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Lucas Cubes and Resonance Graphs of Cyclic Polyphenanthrenes

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Abstract

Several classes of graphs based on Fibonacci strings were introduced in the last 10 years as models for interconnection networks, among them Lucas cubes. The vertex set of a Lucas cube Λ_n is the set of all binary strings of length n without consecutive 1's and 1 in the first and the last bit. Two vertices of the Lucas cube are adjacent if their strings differ in exactly one bit.

Carbon nanotubes were discovered 20 years ago and their unique structure explains their unusual properties such as conductivity and strength. Our interest is in a class of carbon nanotubes, called cyclic polyphenanthrenes. The resonance graph of an aromatic hydrocarbon reflects the structure of its perfect matchings (t.i. Kekulé structures).

The main result of this paper is the following: Lucas cubes are the nontrivial component of the resonance graphs of cyclic polyphenanthrenes. This result has some interesting applications regarding hamiltonicity and observability of the resonance graph of the cyclic polyphenanthrene.

1 Introduction

Several classes of graphs based on Fibonacci strings were introduced as models for interconnection networks. Fibonacci cubes were introduced in 1993 [12, 13] and intensively studied afterwards [3, 22, 25, 31], see also a survey [17], followed with extended Fibonacci cubes [32] and finally Lucas cubes [3, 7, 16, 18, 24]. We are interested in the connection between Lucas cubes and the resonance graphs of chemical structures called cyclic polyphenanthrenes, which are related to non-cyclic fibonacenes.

Fibonacenes are benzenoid graphs, t.i. 2-connected bipartite plane graphs where every inner face is a hexagon (for details see a survey [10]). If we embed a class of fibonacenes called polyphenanthrenes on a surface of a cylinder, we obtain cyclic polyphenanthrenes. They belong to very interesting structures chemically known as carbon nanotubes. Carbon nanotubes vere discovered in 1991 [14] and can be imagined as a C_{70} fullerene with many thousands od carbon rings inserted across its equator, giving a tiny tube with about 1.5 nm of diameter and a length of several microns. In 1996 Smalley group at Rice university successfully synthesized the aligned single-walled nanotubes [30], which are carbon nanotubes with the almost alien property of electrical conductivity and supersteel strength. Carbon nanotubes have attracted great attention in different research fields such as chemistry physics, artificial materials, and so on. For the details, see [4, 5]. Open-ended single-walled nanotubes without caps are also called tubulenes [29].

The resonance graph of a graph G reflects the structure of perfect matchings of G. In [19] authors proved the following theorem: Fibonacci cubes are precisely the resonance graphs of fibonacenes. Our main result is very similar to that one: Lucas cubes are the nontrivial component of the resonance graphs of cyclic polyphenanthrenes.

In the next section we give all the necessary definitions. The third section is about Fibonacci cubes and the resonance graphs, since that result is strongly connected to the main result which is presented in section 4, together with some consequences.

2 Preliminaries

Each open-ended single-walled nanotube can be viewed as a mapping of a graphene sheet onto the surface of a cylinder by rolling up a hexagonal lattice. Let us define nanotubes more precisely. Choose any lattice point in the hexagonal lattice as the origin O. Let $\vec{a_1}$

and $\vec{a_2}$ be the two basic lattice vectors. Choose a vector $\vec{OA} = n\vec{a_1} + m\vec{a_2}$ such that n and m are two integers and at least one of them is not zero. Draw two straight lines L_1 and L_2 passing through O and A perpendicular to OA, respectively. By rolling up the hexagonal strip between L_1 and L_2 and gluing L_1 and L_2 such that A and O superimpose, we can obtain a hexagonal tessellation $\mathcal{H}$ of the cylinder. L_1 and L_2 indicate the direction of the axis of the cylinder. Using the terminology of graph theory, a *nanotube* T is defined to be the finite graph induced by all the hexagons of $\mathcal{H}$ that lie between c_1 and c_2, where c_1 and c_2 are two vertex-disjoint cycles of $\mathcal{H}$ encircling the axis of the cylinder. The vector $\vec{OA}$ is called the *chiral vector* of T, denoted by C_h. The cycles c_1 and c_2 are the two open-ends of T.

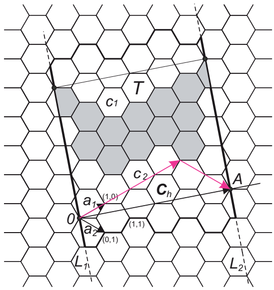

Figure 1: Illustration of a $(4, 2)$-type nanotube.

For any nanotube T, if its chiral vector is $C_h = n\vec{a_1} + m\vec{a_2}$, T will be called an (n, m)-type nanotube, see Figure 1. If $n = m$, nanotube is an *armchair nanotube* and if exactly one of n or m is zero, then it is a *zigzag nanotube*. Let T be a nanotube encircled with cycles c_1 and c_2 and e an edge of T. If e is not in c_1 or c_2, then e is an *inner edge* of T. If every inner edge of T has one end vertex in c_1 and another in c_2, then T is said to be a *catacondensed* nanotube, otherwise it is *pericondensed*. If a vertex u of a nanotube T is not in c_1 or c_2, then u is an *inner vertex* of T.

Cyclic polyphenanthrenes are armchair nanotubes, consisting of polyphenanthrene strips. In this paper we are interested in a single strip cyclic polyphenanthrenes, which are catacondensed (n, n)-type nanotubes and will be denoted with T_{2n} (note that $2n$ is the number of hexagons of T_{2n}), see Figure 2 (a). Instead of a term single strip cyclic polyphenanthrenes we will name them just cyclic polyphenanthrenes. Note, the drawings of cyclic polyphenanthrenes will be as the one of T_8 on Figure 2 (b) with pending edges indicating the cycling structure.

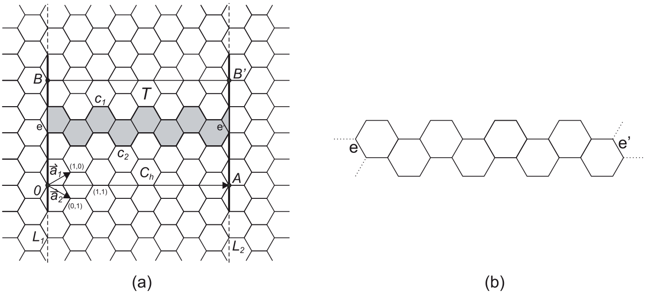

Figure 2: (a) A (single strip) cyclic polyphenanthrene T_8 embedded in a hexagonal lattice, (b) a drawing of T_8 and edges e,e' of the corresponding fibonacene B_8.

If we do the opposite of rolling and gluing the hexagonal lattice, t.i. if we open it, we obtain the usual 2-dimensional hexagonal lattice. More precisely, let T be a nanotube and c_1, c_2 the cycles encircling T. Let P be a path in T such that the end vertices of P belongs to c_1 and c_2, respectively, and all the other vertices of P are inner vertices. By opening the nanotube T through the path P, we obtain a *benzenoid system* B. An edge e of path P is a *tessellation edge* of T and let the corresponding pairwise edge in the benzenoid system B be e', see for example Figure 2 (b) or 3 (c). If T was a cata- or peri-condensed nanotube, so is then B a cata- or pericondensed benzenoid system. For more information on these graphs see [9]. If two hexagons of a benzenoid system share an edge, then they are *adjacent*. If every hexagon of a catacondensed benzenoid system B has at most two adjacent hexagons, then B is a *hexagonal chain*. Note that a hexagon h of a hexagonal chain that is adjacent to two other hexagons contains two vertices of degree two. We say that h is *angularly connected* if its two vertices of degree two are adjacent. Now, a hexagonal chain is called a *fibonacene* if all of its hexagons, apart from the two terminal ones, are angularly connected , cf. Figure 3 (a). Note that there are fibonacenes, that can not be embedded in the hexagonal lattice, but they are not of any interest for us. If T_{2n} is the cyclic polyphenanthrene, cf. Figure 3 (c), then the corresponding benzenoid system is the fibonacene B_{2n} called *polyphenanthrene*, cf. Figure 3 (b).

It is convenient for us to consider a benzenoid system B as a subgraph of the hexagonal lattice from Figures 1 and 2 (a). Then there are three different directions of edges of B called *horizontal*, *positive* (at the angle $60°$) and *negative* (at the angle $-60°$).

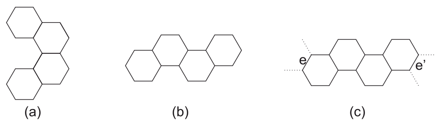

Figure 3: (a) A fibonacene, (b) the polyphenanthrene B_4, (c) the cyclic polyphenanthrene T_4 with the tesselation edge e and its pairwise edge e'.

A *1-factor* or a *perfect matching* of a graph G is a spanning subgraph with every vertex having degree one (in the chemical literature these are known as Kekulé structures); see [1] and [9]. Thus a perfect matching of a graph with $2n$ vertices will consist of n non-touching edges.

Let G be a planar 2-connected bipartite graph. Then the vertex set of the *resonance graph* $R(G)$ of G consist of all perfect matchings of G, and two perfect matchings are adjacent whenever their symmetric difference is the edge set of a face 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 [6, 8] as well as in the mathematical literature [33] under the name Z-transformation graph. On Figure 5 we can see the cyclic polyphenanthrene T_4 together with its resonance graph.

Let h and h' be adjacent hexagons of a catacondensed benzenoid system. Then the two edges of h that have exactly one vertex in h' are called the *link* from h to h' (cf. on Figure 5 there is a link from h_3 to h_2).

The vertex set of the n-dimensional *hypercube* Q_n, $n \geq 1$, 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 Γ_n is the set of all binary strings $b_1 b_2 \ldots b_n$ containing no two consecutive 1's. Two vertices are adjacent in Γ_n if they differ in precisely one bit. A *Lucas cube* Λ_n is very similar to the Fibonacci cube Γ_n. The vertex set of Λ_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 4 we see first four Lucas cubes. Both, Fibonacci and Lucas cubes are subgraphs of hypercubes.

Vertices of the Fibonacci cube Γ_n, $n \geq 1$, are *Fibonacci strings* of length n and the number of all such strings is a *Fibonacci number* $F_{n+2} = |V(\Gamma_n)|$ (F_n is the Fibonacci sequence, where $F_1 = F_2 = 1$). Similary are the vertices of the Lucas cube Λ_n, $n \geq 1$, are *Lucas strings* of length n and the number of all such strings is a *Lucas number* $L_n = |V(\Lambda_n)|$. The following identity is well known: for $n \geq 2$, $L_n = F_{n+1} + F_{n-1}$ $(L_1 = 1)$.

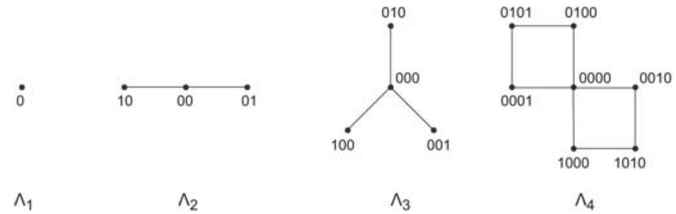

Figure 4: First four Lucas cubes.

3 Fibonacci cubes and the resonance graphs

Our main result is strongly connected with the following result from [19].

Theorem 3.1 *[19] Let B be an arbitrary fibonacene with n hexagons. Then $R(B)$ is isomorphic to the Fibonacci cube Γ_n.*

Since Theorem 3.1 is very important for our main result, let us explain some concepts introduced in [19].

Let B_n be the polyphenanthrene with n hexagons, consecutively labeled $h_1, h_2, \ldots, h_n$. We first establish a bijective correspondence between the vertices of $R(B_n)$ and the vertices of Γ_n. Let $\mathcal{M}(B_n)$ be the set of all perfect matchings of G_n and define a (labeling) function

$$\ell : \mathcal{M}(G_n) \to \{0, 1\}^n$$

as follows. Let M be an arbitrary perfect matching of B_n and let e be an edge of h_1 with end vertices of degree two in the positive direction. Then for $i = 1$ we set

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

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

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

For instance, the fibonacene with four hexagons contains eight perfect matchings. On Figure 5 the labels obtained by ℓ are shown.

For detailed proof of Theorem 3.1 the reader is referred to [19], here we just present a very useful simple argument that the labeling ℓ produces the vertices of Γ_n. This is clearly true for $n = 2$ and $n = 3$. So let the polyphenanthrene B_n be obtained from the polyphenanthrene B_{n-1} with $n-1$ hexagons h_1, h_2, ..., h_{n-1} by adding the hexagon h_n to B_{n-1}.

The perfect matchings of B_n can be partitioned into two disjoint sets $\mathcal{M}_1(B_n)$ and $\mathcal{M}_2(B_n)$, where $\mathcal{M}_1(B_n)$ contains perfect matchings without the link from h_n to h_{n-1}, while $\mathcal{M}_2(B_n)$ contains all other perfect matchings of B_n. Note that each perfect matching M of B_{n-1} can be in a unique way extended to a perfect matching M_1 of $\mathcal{M}_1(B_n)$. Moreover, $\ell(M_1) = \ell(M)0$, where $\ell(M)0$ denotes the concatenation of the label $\ell(M)$ with the symbol 0.

Consider next a perfect matching $M_2 \in \mathcal{M}_2(B_n)$. Then there is no link from h_{n-1} to h_{n-2}. Hence we are interested only in perfect matchings of B_{n-1} without this link. Consequently, $\ell(M_2)$ must have 0 in the last position. Similarly as above, each perfect matching of B_{n-1} without a link from h_{n-1} to h_{n-2} can be in a unique way extended to a perfect matching from $\mathcal{M}_2(B_n)$. The labellings of perfect matchings from $\mathcal{M}_2(B_n)$ are obtained by adding 1 as the nth bit. Hence $\ell(M_2)$ ends with 01. Since the above construction is a well-known procedure for obtaining all the vertices of Γ_n, we conclude that the labeling ℓ indeed produces all the vertices of Γ_n.

4 Main result and some consequences

Here is our main result:

Theorem 4.1 *Let T_{2n} be the cyclic polyphenanthrene, $n \geq 1$. Then the resonance graph of T_{2n} is isomorphic to the union of the Lucas cube Λ_{2n} and two isolated vertices.*

Proof. Let T_{2n} be the cyclic polyphenanthrene with $2n$ hexagons and let B_{2n} be the corresponding polyphenanthrene with a tesselation edge e and its pairwise edge e' in B_{2n}. Further, let us label hexagons of B_{2n} consecutively with $h_1, h_2, \ldots, h_{2n}$ such that e and e' belongs to h_1 and h_{2n}, respectively.

By Theorem 3.1 the perfect matchings of B_{2n} can be represented with the binary strings of length $2n$ without consecutive 1's, obtained by the labeling function ℓ, as de-

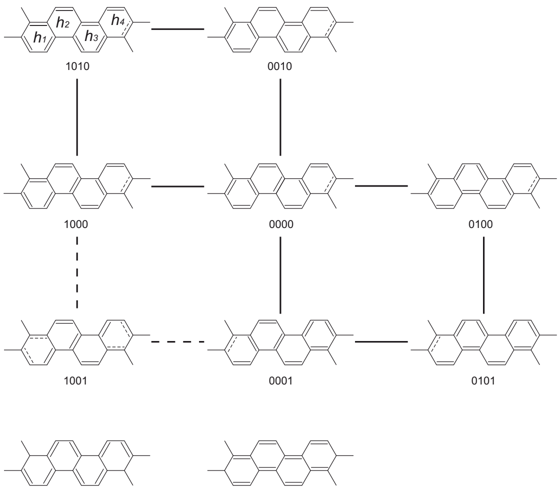

Figure 5: (a) All 8 perfect matchings of a fibonacene B_4 and the contraction to 7 perfect matchings of T_4 together with the 2 additional ones, (b) the resonance graph $R(T_4)$.

scribed above. Then the corresponding resonance graph $R(B_{2n})$ is isomorphic to the Fibonacci cube Γ_{2n}.

Let $\mathcal{M}(B_{2n})$ be the set of perfect matchings of the polyphenanthrene B_{2n} and $\mathcal{M}(T_{2n})$ be the set of perfect matchings of the cyclic polyphenanthrene T_{2n}. Further, let $\mathcal{M}_1(B_{2n})$ be the set of perfect matchings of B_{2n} that contain at least one of edges e and e' and let M be a perfect matching from $\mathcal{M}_1(B_{2n})$. It is straightforward to see, that with removal of either an edge e or e', the perfect matching M can be contracted onto the perfect matching M^T of T_{2n}. Let $\mathcal{M}_1(T_{2n})$ be the set of all such perfect matchings of the cyclic polyphenanthrene T_{2n}.

Now, let M' be a perfect matching from $\mathcal{M}(B_{2n}) \setminus \mathcal{M}_1(B_{2n})$. Then M' does not contain neither edge e nor e' and it can not be contracted to a perfect matching of T_{2n}. Also $(\ell(M'))_1 = (\ell(M'))_{2n} = 1$.

Therefore the subgraph of the resonance graph of B_{2n} (t.i. of a Fibonacci cube Γ_{2n}), induced with the vertex set $\mathcal{M}_1(B_{2n})$ is isomorphic to the Lucas cube Λ_{2n}. Since any $M \in \mathcal{M}_1(B_{2n})$ can be contracted to the perfect matching $M^T \in \mathcal{M}_1(T_{2n})$, the subgraph of the resonance graph of the cyclic polyphenanthrene T_{2n}, induced with the vertex set $\mathcal{M}_1(T_{2n})$, is also isomorphic to Λ_{2n}.

Next, let us consider perfect matchings of T_{2n} that are not in $\mathcal{M}_1(T_{2n})$. Let u_1 and u_2 be the end vertices of the tesselation edge e of T_{2n} and let M_2 be a perfect matching from $\mathcal{M}(T_{2n}) \setminus \mathcal{M}_1(T_{2n})$. Then in M_2 the vertices u_1 and u_2 must be covered with two different edges, say f_1 and f_2, and they can not belong to the same hexagon. So, f_1 must be in the hexagon h_1 and f_2 in the hexagon h_{2n} or vice versa. Then the only way to extend M_2 to the other vertices of T_{2n} is to either choose all edges of T_{2n} in the horizontal direction, or edges of M_2 alternate in a positive and a negative direction, as seen on Figure 5. So, $|\mathcal{M}(T_{2n}) \setminus \mathcal{M}_1(T_{2n})| = 2$. To conclude the proof we observe, the both new perfect matchings are not adjacent to any other perfect matching of T_{2n}. $\square$

For example, on Figure 6 there is the cyclic polyphenanthrene T_6 together with the resonance graph. The nontrivial connected component of the resonance graph $R(T_6)$ is isomorphic to the Lucas cube Λ_6.

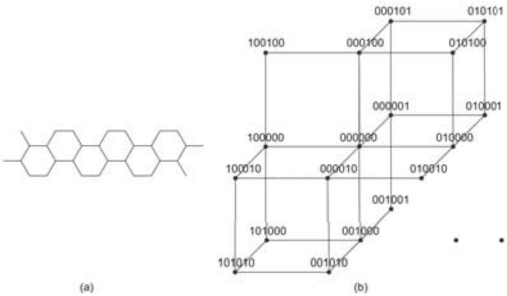

Figure 6: The cyclic polyphenanthrene T_6 with the resonance graph $R(T_6)$.

Let $K(G)$ be the number of perfect matchings (t.i. Kekulé structures) of a bipartite graph G. Enumeration of Kekulé structures in aromatic hydrocarbons has been a great challenge and was first accomplished in 1933 [26]. Since then there were several approaches and methods used in finding the number $K(G)$ for different kind of benzenoid systems G, for example see [27], [21], [28], [11], [34]. Determination of the number of perfect matchings in nanotubes is a complex problem and it was addressed first in [29], [21], [15], after that several methods of enumeration were described in [2], [20]. In [23] the authors deduced a recursive formula for determination $K(G)$ of cyclic polyphenanthrenes . Since we have an explicit formula for the Lucas numbers L_n (see [24] for instance), we immediately have the first corollary of Theorem 4.1.

Corollary 4.2 *Let T_{2n} be the cyclic polyphenanthrene, $n \geq 1$. Then the number of perfect matchings of T_{2n} is*

$$K(T_{2n}) = L_{2n} + 2 = \sum_{i=0}^{n} \binom{2n-i}{i} \frac{2n}{2n-i} + 2\,.$$

In [22] it vas proved that the Fibonacci cubes have a Hamiltonian cycle in the case of even number of vertices. We can not claim the same for the Lucas cubes, since it was proven in [24] that no Lucas cube is a Hamiltonian graph. Therefore the next corollary is also straightforward.

Corollary 4.3 *Let T_{2n} be the cyclic polyphenanthrene, $n \geq 1$. Then the nontrivial connected component of the resonance graph $R(T_{2n})$ is not a Hamiltonian graph.*

Let G be a graph. An edge coloring of G is proper if any two adjacent edges receive different colors and is vertex-distinguishing if distinct vertices are assigned distinct color sets, where the color set of a vertex v is the set of colors assigned to the edges incident to v. The *observability* of G, denoted by $\mathrm{obs}(G)$, is the minimum number of colors to be assigned to the edges of G so that the coloring is proper and vertex-distinguishing.

In [3] the authors proved that the observability of the Lucas cube Λ_n is n, for $n \geq 2$. Therefore we present our last corollary.

Corollary 4.4 *Let T_{2n} be the cyclic polyphenanthrene, $n \geq 1$. Then the observability of the resonance graph of T_{2n} is*

$$\mathrm{obs}(R(T_{2n})) = 2n\,.$$

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