FIBONACCI CUBES ARE THE RESONANCE GRAPHS OF FIBONACCENES

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ABSTRACT

Fibonacci cubes were introduced in 1993 and intensively studied afterwards. This paper adds the following theorem to these studies: Fibonacci cubes are precisely the resonance graphs of fibonaccenes. Here fibonaccenes are graphs that appear in chemical graph theory and resonance graphs reflect the structure of their perfect matchings. Some consequences of the main result are also listed.

1. FIBONACCI CUBES

Fibonacci cubes were introduced in [12, 13] as a model for interconnection networks and have been intensively studied afterwards—in [5, 16, 18, 19] several interesting properties have been obtained. For instance, the Fibonacci cubes poses a useful recursive structure [13] (not surprisingly closely connected to the Fibonacci numbers). In addition, one can define a related Fibonacci semilattice [18], as well as to determine several graph parameters of these graphs, for instance the independence number [18] and the observability [5].

Figure 1: The first four Fibonacci cubes.

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 ones. Two vertices are adjacent in Γ_n if they differ in precisely one bit. The Fibonacci cubes Γ_1, Γ_2, Γ_3, and Γ_4 are shown on Figure 1.

A motivation for the definition of the Fibonacci cubes comes from the well-known Zeckendorf's theorem [23], cf. also [8]. The theorem asserts that every non-negative integer can be uniquely represented as the sum of non-consecutive Fibonacci numbers. More precisely, given an integer i, if $0 \leq i < F_n$, the following representation is unique:

$$i = \sum_{j=2}^{n-1} a_j F_j;\ a_j \in \{0,1\},\ a_j a_{j+1} = 0\,.$$

Clearly, the representations for the integers i with $0 \leq i < F_n$ correspond to the vertices of the Fibonacci cube Γ_{n-2}. Consequently, $|V(\Gamma_n)| = F_{n+2}$.

2. FIBONACCENES AND RESONANCE GRAPHS

Another graph-theoretic concept that we consider here are the so-called fibonaccenes. The earliest reference to this family of chemicals is [1], cf. also [2, 10]. For more background on chemical graph theory we refer to the book of Trinajstić [22].

Figure 2: Some examples of fibonaccenes with six hexagons.

A *hexagonal chain* G with h hexagons is a graph defined recursively as follows. If $h = 1$ then G is the cycle on six vertices. For $h > 1$ we obtain G from a hexagonal chain H with $h-1$ hexagons by attaching the h^{th} hexagon along an edge e of the $(h-1)^{\text{st}}$ hexagon, where the endvertices of e are of degree 2 in the hexagonal chain H. Note that a hexagon r of a hexagonal chain that is adjacent to two other hexagons (that is, an inner hexagon) contains two vertices of degree two. We say that r is *angularly connected* if its two vertices of degree two are adjacent. Now, a hexagonal chain is called a *fibonaccene* if all of its hexagons, apart from the two terminal ones, are angularly connected. On Figure 2 we can see three non-isomorphic fibonaccenes with six hexagons, where the fibonaccenes (a) and (b) admit a planar representation as a subgraph of a hexagonal (graphite) lattice, while the fibonaccene (c) possess no such representation.

A *1-factor* or *perfect matching* of a graph G is a spanning subgraph with every vertex having degree one. Thus a 1-factor of a graph with $2n$ vertices will consist of n non-touching edges. It is well-known that a fibonaccene with n hexagons contains precisely F_{n+2} 1-factors (in the chemical literature these are known as Kekulé structures); see [1] and [10, Section 5.1.2]. F_{n+2} is also the number of vertices of the Fibonacci cube Γ_n. (For related results see [3, 7, 11, 20, 21].) In this paper we will demonstrate that a connection between the Fibonacci cubes and the fibonaccenes is much deeper. For this sake we need to introduce another concept.

Let G be a hexagonal chain. Then the vertex set of the *resonance graph* $R(G)$ of G consists of all 1-factors of G, and two 1-factors are adjacent whenever their symmetric difference is the edge set of a hexagon of G. On Figure 3 we can see the resonance graph of fibonaccenes from the Figure 2.

Figure 3: The resonance graph of fibonaccenes from the Figure 2.

In fact, the concept of the resonance graph can be defined much more generally, for instance, one can define the analogous concept for plane 2-connected graph [15]. 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 [6,9] as well as in the mathematical literature [24].

Figure 4: The link from r to r'.

In the next section we will also use the following terminology. Let r and r' be adjacent hexagons of a fibonaccene. Then the two edges of r that have exactly one vertex in r' are called the *link* from r to r' (see Figure 4).

3. THE CONNECTION

Our main result in the following.

Theorem 1: *Let G be an arbitrary fibonaccene with n hexagons. Then $R(G)$ is isomorphic to the Fibonacci cube Γ_n.*

In the rest of this section we prove the theorem. Let $r_1, r_2, \ldots, r_n$ be the hexagons of G, where r_1 and r_n are the terminal hexagons. So all the other hexagons of G are angularly connected.

We first establish a bijective correspondence between the vertices of $R(G)$ and the vertices of Γ_n. Let $\mathcal{F}(G)$ be the set of all 1-factors of G and define a (labeling) function

$$\ell : \mathcal{F}(G) \to \{0,1\}^n$$

as follows. Let F be an arbitrary 1-factor of G and let e be the edge of r_1 opposite to the common edge of r_1 and r_2. Then for $i = 1$ we set

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

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

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

For instance, the fibonaccene with three hexagons contains five 1-factors. On Figure 5 the labels obtained by ℓ are shown.

Note first that $(\ell(F))_1 = 1$ implies $(\ell(F))_2 = 0$. Moreover, in any three consecutive hexagons r_i, r_{i+1}, r_{i+2}, the 1-factor F cannot have both the link from r_{i+2} to r_{i+1} and the link from r_{i+1} to r_i. It follows that in $\ell(F)$ we do not have two consecutive ones. In addition, it is easy to see that for different 1-factors F and F', $\ell(F) \neq \ell(F')$. Since it is well-known that G contains F_{n+2} 1-factors (cf. [10]), it follows that the vertices of $R(G)$ bijectively correspond to the vertices of Γ_n (via the labeling ℓ).

For binary strings b and b', let $H(b, b')$ be the *Hamming distance* between b and b', that is, the number of positions in which they differ. To conclude the proof we need to show that for 1-factors F and F' of G the following holds:

$$F \text{ is adjacent to } F' \text{ if and only if } H(\ell(F), \ell(F')) = 1\,.$$

Suppose that F and F' are adjacent in $R(G)$. If the symmetric difference of F and F' contains the edges of r_1, then $\ell(F)$ and $\ell(F')$ differ in the first position and coincide in all the others. Assume now that the symmetric difference of F and F' contains the edges of r_i, $i \geq 2$. Then exactly one of the 1-factors F and F' must have a link from r_i to r_{i-1}, we may assume it is F. Then $(\ell(F))_i = 1$ and $(\ell(F'))_i = 0$, while $(\ell(F))_j = (\ell(F'))_j$ for $j \neq i$.

Conversely, suppose that $H(\ell(F), \ell(F')) = 1$. Then F and F' differ at precisely one hexagon, say r_i. Suppose $i = 1$. Then neither F nor F' contain the link from r_2 to r_1 which immediately implies that the symmetric difference of F and F' is the edge set of r_1. Since F and F' coincide in all the other hexagons, they are adjacent in $R(G)$. Assume next that $2 \leq i \leq n-1$. Then neither F nor F' contain the link from r_{i+1} to r_i as well as the link from r_{i-1} to r_i. Hence the symmetric difference of F and F' is the edge set of r_i. Finally, the case $i = n$ is treated analogously as the case $i = 1$.

Figure 5: The labelings corresponding to the fibonaccene with three hexagons.

This completes the proof.

To conclude the section we give an alternative argument that the labeling ℓ produces the vertices of Γ_n. This is clearly true for $n = 2$ and $n = 3$. So let G be obtained from a fibonaccene H with $n-1$ hexagons r_1, r_2, ... , r_{n-1} by adding the hexagon r_n to H in such a way that r_{n-1} becomes angularly connected.

The 1-factors of G can be divided into $\mathcal{F}_1(G)$ and $\mathcal{F}_2(G)$, where $\mathcal{F}_1(G)$ contains the 1-factors without the link from r_n to r_{n-1}, while $\mathcal{F}_2(G)$ contains the other 1-factors of G. Note that each 1-factor F of H can be in a unique way extended to a 1-factor F_1 of $\mathcal{F}_1(G)$. Moreover, $\ell(F_1) = \ell(F)0$, where $\ell(F)0$ denotes the concatenation of the label $\ell(F)$ with the symbol 0, see Figure 6.

Consider next a 1-factor $F_2 \in \mathcal{F}_2(G)$. Then there is no link from r_{n-1} to r_{n-2}. Hence we are interested only in 1-factors of H without this link. Consequently, $\ell(F_2)$ must have 0 in the last position. Similarly as above, each 1-factor of G without a link from r_{n-1} to r_{n-2} can be in a unique way extended to a 1-factor from $\mathcal{F}_2(G)$. The labelings of 1-factors from $\mathcal{F}_2(G)$ are obtained by adding 1 as the n^{th} bit. Hence $\ell(F_2)$ ends with 01, cf. Figure 6. 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.

Figure 6: Fixed edges of 1-factors from $\mathcal{F}_1(G)$ and $\mathcal{F}_2(G)$ with associated labelings.

4. SOME APPLICATIONS

In this section we list several consequences of our main result that follow from the fact that the Fibonacci cubes are median graphs. Since median graphs are closely related to hypercubes, cf. [14, 17], we first introduce the latter class of graphs.

The vertex set of the *n-cube* Q_n consists of all n-tuples $b_1b_2\ldots b_n$ with $b_i \in \{0,1\}$. Two vertices are adjacent if the corresponding tuples differ in precisely one place. Q_n is also called a *hypercube of dimension* n. Note that $Q_1 = K_2$ and $Q_2 = C_4$.

Let G be a graph. Then a *median* of vertices u, v, and w is a vertex that simultaneously lies on a shortest u,v-path, on a shortest u,w-path, and on a shortest v,w-path. A connected graph is called a *median graph* if every triple of its vertices has a unique median. Standard examples of median graphs are trees and hypercubes. For basic results about median graphs see [14].

In [15] it is proved that the so-called catacondensed even ring systems have median resonance graphs. Since fibonaccenes form a (very) special subclass of catacondensed even ring systems, their resonance graphs are median as well. Hence Theorem 1 implies:

Corollary 1: *For any $n \geq 1$, Γ_n is a median graph.*

As median graphs embed isometrically into hypercubes [17], we note in passing that the Fibonacci cubes can be isometrically embedded into hypercubes as well.

The set X of vertices of a graph G is called *independent* if no two vertices of X are adjacent. The size of a largest independent set is called the *independence number* of G and denoted by $\alpha(G)$.

Since Γ_n is an (isometric) subgraph of a (bipartite) hypercube Q_n, its bipartition is induced by the set of vertices E_n containing an even number of ones and the set of vertices O_n containing an odd number of ones. Let $e_n = |E_n|$ and $o_n = |O_n|$. Chen and Zhang [4] proved that the resonance graph of a catacondensed hexagonal graph contains a Hamilton path. In particular this is true for the fibonaccenes which in turn implies that any Fibonacci cube contains a Hamilton path. As Γ_n is bipartite with the bipartition $E_n + O_n$ we obtain Theorem 1 of [18]:

Corollary 2: *For* $n \geq 1$, $\alpha(\Gamma_n) = \max\{e_n, o_n\}$.

We conclude the paper with an application concerning representations of integers using Fibonacci numbers that might be of some independent interest. Let i_1, i_2, and i_3 be non-negative integers and let

$$i_1 = \sum_{j=2}^{n-1} a_j F_j;\ a_j \in \{0,1\},\ a_j a_{j+1} = 0\,,$$

$$i_2 = \sum_{j=2}^{n-1} b_j F_j;\ b_j \in \{0,1\},\ b_j b_{j+1} = 0\,,$$

and

$$i_3 = \sum_{j=2}^{n-1} c_j F_j;\ c_j \in \{0,1\},\ c_j c_{j+1} = 0\,,$$

be their Zeckendorf's representations. Then we say that i_3 is an *F-intermediate integer* for i_1 and i_2 if for any index j, the equality $a_j = b_j$ implies $c_j = a_j$.

Let G be a median graph isometrically embedded into Q_n. Let u, v, and w be vertices of G that are mapped to vertices $u_1 u_2 \ldots u_n$, $v_1 v_2 \ldots v_n$, and $w_1 w_2 \ldots w_n$ of Q_n, respectively. (Recall that vertices of Q_n are n-tuples over $\{0,1\}$.) Then it is well known (cf. the proof of [14, Proposition 1.29]) that the median of the triple in Q_n is obtained by the majority rule: the i^{th} coordinate of the median is equal to the element that appears at least twice among the u_i, v_i, and w_i. Hence, we have the following result:

Corollary 3: *Let i_1, i_2, and i_3 be arbitrary non-negative integers. Then there exists a unique non-negative integer i such that i is*

an F-intermediate integer for i_1 and i_2,
an F-intermediate integer for i_1 and i_3, and
an F-intermediate integer for i_2 and i_3.

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