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Resonance Graphs of Kinky Benzenoid Systems Are Daisy Cubes

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Abstract

In [10] introduced daisy cubes are interesting isometric subgraphs of n-cubes Q_n, induced with intervals between the maximal elements of a poset $(V(Q_n), \leq)$ and the vertex $0^n \in V(Q_n)$. In this paper we show that the resonance graph, which reflects the interaction between Kekulé structures of aromatic hydrocarbon molecules, is a daisy cube, if the molecules considered can be modeled with the so called kinky benzenoid systems, i.e. catacondensed benzenoid systems without linear hexagons.

1 Introduction

Klavžar and Mollard just recently introduced in [10] a cube like structures called daisy cubes. The daisy cube $Q_n(X)$ is defined as the subgraph of n-cube Q_n induced by the intersection of the intervals $I(x, 0^n)$ over all $x \in X$. Daisy cubes are partial cubes that include among others Fibonacci cubes, Lucas cubes, and bipartite wheels. The authors in [10] also introduced a bivariate polynomial called distance cube polynomial and showed that for a daisy cubes it is connected with the cube polynomial.

Fibonacci and Lucas cubes are a Fibonacci strings based graphs introduced as models for interconnection networks (see [5, 6, 9] for more details). Both structures are surprisingly connected with the chemical molecules made of hydrogen and carbon atoms. Benzenoid hydrocarbons are molecules composed of benzene hexagonal rings and can be viewed as subgraphs of a hexagonal lattice. If we embed them on the surface of a cylinder

and roll up a hexagonal lattice we obtain carbon nanotubes - interesting molecules discovered in 1991 [7]. Benzenoid hydrocarbons and carbon nanotubes are aromatic molecules and the interaction between theirs Kekulé structures can be modeled with the resonance graph. In [12] the authors showed that the resonance graph of a class of benzenoid hydrocarbons called fibonaccenes is isomorphic to a Fibonacci cube. Later a similar result was shown for a class od carbon nanotubes, but this time it was proven that the largest connected component of the resonance graph is isomorphic to a Lucas cube, see [20]. Since both classes of cubes, i.e. Fibonaci and Lucas cubes, are daisy cubes, we were interested in a problem, for which class of chemical graphs the resonance graph is a daisy cube.

In the next section all the necessary definitions are given, followed with the section on the main result of this paper. The main result of this paper says, that the resonance graphs of a fibonaccene-like benzenoid hydrocarbons, called kinky benzenoid systems, are daisy cubes.

2 Preliminaries

Let us first describe the concept of a daisy cube. If $G = (V(G), E(G))$ is a graph and $X \subseteq V(G)$, then $\langle X \rangle$ denotes the subgraph of G induced by X. Further, for a word u of length n over $B = \{0, 1\}$, i.e., $u = (u_1, \ldots, u_n) \in B^n$ we will briefly write u as $u_1 \ldots u_n$. The n-cube Q_n has the vertex set B^n, vertices $u_1 \ldots u_n$ and $v_1 \ldots v_n$ being adjacent if $u_i \neq v_i$ for exactly one $i \in [n]$, where $[n] = \{1, \ldots, n\}$. Let $\leq$ be a partial order on B^n defined with $u_1 \ldots u_n \leq v_1 \ldots v_n$ if $u_i \leq v_i$ holds for all $i \in [n]$. For $X \subseteq B^n$ we define the graph $Q_n(X)$ as the subgraph of Q_n with $Q_n(X) = \langle \{u \in B^n; u \leq x \,\text{for some}\, x \in X\} \rangle$ and say that $Q_n(X)$ is a *daisy cube* (generated by X). The vertex sets of daisy cubes are also known as hereditary or downwards closed sets, see [8]. For vertices u and v of a graph G let $d_G(u, v)$ be the *distance* between u and v in G. Further, the *interval* $I_G(u, v)$ between u and v (in G) is the set of vertices lying on shortest u, v-paths, so $I_G(u, v) = \{w; d_G(u, v) = d_G(u, w) + d_G(w, v)\}$.

Benzenoid systems are 2-connected plane graphs such that every interior face is a hexagon. Two hexagons of a benzenoid system G are said to be *adjacent*, if they share an edge. A hexagon of G is *terminal* if it is adjacent to only one other hexagon in G. If every vertex of a benzenoid system G belongs to at most two hexagons, then G is said to be catacondensed; otherwise it is pericondensed. Note that hexagon h of a catacondensed

benzenoid system that is adjacent to two other hexagons contains two vertices of degree two. If these two vertices are adjacent, then hexagon h is called a *kink* or *angularly connected hexagon*, otherwise h is *linearly connected hexagon*. A catacondensed benzenoid system with no linearly connected hexagons is called a *kinky benzenoid system*.

A *1-factor* of a benzenoid system G is a spanning subgraph of G such that every vertex has degree one. The edge set of a 1-factor is called a *perfect matching* of G, which is a set of independent edges covering all vertices of G. In chemical literature, perfect matchings are known as Kekulé structures (see [4] for more details). A hexagon h of a benzenoid system G is *M-alternating* if the edges of h appear alternately in and off the perfect matching M. Set S of disjoint hexagons of G is a *resonant set* of G if there exists a perfect matching M such that all hexagons in S are M-alternating.

Next we will briefly describe the binary coding of perfect matchings of catacondensed benzenoid system G with n hexagons introduced in [11]. First we order the hexagons of a catacondensed benzenoid system with the use of the depth–first search algorithm (DFS) or by the breadth–first search algorithm (BFS) ([14]) performed on the inner dual T of G, starting at an arbitrary leaf of T. Let h and h' be adjacent hexagons of G and M a perfect matching of G. Then the two edges of M in h that have exactly one vertex in h' are called the *link* from h to h'. For example, on Figure 1 we can see the link from hexagon h_3 to hexagon h_2. Note that a result from [13] says that either both edges of a link belong to some perfect matching of a catacondensed benzenoid system or none. Further, let $\mathcal{M}(G)$ be the set of all perfect matchings of G and we define a (labeling) function

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

as follows. Let M be an arbitrary perfect matching of G and let e be the edge of hexagon h_1 opposite to the common edge of hexagons h_1 and h_2 (see Figure 1). Then for $i = 1$ we set

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

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

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

On Figure 1 we can see a kinky benzenoid system with ordered hexagons, a perfect matching M and the label of M.

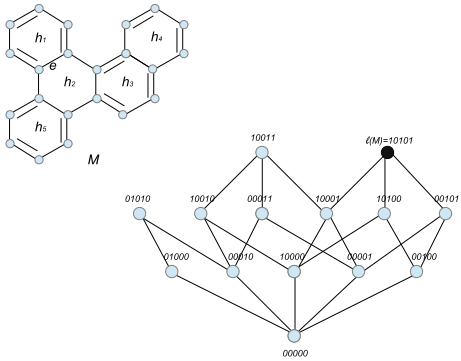

Figure 1. A kinky benzenoid system with ordered hexagons, perfect matching M and the resonance graph with labeled vertices.

Let $\mathcal{L}(G)$ be the set of all binary labels of perfect matchings of a catacondensed benzenoid system G. Clearly, $\mathcal{L}(G)$ is a subset of $B^n = \{0,1\}^n$ and since $(B^n, \leq)$ is a poset, so is $(\mathcal{L}(G), \leq)$.

The vertex set of the *resonance graph* $R(G)$ of G consists of all perfect matchings of G, two vertices being adjacent whenever their symmetric difference forms the edge set of a hexagon of G (see Figures 1, 2). The concept of the resonance graph was introduced independently in mathematics (under the name Z-transformation graph) in [19] as well in chemistry [1, 3, 15, 16]. We can also introduce the *resonance digraph* $\overrightarrow{R}(G)$ of G by orienting the edge M_1M_2 of $R(G)$. An ordered pair (M_1, M_2) is an arc from M_1 to M_2 in $\overrightarrow{R}(G)$ if for some i we have $(\ell(M_1))_i = 0$ and $(\ell(M_2))_i = 1$, and the labels of M_1 and M_2 on all other positions (different from i-th) coincide. Since the resonance graph of a catacondensed benzenoid system with n hexagons can be isometrically embedded into the n-cube (in fact it is also a median graph, see [13]) and function ℓ is the labeling of the vertices of the resonance (di)graph for that embedding, it naturally follows that the Hasse diagram of the poset $(\mathcal{L}(G), \leq)$ is isomorphic to the resonance digraph $\overrightarrow{R}(G)$.

3 The main result

In this section G is a kinky benzenoid system with n hexagons $\{h_i, h_2, \ldots, h_n\}$ indexed accordingly to the DFS (or BFS) algorithm performed on the inner dual T of G . Hexagons of G are then numbered so that h_i is a predecessor of h_j in T if and only if $i < j$.

Lemma 3.1 *Let G be a kinky benzenoid system and let S be a maximal resonant set of G. If h is a hexagon of G that does not lie in S, then one of its adjacent hexagons lies in S.*

Proof. Let G be a kinky benzenoid system with a maximal resonant set S, where M is a perfect matching of G such that every hexagon in S is M-alternating.

Let h be a non-terminal hexagon of G and h_1, h_2 (and if exists - h_3) hexagons adjacent to h. If h is an M-alternating hexagon, we are done. Suppose h is not in S. Then there must be a link in M from at least one of hexagons h_1, h_2 (or h_3) to hexagon h and consequently this hexagon is M-alternating. By the maximality of S it must also belong to S.

Similar holds if h is a terminal hexagon. Let h_1 be the hexagon adjacent to h. Since G is kinky benzenoid system at least one of hexagons h_1 and h is M-alternating and therefore belongs to S.

We can assign in a natural way a binary label to a resonant set of a benzenoid system.

Definition 3.2 *Let G be a benzenoid system with n hexagons h_i, $i \in [n]$. If S is a resonant set of G, then its* binary representation *$b(S)$ is a binary string of length n where*

$$(b(S))_j = \begin{cases} 1 \;\; ; & h_j \in S, \\ 0 \;\; ; & otherwise\,. \end{cases}$$

Lemma 3.3 *Let G be a kinky benzenoid system and S a resonant set of G. Then S is a maximal resonant set of G if and only if $b(S)$ is a maximal element in $(\mathcal{L}(G), \leq)$.*

Proof. First, let S be a maximal resonant set of a kinky benzenoid system G and $b(S)$ its binary label. Then we can construct a perfect matching M of G such that $b(S) = \ell(M)$. Namely, if $(b(S))_i = 1$ for some $i \in [n]$, then we insert a link from hexagon h_i to its adjacent predecessor and $(\ell(M))_i = 1$ (the same holds if $i = 1$ - then we insert a link from h_1 to h_2).

On the other side, if $(b(S))_j = 0$ then due to Lemma 3.1 at least one of the hexagons adjacent to hexagon h_j must be in S, let it be hexagon $h_{j'}$, so $(b(S))_{j'} = 1$. We again insert a link from hexagon $h_{j'}$ to its adjacent predecessor and $(\ell(M))_{j'} = 1$ (the same holds if $j' = 1$ - then we insert a link from $h_{j'} = h_1$ to h_j). If $j < j'$, hexagon h_j can not have a link to its adjacent predecessor and consequently $(\ell(M))_j = 0$. Also in the case when $j' < j$ there is no link from hexagon h_j to hexagon $h_{j'}$ and again $(\ell(M))_j = 0$.

Suppose $\ell(M)$ is not a maximal element in $(\mathcal{L}(G), \leq)$. Then there exists a perfect matching M' of G such that $\ell(M) \leq \ell(M')$ and $\ell(M) \neq \ell(M')$. More precisely, there exists $j \in [n]$ so that $(\ell(M'))_j = 1$ and $(\ell(M))_j = 0$. Hexagon h_j then does not belong to S and if h_j is a non terminal hexagon, it is adjacent to one predecessor h_{j_0} and at most two successors h_{j_1}, h_{j_2}. If h_j is a terminal hexagon it has either only one adjacent successor h_{j_1} or only one adjacent predecessor h_{j_0}.

If h_j is a non terminal hexagon, then since $(\ell(M'))_j = 1$ there is a link from hexagon h_j to hexagon h_{j_0} and since G is kinky benzenoid system, there are no links from h_{j_1}, h_{j_2} to h_j or from h_{j_0} to its adjacent predecessor. Consequently $(\ell(M'))_{j_k} = 0, k = 0, 1, 2$. Also if h_j is a terminal hexagon adjacent either to one successor h_{j_1} or one predecessor h_{j_0}, again $(\ell(M'))_{j_1} = 0$ and $(\ell(M'))_{j_0} = 0$, respectively.

Let us now consider the label of M, $\ell(M)$, and suppose h_j is a non terminal hexagon. Since h_j is not contained in S, then by Lemma 3.1 at least one of the adjacent hexagons must be in S and is therefore M-alternating. So, at least one of the positions $(\ell(M))_{j_k} = 1$, $k = 0, 1, 2$, and consequently $\ell(M')$ and $\ell(M)$ are incomparable elements in $(\mathcal{L}(G), \leq)$. The same argument holds if h_j is a terminal hexagon.

For the if part of the proof suppose S is not a maximal resonant set, so there exists a resonant set S'' of G such that $S \subset S''$. By the same argument as above, there exist perfect matchings M and M'' so that $b(S) = \ell(M)$ and $b(S'') = \ell(M'')$. But then $\ell(M) \leq \ell(M'')$ and therefore $\ell(M) = b(S)$ is not a maximal element in $(\mathcal{L}(G), \leq)$.

Lemma 3.4 *Let G be a kinky benzenoid system and $\ell(M)$ a maximal element in $(\mathcal{L}(G), \leq)$. Then there exists a maximal resonant set S of G such that $b(S) = \ell(M)$.*

Proof. Let G be a kinky benzenoid system with n hexagons denoted with h_i, $i \in [n]$. Let $\ell(M)$ be a maximal element in $(\mathcal{L}(G), \leq)$, where M is a perfect matching of a G. Then for all $i \in [n]$ such that $(\ell(M))_i = 1$, the hexagon h_i is an M-alternating hexagon of G. Let S be the set of all M-alternating hexagons of G. If $(\ell(M))_j = (\ell(M))_k = 1$ for some $j \neq k$, then hexagons h_j and h_k can not be adjacent, since there are links in M from hexagons h_j and h_k to theirs adjacent predecessors. Therefore S is a resonant set. Suppose now S is not a maximal resonant set. Then there exists a hexagon h' of G such that $h \notin S$. By Lemma 3.1, $S' = S \cup \{h'\}$ is a resonant set and $b(S) \leq b(S')$. But then we have a perfect matching M' in G such that $b(S') = \ell(M')$ and $\ell(M) \leq \ell(M')$ contradicts the maximality of M.

Theorem 3.5 *The resonance graph of a kinky benzenoid system is a daisy cube.*

Proof. It was shown in [10] that the daisy cube $Q_n(X)$ induced on set X is isomorphic to $\langle \cup_{x\in\hat{X}} I_{Q_n}(x, 0^n)\rangle$, where $\hat{X}$ is an antichain consisting of all maximal elements of X.

Let G be a kinky benzenoid system with n hexagons and let $X = \mathcal{L}(G)$ and $\widehat{X}$ the set of all maximal elements of $(\mathcal{L}(G), \leq)$. By Lemmas 3.3 and 3.4 for each $x = \ell(M) \in \widehat{X}$ there is a maximal resonant set S of G such that $b(S) = \ell(M)$. Further, for $x = \ell(M) = b(S) \in \widehat{X}$ the graph induced on interval $I_{R(G)}(\ell(M), 0^n)$ is the subgraph of the resonance graph $R(G)$ isomorphic to the k-cube, where k equals the number of $1'$s in $\ell(M)$ i.e. $k = |S|$ (similar result was shown in [17]). Since for every vertex $\ell(M')$ of the resonance graph $R(G)$ there exists $x' \in \widehat{X}$ such that $\ell(M') \leq x'$, we are done.

On Figure 1 we can see a kinky benzenoid system with the resonance graph that is a daisy cube, and on Figure 2 we have a benzenoid system with linear hexagons where the resonance graph is not a daisy cube.

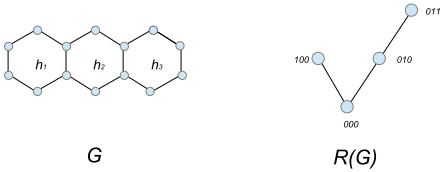

Figure 2. A benzenoid system G with linear hexagon and the resonance graph $R(G)$ which is not a daisy cube.

Obviously the converse does not hold. For example, the largest connected component of the resonance graph of benzenoid like structures called cyclic polyphenantrenes (they are simple carbon nanotubes) is isomorphic to a Lucas cube ([20]), which are daisy cubes.

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References

[1] S. El-Basil, Kekulé structures as graph generators, *J. Math. Chem.* **14** (1993) 305–318.

[2] E. Dedó, D. Torri, N. Zagaglia Salvi, The observability of the Fibonacci and the Lucas cubes, *Discr. Math.* **255** (2002) 55–63.

[3] W. Gründler, Signifikante Elektronenstrukturen fur benzenoide Kohlenwasserstoffe, *Wiss. Z. Univ. Halle* **31** (1982) 97–116.

[4] I. Gutman, S. J. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons*, Springer, Berlin, 1989.

[5] W. J. Hsu, Fibonacci cubes - A new interconnection topology, *IEEE Trans. Parallel Distr. Sys.* **4** (1993) 3–12.

[6] W. J. Hsu, C. V. Page, J. S. Liu, Fibonacci cubes – A class of self–similar graphs, *Fibonacci Quart.* **31** (1993) 65–72.

[7] S. Iijima, Helical microtubules of graphitic carbon, *Nature* **354** (1991) 56–58.

[8] S. Jukna, *Extremal Combinatorics – with Applications in Computer Science*, Springer, Heidelberg, 2011.

[9] S. Klavžar, Structure of Fibonacci cubes: a survey, *J. Comb. Optim.* **25** (2013) 505–522.

[10] S. Klavžar, M. Mollard, Daisy cubes and distance cube polynomial, *Eur. J. Comb.*, to appear.

[11] S. Klavžar, A. Vesel, P. Žigert, I. Gutman, Binary coding of Kekulé structures of catacondensed benzenoid hydrocarbons, *Comput. Chem.* **25** (2001) 569–575.

[12] S. Klavžar, P. Žigert, Fibonacci cubes are the resonance graphs of fibonaccenes, *Fibonacci Quart.* **43** (2005) 269–276.

[13] S. Klavžar, P. Žigert, G. Brinkmann, Resonance graphs of catacondensed even ring systems are median, *Discrete Math.* **253** (2002) 35–43.

[14] D. C. Kozen, *The Design and Analysis of Algorithms*, Springer-Verlag, New York, 1992.

[15] M. Randić, Resonance in catacondensed benzenoid hydrocarbons, *Int. J. Quantum Chem.* **63** (1997) 585–600.

[16] M. Randić, D. J. Klein, S. El–Basil, P. Calkins, Resonance in large benzenoid hydrocarbons, *Croat. Chem. Acta.* **69** (1996) 1639–1660.

[17] A. Taranenko, P. Žigert, Resonant sets of benzenoid graphs and hypercubes of their resonance graphs, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 65–77.

[18] H. Zhang, Z-transformation graphs of perfect matchings of plane bipartite graphs: a survey, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 457–476.

[19] F. Zhang, X. Guo, R. Chen, *Z*-transformation graphs of perfect matchings of hexagonal systems, *Discr. Math.* **72** (1988) 405–415.

[20] P. Žigert, M. Berlič, Lucas cubes and resonance graphs of cyclic polyphenantrenes, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 77–90.