On the role of hypercubes in the resonance graphs of benzenoid graphs

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Abstract

The resonance graph $R(B)$ of a benzenoid graph B has the perfect matchings of B as vertices, two perfect matchings being adjacent if their symmetric difference forms the edge set of a hexagon of B. A family $\mathcal{P}$ of pair-wise disjoint hexagons of a benzenoid graph B is *resonant* in B if $B-\mathcal{P}$ contains at least one perfect matching, or if $B-\mathcal{P}$ is empty. It is proven that there exists a surjective map f from the set of hypercubes of $R(B)$ onto the resonant sets of B such that a k-dimensional hypercube is mapped into a resonant set of cardinality k.

Key words: Benzenoid graph, perfect matching, resonance graph, hypercube

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1 Introduction

The concept of resonance graph has been introduced in chemistry for the first time by Gründler [5,6] and later reinvented by El-Basil [3,4] as well as by Randić with co-workers [17,18]. Independently, Zhang, Guo, and Chen introduced this concept to mathematics, more precisely to graph theory, under the name Z-transformation graphs [21].

Resonance graphs of benzenoid graphs have been studied in [21], where it is proven that such graphs (provided they contain at least one vertex) are connected, bipartite, and either isomorphic to a path or have girth 4. Restricting to the catacondensed benzenoid graphs even more is known about the structure of their resonance graphs. In particular, every such graph has a Hamilton path [2,11] and belongs to the class of median graphs [14]. The latter result forms the basis for an algorithm that assigns a binary code to every perfect matching of a catacondensed benzenoid graph [12].

Very recently Lam, Shiu, and Zhang [16] widely generalized these results by proving that the resonance graph of a plane weakly-elementary bipartite graph is a median graph. This in particular means that the resonance graph of an arbitrary benzenoid graph is a median graph. We also add that a decomposition theorem for the resonance graphs of catacondensed benzenoid graphs is reported in [11]. It would be interesting to see if such a decomposition can be obtained for all benzenoid graphs.

Median graphs form a well-studied class of graphs, see the survey [10] and references therein. In view of this, it is no surprise that knowing that the resonance graphs of (catacondensed) benzenoid graphs are median resulted in new insights into their structure [11–13,15]. Since, roughly speaking, median graphs are glued together from hypercubes, a detailed consideration of subgraphs of resonance graphs isomorphic to hypercubes seems a natural step to gain more structure information about these resonance graphs.

Hansen and Zheng [9] formulated the (computation of the) Clar number of benzenoid graphs as an integer linear program. Later Abeledo and Atkinson [1] were able to relax the Clar number to a linear program which, in particular, implies that the determination of the Clar number of a benzenoid graph is a polynomial problem. On the other hand, the Clar number of a benzenoid graph is equal to the dimension of a largest hypercube in its resonance graph [15]. Hence there are good reasons to study hypercubes in resonance graphs.

In the next section we formally introduce the concepts and notations of this note. The results are given in Section 3. Let B be a benzenoid graph and $R(B)$ its resonance graph. Then our main result asserts that there exists a surjective map f from the set of hypercubes of $R(B)$ onto the resonant sets of B, such that a k-dimensional hypercube is mapped into a resonant set of cardinality k. This result in particular implies that the Clar number of a benzenoid graph B with at least one perfect matching equals the largest k such that the resonance graph of B contains a k-dimensional hypercube as a subgraph.

2 Preliminaries

Benzenoid graphs 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*. We refer to the book [8] for more information on these graphs, especially for their chemical meaning as representations of benzenoid hydrocarbons.

A *matching* of a graph G is a set of edges no two of which have shared endpoints. A matching is *perfect*, if it covers all the vertices of G. Let B be a benzenoid graph possessing at least one perfect matching. Then the vertex set of the *resonance graph* $R(B)$ of B consists of the perfect matchings of B, two vertices (= perfect matchings) being adjacent whenever their symmetric difference forms the edge set of a hexagon of B.

Let $\mathcal{P} = \{H_1, H_2, \ldots, H_i\}$, $i \geq 1$, be a family of pair-wise disjoint hexagons of a benzenoid graph B. Then by $B - \mathcal{P}$ we mean the graph obtained from B by removing the vertices of the hexagons from $\mathcal{P}$ and all incident edges. The family $\mathcal{P}$ (of pair-wise disjoint hexagons) is said to be *resonant* [7] in B if $B - \mathcal{P}$ contains at least one perfect matching, or if $B - \mathcal{P}$ is empty (without vertices). Alternatively, the family $\mathcal{P}$ (of pair-wise disjoint hexagons) is resonant in B if there exists a perfect matching of B that contains a perfect matching of each hexagon in $\mathcal{P}$ [1]. A perfect matching of a hexagon is sometimes called a *sextet*. The *Clar number*, $CL(B)$, of a benzenoid graph B, is defined as the cardinality of a largest resonant set of B.

We note that in [7] it has been proven that if $\mathcal{P}$ is a maximal resonant set of a catacondensed benzenoid graph B, then $B - \mathcal{P}$ contains a unique perfect matching or is empty. In the case of (general) benzenoid graphs the results is no longer true, see [7] for an example, but remains true if maximal is replaced by maximum, as it is proved in [20].

The *k-cube* Q_k, $k \geq 1$, (or the *k-dimensional hypercube*) is the graph whose vertices are all binary strings of length k, two strings being adjacent whenever they differ in precisely one position. Clearly, Q_k has 2^k vertices and is a k-regular graph. Note also that Q_1 is the complete graph on two vertices K_2, and Q_2 is the 4-cycle C_4.

Finally, for a graph G, let $\mathcal{H}(G)$ be the set of all hypercubes of G, and for a benzenoid graph B let $\mathcal{RS}(B)$ be the set of all resonant sets of B.

3 Hypercubes in resonance graphs

For the proof of our main result, the following lemma will be useful.

Lemma 1 *Let B be a benzenoid graph possessing at least one perfect matching and $R(B)$ be its resonance graph. Let $uvwxu$ be a 4-cycle of $R(B)$. Then the hexagon that corresponds to the edge uv is the same as the hexagon that corresponds to the edge xw.*

PROOF. Let the hexagons that correspond to the edges uv, ux, and xw be denoted by H, H', and H'' respectively. See Fig. 1.

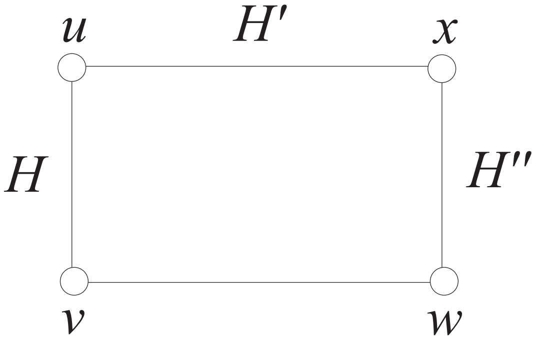

Fig. 1. A 4-cycle of $R(B)$.

Since x and v are distinct, H and H' are distinct. Since u and w are distinct, H' and H" are distinct. Assume that H and H" are distinct. We consider all the possible cases of how the hexagons H, H' and H" are positioned relative to each other and show that we always obtain a contradiction. Hence $H = H$". The details of the proof are tedious and, therefore, are omitted here, but they can be found in [19]. However, we discuss one of these possible cases for an illustration. Case: H and H' are disjoint. Subcase: H" is not disjoint with H but it is disjoint with H'. Since H" and H are distinct, they are adjacent. See Fig. 2, where an oval is drawn inside each hexagon that has a sextet contained in the respective perfect matching.

Since vw is an edge of $R(B)$, we can move along it by rotating a sextet of a hexagon. Since e is matched in v but not matched in w, that hexagon contains e. But none of the hexagons that contain e has a sextet in w, a contradiction. $\square$

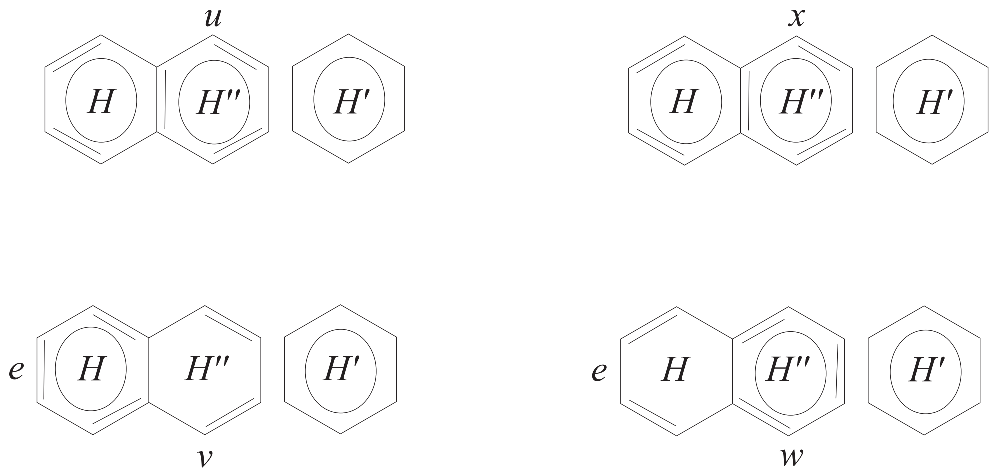

Fig. 2. One possible case of the hexagons H, H' and H" are positioned relative to each other and the perfect matchings u, v, w, and x.

Here is our main result.

Theorem 2 *Let B be a benzenoid graph possessing at least one perfect matching. Then there exists a surjective map*

$$f : \mathcal{H}(R(B)) \to \mathcal{R}S(B)\,,$$

where $|f(Q)| = k$ for a k-dimensional hypercube Q of $R(B)$.

PROOF. First, we construct a bijective map from $\mathcal{R}S(B)$ to a subset of $\mathcal{H}(R(B))$. Let $\mathcal{P} = \{R_1, R_2, \ldots, R_m\}$ be a resonant set of B of cardinality m. Then the hexagons in $\mathcal{P}$ are pair-wise disjoint and $B - \mathcal{P}$ is either empty or has a perfect matching (possibly more than one). If $B - \mathcal{P}$ is nonempty, let M be a perfect matching of $B - \mathcal{P}$ (If $B - \mathcal{P}$ has more than one perfect matching, select one arbitrarily), otherwise, let M be the empty set. Then on every hexagon of $\mathcal{P}$, we have exactly two possibilities how to extend M to the hexagon. Let us call these "possibility 0" and "possibility 1". In this way, we obtain 2^m perfect matchings of B and they can be coded with binary strings $b_1, b_2, \ldots, b_m$ of length m, where $b_i = 0$ if on R_i possibility 0 is selected, and $b_i = 1$ otherwise. If two such binary strings (two such perfect matchings) differ in exactly one position, then their symmetric difference is a hexagon and consequently they are adjacent in $R(B)$. It follows that these 2^m perfect matchings are the vertices of an m-dimensional hypercube that is a subgraph of $R(B)$. Let us denote this hypercube with $Q^{\mathcal{P}}$.

Let $\mathcal{H}_0 = \{Q^{\mathcal{P}} \mid \mathcal{P}$ is a resonant set of $\mathcal{P}\}$ and define a map $g : \mathcal{R}S(B) \to \mathcal{H}_0$ by $g(\mathcal{P}) = Q^{\mathcal{P}}$. We show that this map is bijective. It is clear that this map is surjective. It remains to show that it is injective. Let $\mathcal{P}$ and $\mathcal{P}'$ be distinct resonant sets of B. If $\mathcal{P}$ and $\mathcal{P}'$ have distinct cardinalities then $Q^{\mathcal{P}}$ and $Q^{\mathcal{P}'}$ are distinct. If $\mathcal{P}$ and $\mathcal{P}'$ have the same cardinality, m say, let $\mathcal{P} =$

$\{R_1, R_2, \ldots, R_m\}$ and $\mathcal{P}' = \{R_1', R_2', \ldots, R_m'\}$, where the notation is selected such that $R_1 \notin \mathcal{P}'$. Let $\mathcal{M}$ be the set of the 2^m perfect matchings of B that correspond to the vertices of $Q^{\mathcal{P}}$ and let $\mathcal{M}'$ be the set of the 2^m perfect matchings of B that correspond to the vertices of $Q^{\mathcal{P}'}$. Let u, v, w be three consecutive vertices of R_1. If uv is in no perfect matching of $\mathcal{M}'$, then clearly $Q^{\mathcal{P}}$ and $Q^{\mathcal{P}'}$ are distinct. If uv is in some perfect matching of $\mathcal{M}'$, we consider two subcases. Assume that for some j, uv is in R_j'. Note that $R_1 \neq R_j'$. This implies that R_1 and R_j' are adjacent with uv being their common edge. Hence, vw is in no perfect matching of $\mathcal{M}'$ and so $Q^{\mathcal{P}}$ and $Q^{\mathcal{P}'}$ are distinct. Assume that uv does not belong to any hexagon in $\mathcal{P}'$. Then uv is not incident to a vertex of a hexagon in $\mathcal{P}'$ and therefore it belongs to $B - \mathcal{P}'$. Hence, uv belongs to all the perfect matchings in $\mathcal{M}'$ and vw belongs to none of them which implies that $Q^{\mathcal{P}}$ and $Q^{\mathcal{P}'}$ are distinct. This completes the proof that g is bijective.

The map $g^{-1} : \mathcal{H}_0 \to \mathcal{RS}(B)$ is also bijective. It is clear that g^{-1} maps a k-dimensional hypercube to a resonant set of cardinality k. If $\mathcal{H}_0 = \mathcal{H}(R(B))$, the proof of Theorem 2 is complete. If $\mathcal{H}_0$ is a proper subset of $\mathcal{H}(R(B))$, we can define an extension, f say, of g^{-1} to $\mathcal{H}(R(B))$ as will be shown. This extension f is clearly surjective.

Let Q be a subgraph of $R(B)$ isomorphic to Q_k, $k \geq 1$ and $Q \notin \mathcal{H}_0$. The vertices of Q can be identified (put in 1-1 correspondence) with the 0-1 strings $\langle u_1 u_2 \ldots u_k \rangle$, so that vertices $\langle u_1 u_2 \ldots u_k \rangle$ and $\langle v_1 v_2 \ldots v_k \rangle$ of Q are adjacent in Q (and hence in $R(B)$) if and only if they differ in precisely one position. Due to symmetries of hypercubes, there are several ways to make this identification, but we select one and fix it in the rest.

Consider the following vertices of Q: $u = \langle 000 \ldots 0 \rangle$, $v^1 = \langle 100 \ldots 0 \rangle$, $v^2 = \langle 010 \ldots 0 \rangle$, $\ldots$, $v^k = \langle 000 \ldots 1 \rangle$. Then uv^i , $i = 1, 2, \ldots, k$, is an edge of Q . By definition of $R(B)$, the symmetric difference of the perfect matchings corresponding to u and v^i is a hexagon of B, we denote it by H_i. Set

$$f(Q) = \{H_1, H_2, \ldots, H_k\} \, .$$

To complete the proof we must show that $f(Q) = \{H_1, H_2, \ldots, H_k\}$ is a resonant set of cardinality k, that is, (i) the hexagons in $\{H_1, H_2, \ldots, H_k\}$ are pairwise disjoint and their number is k and (ii) there exists a perfect matching of B that contains a sextet of each of the hexagons in $\{H_1, H_2, \ldots, H_k\}$.

Claim A. *The hexagons* H_i , $1 \leq i \leq k$, *are pairwise disjoint and their number is* k.

If $k = 1$ there is nothing to prove. So let $k \geq 2$ and select arbitrary indices i and j, where $1 \leq i, j \leq k$, $i \neq j$. Let M, M_i, and M_j be the perfect matchings corresponding to the vertices u, v^i, and v^j, respectively.

Assume $H_i = H_j$. Then, as v^i and v^j are both adjacent to u, we infer that $M_i = M_j$. But since v^i and v^j are distinct, M_i and M_j are distinct, a contradiction. Suppose next that H_i and H_j share an edge. Then we first observe that the common edge of H_i and H_j belongs to M, cf. Fig. 3. Then M_i and M_j are as shown in the same figure.

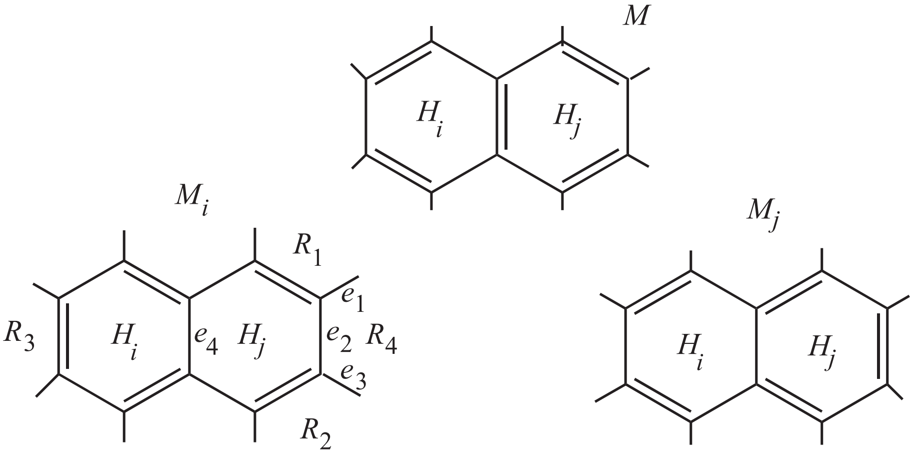

Fig. 3. Situation if H_i and H_j would share an edge.

Let w be a 0-1 string of length k having exactly two 1's and these are in the i-th and j-th positions. Note that w is adjacent to both of v^i and v^j and that it is distinct from u. Let M_w be the perfect matching corresponding to w. Since w and v^i are adjacent, we can obtain M_w from M_i by rotating a sextet. That sextet cannot be that of H_i otherwise $M_w = M$, contradicting that w and u are distinct. Also, H_j does not have a sextet contained in M_i. Hence, that sextet is in a hexagon that is either adjacent to H_i or H_j, possibilities are R_1, R_2, or R_3 (see Fig. 3), or disjoint from them. In any case, e_2, e_4, and at least one of e_1 and e_3 (see Fig. 3) do not belong to M_w. Consequently, neither H_j nor R_4 has a sextet contained in M_w. Since w and v_j are adjacent, we can obtain M_w from M_j by rotating a sextet. Since e_2 does not belong to M_w but belongs to M_j, that sextet is either in H_j or R_4, a contradiction. This completes the proof of Claim A.

We next demonstrate that there exists a perfect matching of B that contains a sextet of each hexagon in $\{H_1, H_2, \dots, H_k\}$. We first show:

Claim B. *Let xy be an edge of Q. Let the binary representations of x and y differ at the j-th place. Then the symmetric difference of the corresponding perfect matchings in $R(B)$ is the hexagon H_j.*

Without loss of generality, as will be explained, we may assume that $j = 1$. We can rotate the coordinates of each vertex of the hypercube Q so that the

j-th coordinate becomes the first. This is an alternative identification of the vertices of Q with the 0-1 strings of length k so that two vertices are adjacent in Q if and only if they differ in exactly one coordinate. Note that as a result of this renaming of the vertices, the H_i's get renamed as well, in particular, H_j becomes H_1.

Let $x = \langle 0 \ldots \rangle$ and $y = \langle 1 \ldots \rangle$. Let s be the number of 1's in x. If $s = 0$, then $x = u$ and $y = v^1$ and so the claim follows from the definition of H_1. If $s > 0$, consider the path $x^0, x^1, x^2, \ldots, x^s$ in Q, where x^i has exactly i 1's and these are in the same positions as the first i 1's in x and also, consider the path $y^0, y^1, y^2, \ldots, y^s$ in Q, where y^i differ from x^i in precisely the first position. Note that x^i and y^i are adjacent in Q and also, note that $x^0 = u$, $y^0 = v^1$, $x^s = x$, and $y^s = y$. We show that the symmetric difference of x^i and y^i is the hexagon H_1, where $i = 0, 1, \ldots, s$. We use induction to prove this statement. Initial Step: Let $i = 0$. The symmetric difference of $x^0 = u$ and $y^0 = v^1$ is the hexagon H_1 by definition of H_1. Inductive Step: Assume that the statement is true for $i = r$, that is, the symmetric difference of x^r and y^r is the hexagon H_1, where $r = 0, 1, \ldots, s-1$. Consider the 4-cycle $x^r y^r y^{r+1} x^{r+1} x^r$. By the inductive assumption and Lemma 1, the symmetric difference of x^{r+1} and y^{r+1} is the hexagon H_1, i.e., the statement is true for $i = r + 1$. This completes the inductive proof. In particular, the symmetric difference of $x^s = x$ and $y^s = y$ is the hexagon H_1 and this completes the proof of Claim B.

Consider now the path $u^0 = \langle 000 \ldots 0 \rangle$, $u^1 = \langle 100 \ldots 0 \rangle$, $u^2 = \langle 110 \ldots 0 \rangle$, $\ldots$, $u^k = \langle 111 \ldots 1 \rangle$ in Q . Then, by Claim B, the edge $u^i u^{i+1}$, $0 \leq i \leq k-1$, corresponds to the hexagon H_{i+1} . So going from u^0 to u^k the perfect matchings only change in the pair-wise disjoint hexagons $H_1, H_2, \ldots, H_k$. It follows that the perfect matching u^k contains a sextet of each of the hexagons in $\{H_1, H_2, \ldots, H_k\}$, implying that $f(Q)$ is a resonant set of B and the proof is complete. $\square$

Recall that the Clar number $CL(B)$ is the size of a largest resonant set of B . Hence Theorem 2 implies the following result from [15].

Corollary 3 *Let B be a benzenoid graph possessing at least one perfect matching and $R(B)$ its resonance graph. Then $CL(B)$ equals the largest k such that $R(B)$ contains a k-dimensional hypercube as a subgraph.*

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