properties of benzenoid systems. XIX. Contributions to the aromatic sextet theory, *Wiss. Z. Techn. Hochsch. Ilmenau* **29** (1983) 57–65.
- [9] I. Gutman, S. J. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons*, Springer-Verlag, Berlin, 1989.
- [10] I. Gutman, S. Klavžar, Chemical graph theory of fibonacenes, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 39–54.
- [11] W. J. Hsu, Fibonacci cubes – A new interconnection topology, *IEEE Trans. Parallel Distr. Sys.* **4** (1993) 3–12.
- [12] W. J. Hsu, C. V. Page, J. S. Liu, Fibonacci cubes – A class of self-similar graphs, *Fibonacci Quart.* **31** (1993) 65–72.
- [13] S. Iijima, Helical microtubules of graphitic carbon, *Nature* **354** (1991) 56–58.
- [14] S. Klavžar, Structure of Fibonacci cubes: a survey, *J. Comb. Optim.*, in press.

- [15] S. Klavžar, On median nature and enumerative properties of Fibonacci-like cubes, *Discr. Math.* **299** (2005) 145–153.
- [16] S. Klavžar, I. Gutman, Chemical graph theory of fibonacenes, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 39–54.
- [17] S. Klavžar, K. Salem, A. Taranenko, Maximum cardinality resonant sets and maximal alternating sets of hexagonal systems, *Comput. Math. Appl.* **59** (2010) 506–513.
- [18] S. Klavžar, A. Vesel, P. Žigert, I. Gutman, Binary coding of Kekulé structures of catacondensed benzenoid hydrocarbons, *Comput. & Chem.* **25** (2001) 569–575.
- [19] S. Klavžar, P. Žigert, Fibonacci cubes are the resonance graphs of fibonacenes, *Fibonacci Quart.* **43** (2005) 269–276.
- [20] M. Mollard, Maximal hypercubes in Fibonacci and Lucas cubes, *submitted*.
- [21] E. Munarini, C. P. Cippo, N. Z. Salvi, On the Lucas cubes, *Fibonacci Quart.* **39** (2001) 12–21.
- [22] K. Salem, H. Abeledo, A maximal alternating set of a hexagonal system, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 159–176.
- [23] K. Salem, S. Klavžar, I. Gutman, On the role of hypercubes in the resonance graphs of benzenoid graphs, *Discr. Math.*, **306** (2006) 699–704.
- [24] K. Salem, S. Klavžar, A. Vesel, P. Žigert, The Clar formulas of a benzenoid system and the resonance graph, *Discr. Appl. Math.* **157** (2009) 2565–2569.
- [25] K. Salem, I. Gutman, The unfixed subgraph of a catacondensed hexagonal system obtained by fixing an alternating set, *J. Math. Chem.* **38** (2005) 503–510.
- [26] A. Taranenko, P. Žigert, Resonant sets of benzenoid graphs and hypercubes of their resonance graphs, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 65–77.
- [27] H. Zhang,  $Z$ -transformation graphs of perfect matchings of plane bipartite graphs: a survey, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 457–476.
- [28] F. Zhang, X. Guo, R. Chen,  $Z$ -transformation graphs of perfect matchings of hexagonal systems, *Discr. Math.* **72** (1988) 405–415.
- [29] H. Zhang, G. Wang, Embeddability of open-ended carbon nanotubes in hypercubes, *Comp. Geom. – Theor. Appl.* **43** (2010) 524–534.
- [30] P. Žigert, M. Berlič, Lucas cubes and resonance graphs of cyclic polyphenantrenes, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 77–90.