A min-max result on catacondensed benzenoid graphs

Sandi Klavžar* and Petra Žigert
Department of Mathematics, PEF, University of Maribor
Koroška cesta 160, 2000 Maribor, Slovenia
sandi.klavzar@uni-lj.si
petra.zigert@uni-mb.si

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Abstract

The resonance graph of a benzenoid graph G has the 1-factors of G as vertices, two 1-factors being adjacent if their symmetric difference forms the edge set of a hexagon of G. It is proved that the smallest number of elementary cuts that cover a catacondensed benzenoid graph equals the dimension of a largest induced hypercube of its resonance graph.

Keywords: benzenoid graph, perfect matching, resonance graph, hypercube

1 Introduction

Benzenoid graphs (in the mathematical literature also called *hexagonal systems*) are 2-connected subgraphs of the hexagonal lattice so that every bounded face is a hexagon. If all vertices of a benzenoid graph G lie on its *perimeter*, then G is said to be *catacondensed*; otherwise it is *pericondensed*. For more information on these graphs, in particular for their chemical meaning as benzenoid hydrocarbons, see the book of Gutman and Cyvin [6].

A *matching* of a graph G is a set of pairwise independent edges. A matching is *perfect* or a *1-factor*, if it covers all the vertices of G. Let G be a benzenoid graph. 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.

The concept of the resonance graph is very natural, hence it is not surprising that it was independently introduced several times. In the chemical literature, the first known references are due to Gründler [4, 5]. The concept was later reinvented by El-Basil in [2, 3], and Randić with co-workers in [14, 13]. In the mathematical literature, again

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independently, Zhang, Guo, and Chen introduced resonance graphs under the name of Z-transformation graphs [15]. They proved among others that the resonance graph of a benzenoid graph with at least one 1-factor is connected, bipartite, and is either a path or has girth 4. Chen and Zhang [1] proved that the resonance graph of a catacondensed benzenoid graph has a Hamilton path.

In [10] it is proved that the resonance graphs of the catacondensed benzenoid graphs possess much of a structure, namely, they belong to the class of median graphs. (For more information on the well developed theory of median graphs see [7, 8, 12].) This result was in [11] extended to a larger class of planar graphs—to the so-called even ring systems. The structure of the resonance graphs of the catacondensed benzenoid graphs as described in [10] (or in [11]) led to an algorithm that assigns a unique and quite short binary code to every 1-factor of a catacondensed benzenoid graph [9].

Let e be an edge of a benzenoid graph G lying on its perimeter. Then the *elementary cut* C_e corresponding to e is the set of edges so that $e \in C_e$ and with every edge f of C_e also the opposite edge with respect to a hexagon containing f belongs to C_e. Note that the set of elementary cuts partitions the edge set of G. For instance, in $G = C_6$ there are three elementary cuts, each consisting of two opposite edges of C_6. We say that a subset $\mathcal{C}$ of elementary cuts *covers* G if for any hexagon A of G, there is a $C \in \mathcal{C}$ that meets A in two opposite edges. The above definitions can be extended to larger classes of graphs (just replacing hexagons with any even cycles), in particular to the so-called even ring systems to be mentioned at the end of this note.

The *Cartesian product* $G \Box H$ of graphs G and H is the graph with the vertex set $V(G) \times V(H)$ and $(a,x)(b,y) \in E(G \Box H)$ whenever $ab \in E(G)$ and $x = y$, or, if $a = b$ and $xy \in E(H)$. The Cartesian product of n copies of the complete graph on two vertices K_2 is the *n-cube* Q_n. In other words, the vertex set of Q_n consists of all n-tuples $b_1 b_2 \ldots b_n$ with $b_i \in \{0,1\}$, and two vertices are adjacent if the corresponding tuples differ in precisely one place.

In this note we prove the following result:

Theorem 1 *Let G be a catacondensed benzenoid graph. Then the smallest number of elementary cuts that cover G equals the dimension of a largest induced hypercube of $R(G)$.*

Let H be a fixed subgraph of a graph G, $H \subseteq G$. Then the *local Cartesian product* $G \Box_\ell H$ is the graph obtained from the disjoint union of G and H, in which every vertex of H is joined by an edge with the corresponding vertex of $H \subseteq G$. Finally, the notation $G[X]$ is used to denote the subgraph of G induced by the set X.

2 Proof of the theorem

Let G be a catacondensed benzenoid graph. An edge of G that lies on its perimeter will be called a *b-edge* and an edge with end vertices of degree three that belongs to a pendant hexagon will be called a *join edge*. If A and B are incident hexagons of G, then the two edges on the boundary of A that have exactly one vertex on the boundary of B are called the *link* of A to B.

Let e be a join edge of G. Denote by $\mathcal{F}_e(G)$ the set of 1-factors of G that contain e and by $\mathcal{F}_{\overline{e}}(G)$ the set of those 1-factors of G that do not contain e. Let A be the pendant hexagon of G containing e. Then the 1-factors of $\mathcal{F}_{\overline{e}}(G)$ either contain the link of A to its neighboring hexagon or not. We denote the corresponding sets of 1-factors with $\mathcal{F}_{\overline{e}}^{\ell}(G)$ and $\mathcal{F}_{\overline{e}}^{\overline{\ell}}(G)$, respectively. Thus, the 1-factors of G can be partitioned as

$$V(R(G)) = \mathcal{F}_e(G) \cup \mathcal{F}_{\overline{e}}^{\overline{\ell}}(G) \cup \mathcal{F}_{\overline{e}}^{\ell}(G).$$

The following lemma is (implicitly) contained in [10], cf. also [11]. For the sake of completeness we include its proof.

Lemma 2 *Let e be a join edge of a catacondensed benzenoid graph G and let H be the benzenoid graph obtained from G by removing the pendant hexagon containing e. Then $R(G)[\mathcal{F}_e(G)]$ is isomorphic with $R(G)[\mathcal{F}_{\overline{e}}^{\ell}(G)]$. Moreover,*

$$R(G) = R(H)\Box_{\ell}R(G)[\mathcal{F}_e(G)] \qquad \text{(cf. Fig. 1)}\,.$$

Proof. Note first that $R(H) = R(G)[\mathcal{F}_e(G) \cup \mathcal{F}_{\overline{e}}^{\overline{\ell}}(G)]$. Indeed, the 1-factors of $\mathcal{F}_e(H)$ one-to-one correspond to the 1-factors of $\mathcal{F}_e(G)$ and the remaining 1-factors of H to $\mathcal{F}_{\overline{e}}^{\overline{\ell}}(G)$.

Consider now a 1-factor F of $\mathcal{F}_{\overline{e}}^{\ell}(G)$. In $R(G)$ it is adjacent to a unique 1-factor $\overline{F}$ from the set $R(G)[\mathcal{F}_e(G)]$. Moreover, two 1-factors F_1 and F_2 of $\mathcal{F}_{\overline{e}}^{\ell}(G)$ are adjacent if and only if the corresponding 1-factors $\overline{F_1}$ and $\overline{F_2}$ of $\mathcal{F}_e(G)$ are adjacent. Therefore $R(G)[\mathcal{F}_e(G)]$ and $R(G)[\mathcal{F}_{\overline{e}}^{\ell}(G)]$ are isomorphic and $R(G) = R(H)\Box_{\ell}R(G)[\mathcal{F}_e(G)]$. ∎

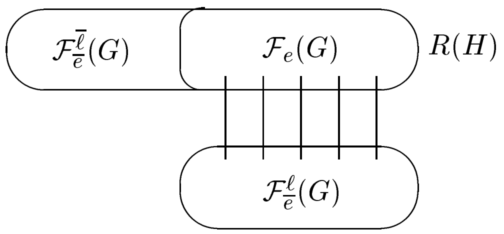

Figure 1: The structure of $R(G)$.

Let e be a join edge of a catacondensed benzenoid graph G and let f and f' be the b-edges of the elementary cut C_e, where f' belongs to the pendant hexagon containing e. Let H be the graph obtained from G by removing all hexagons (their edges and vertices) intersected by C_e, except the two edges, that are incident with f. We call these two edges the *turn-edges* of e. Then H consists of two connected components, we will denote them by G_e^1 and G_e^2, see Fig. 2.

Note that if a turn-edge is a b-edge, then the corresponding component of H is K_2, otherwise it is a benzenoid graph. We define $R(K_2) = K_1$.

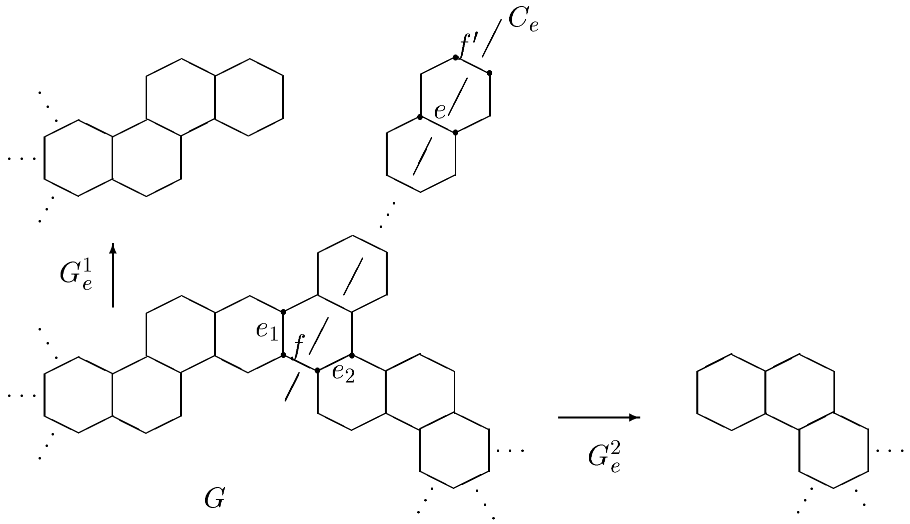

Figure 2: A benzenoid graph G and components G_e^1, G_e^2.

Lemma 3 *Let e be a join edge of a catacondensed benzenoid graph G. Then*

$$R(G)[\mathcal{F}_{\overline{e}}^{\ell}(G)] = R(G_e^1)\square R(G_e^2).$$

Proof. Let F be a 1-factor from $\mathcal{F}_{\overline{e}}^{\ell}(G)$ and let e_1 and e_2 be the turn-edges of e. Then F is fixed on all the hexagons intersected by C_e except on the last one, that is the one containing e_1 and e_2. If e_1 or e_2 is also a b-edge, then it lies in F. Let f be the edge incident with e_1 and e_2, cf. Fig. 2. Then f does not belong to F, for otherwise F cannot be extended to a 1-factor of G since we would need to cover an odd number of vertices. Thus, selecting a 1-factor F_1 of G_e^1 and a 1-factor F_2 of G_e^2, there is a unique way to extend it to a 1-factor from $\mathcal{F}_{\overline{e}}^{\ell}(G)$. Therefore, the 1-factors of $\mathcal{F}_{\overline{e}}^{\ell}(G)$ are in one-to-one correspondence with the pairs (F_1, F_2), where F_1 is a 1-factor of G_e^1 and F_2 a 1-factor of G_e^2. But then the conclusion of the lemma follows immediately from the definition of the Cartesian product. ∎

We are now ready for the proof of Theorem 1. Let n be the number of hexagons of G. We proceed by induction on n. For $n = 1$ we have $G = C_6$ and $R(C_6) = K_2 = Q_1$.

Let $n > 1$. Let A be a pendant hexagon of G and H the benzenoid graph obtained from G by removing A. Let k be the smallest number of elementary cuts that cover H. Then, by the induction assumption, $R(H)$ contains a k-cube, but not an r-cube with $r > k$. We distinguish two cases.

Case 1. $k + 1$ elementary cuts are needed to cover G.
In this case, C_e intersects precisely 2 hexagons. We need to show that Q_{k+1} is a largest subcube of G. Let k_1 be the smallest number of elementary cuts that cover G_e^1 and k_2 be the smallest number of elementary cuts that cover G_e^2. In the case that G_e^1 or G_e^2 is isomorphic to K_2, we set $k_1 = 0$ or $k_2 = 0$. Then $k_1 + k_2 = k$. By the induction

assumption, $R(G_e^1)$ contains Q_{k_1} and $R(G_e^2)$ contains Q_{k_2}. By Lemma 3 we thus infer that $R(G)[\mathcal{F}_{\overline{e}}^{\ell}(G)]$ contains Q_k (and no larger hypercube) and from Lemma 2 we infer that Q_{k+1} is an induced subgraph of G.

Case 2. k elementary cuts suffice to cover G.
Let $\mathcal{C}$ be a cover of G containing k elementary cuts. Then $C_e \in \mathcal{C}$, for otherwise C_e would cover only the hexagon A and hence $\mathcal{C} \setminus C_e$ would be a cover of H with $k-1$ elementary cuts. Since $R(H)$ is a subgraph of $R(G)$, and $R(H)$ contains Q_k, we need to show that there is no larger hypercube in $R(G)$. $\mathcal{C} \setminus C_e$ is a cover of $R(G_e^1)$ and $R(G_e^2)$, say with k_1 elementary cuts in $R(G_e^1)$ and with k_2 elementary cuts in $R(G_e^2)$. Note that $k_1 + k_2 = k - 1$. Thus, by the induction assumption, the dimension of a largest hypercube of $R(G_e^1)$ and $R(G_e^2)$ is bounded by k_1 and k_2, respectively. By Lemma 3 we thus infer that the dimension of a largest hypercube of $R(G)[\mathcal{F}_{\overline{e}}^{\ell}(G)]$ is at most $k-1$ and so Lemma 2 implies that in $R(G)$ the dimension of a largest hypercube is bounded by k. On the other hand, in $R(H)$ we have an induced Q_k, thus we have an induced Q_k in $R(G)$. Case 2 is settled, and the proof of the theorem is complete.

3 Concluding remark

Theorem 1 cannot be extended to the catacondensed even ring systems (see [11] for the definition), consider, for instance, the example from Fig. 3.

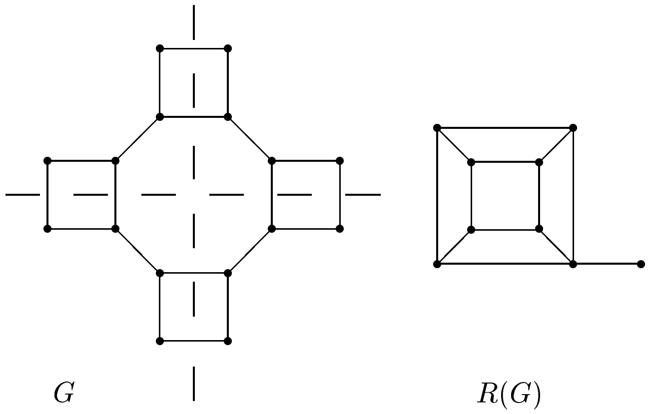

Figure 3: A catacondensed even ring system G and its resonance graph.

The graph G from the figure is a catacondensed even ring system that can be covered by two elementary cuts. However, in its resonance graph (also shown in Fig. 3) we find an induced Q_3.

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