Resonance Graphs and Daisy Cubes – Part I

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Perfect matchings

Definition

A **perfect matching** M of a graph G is a subset of $E(G)$ such that every vertex of G is incident with exactly one edge from M.

In chemistry, perfect matchings are known as **Kekulé structures**.

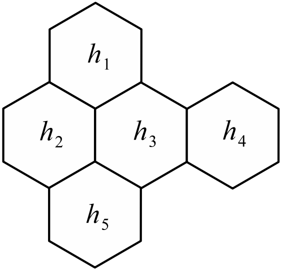
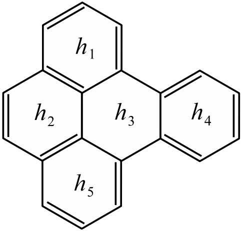
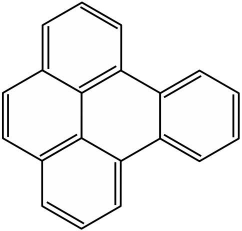


Figure: Benzenoid graph G.

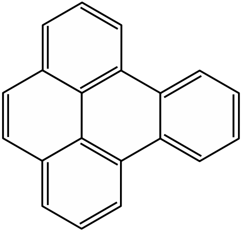
Perfect matchings of G



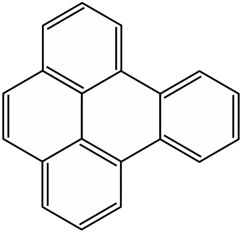
M_1



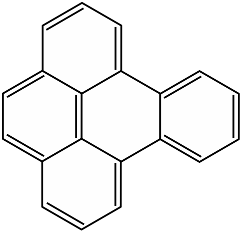
M_2



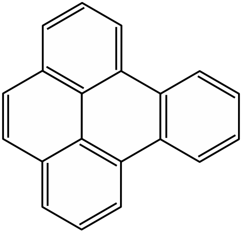
M_3



M_4

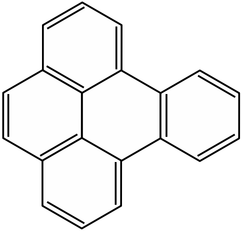


M_5

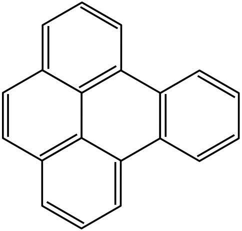


M_6

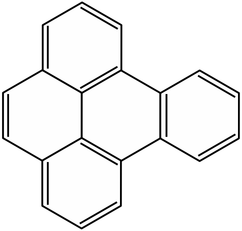
Perfect matchings of G



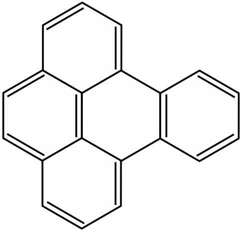
M_7



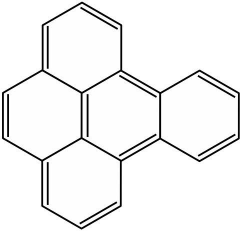
M_8



M_9



M_{10}



M_{11}

Resonance graphs

Resonance graphs were first introduced independently by chemists Gründler (1982) and El-Basil (1993) and also by mathematicians F. Zhang, X. Guo, and R. Chen (1988). While the research on resonance graphs initially revolved around benzenoid graphs, the concept was later extended to plane bipartite graphs.

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Definition

The **resonance graph** (also called Z-**transformation graph**) $R(G)$ of a plane bipartite graph G is a graph whose vertices are the perfect matchings of G, and two perfect matchings M_1, M_2 are adjacent whenever their symmetric difference $M_1 \oplus M_2$ forms exactly one cycle that is the periphery of some finite face s of G. In this case, we say that the edge M_1M_2 of $R(G)$ has the **face-label** s.

Symmetric difference: $M_1 \oplus M_2 = (M_1 \cup M_2) \setminus (M_1 \cap M_2)$

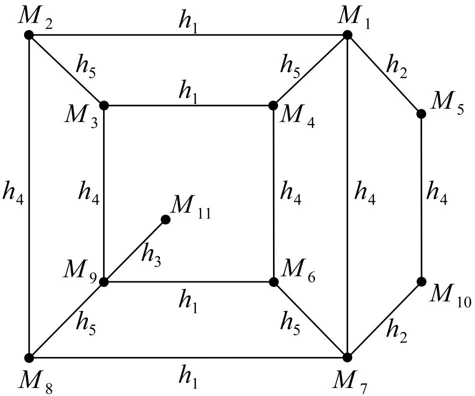


Figure: The resonance graph $R(G)$.

Perfect matchings M_1 and M_2 are adjacent in $R(G)$ (with face-label h_1) because M_2 can be obtained from M_1 by rotating the three edges of hexagon h_1 that belong to M_1.

Hypercubes

Hypercubes can be defined by using binary codes. Let $\mathcal{B} = \{0, 1\}$ and $\mathcal{B}^n$ be the set of all **binary codes** of length $n \geq 1$. Then a **hypercube** Q_n of dimension n has the vertex set $\mathcal{B}^n$, and two vertices of Q_n are adjacent if the corresponding binary codes differ in precisely one position.
Additionally, a hypercube Q_0 of dimension 0 is the one-vertex graph K_1.

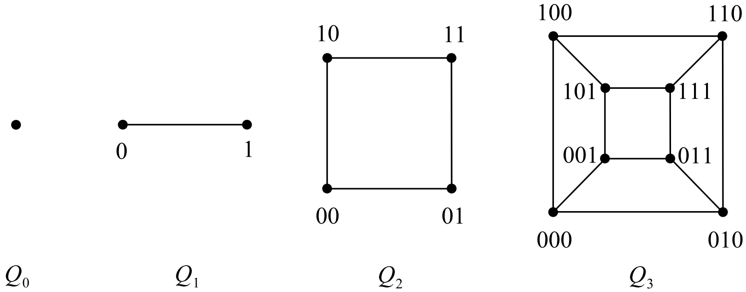


Figure: Hypercubes.

Partial cubes

- A subgraph H of a graph G is an **isometric subgraph** if for all $u, v \in V(H)$, $d_H(u, v) = d_G(u, v)$.
- Isometric subgraphs of hypercubes are called **partial cubes**.
- If a graph is isomorphic to an isometric subgraph of Q_n, we say that it can be **isometrically embedded** in Q_n.
- The **isometric dimension** of a partial cube G, denoted by $\mathrm{idim}(G)$, is the least integer n for which G embeds isometrically into a hypercube Q_n.

Daisy cubes

Daisy cubes are a subclass of partial cubes. They were introduced by Klavžar and Mollard in 2019.

- Let $\mathcal{B} = \{0, 1\}$ and $\mathcal{B}^n$ be the set of all binary codes (or binary strings) of length $n \geq 1$.
- A partial order $\leq$ can be defined on $\mathcal{B}^n$ with $u_1 u_2 \ldots u_n \leq v_1 v_2 \ldots v_n$ if $u_i \leq v_i$ for all $1 \leq i \leq n$.
- Let $X \subseteq \mathcal{B}^n$. A **daisy cube (generated by X)** is an induced subgraph of Q_n defined as $Q_n(X) = \langle \{u \in \mathcal{B}^n \mid u \leq x \text{ for some } x \in X\} \rangle$.

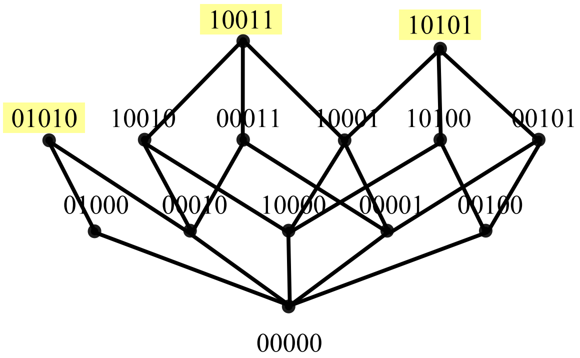


Figure: Daisy cube generated by $X = \{01010, 10011, 10101\}$.

The authors of the seminal paper observed the following:

- daisy cubes are partial cubes;
- $\mathrm{idim}(Q_n(X)) = \deg_{Q_n(X)}(0^n)$.

Outerplane bipartite graphs

An **outerplane graph** is a plane graph whose vertices are all exterior vertices (so all the vertices belong to the infinite face).

Definition

A **catacondensed benzenoid graph** is a 2-connected outerplane bipartite graph whose each vertex has degree at most 3 and in which any inner face is bounded by a 6-cycle.

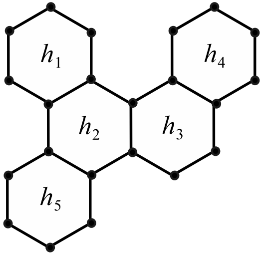


Figure: Catacondensed benzenoid graph.

Angularly and linearly connected triples of faces

- Let $d_{L(G)}(e, f)$ be the distance between two edges $e, f \in E(G)$ in the line graph $L(G)$ of G.
- The adjacent triple of finite faces (s, s', s'') is **angularly connected** if $d_{L(G)}(e, f)$ is even, and **linearly connected** otherwise.

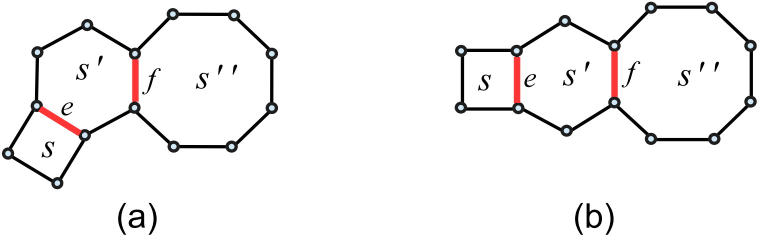


Figure: (a) Angularly connected adjacent triple of finite faces and (b) linearly connected adjacent triple of finite faces.

Previous results: catacondensed benzenoid graphs

Theorem (Žigert Pleteršek; 2018)

Let G be a catacondensed benzenoid graph without any linearly connected hexagons. Then the resonance graph $R(G)$ is a daisy cube.

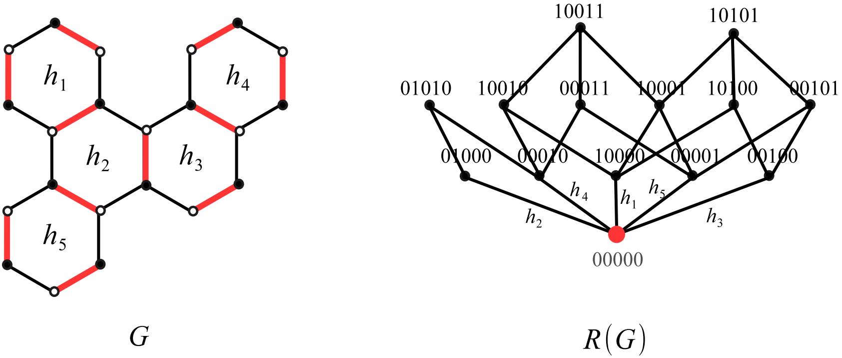


Figure: The resonance graph of a kinky benzenoid graph. Edges of G colored with red form a perfect matching corresponding to the vertex of $R(G)$ with the binary code 00000.

Previous results: outerplane bipartite graphs

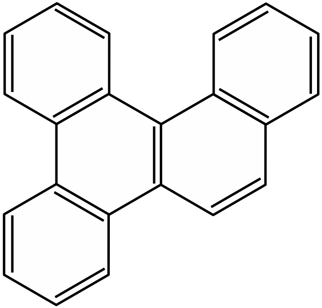
Theorem (S. Brezovnik, N. Tratnik, P. Žigert Pleteršek; 2023)

Let G be a 2-connected outerplane bipartite graph. Then the resonance graph $R(G)$ is a daisy cube if and only if G does not have any adjacent triple of finite faces that is linearly connected.

Plane elementary bipartite graphs

We firstly characterize plane elementary bipartite graphs whose resonance graphs are daisy cubes.

- An edge of a graph is called **allowed** if it is contained in some perfect matching of the graph, and **forbidden** otherwise.
- A bipartite graph is **elementary** if and only if it is connected and each edge is allowed (L. Lovasz, M. D. Plummer; 1986).



M

Figure: Plane elementary bipartite graph.

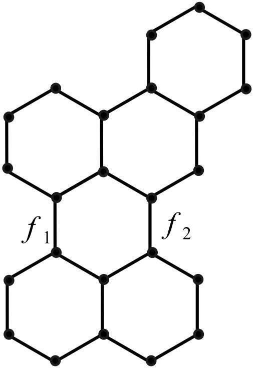


Figure: Graph G with forbidden edges f_1 and f_2.

Alternating cycles and resonant faces

- Let G be a graph, C a cycle of G, and M a perfect matching of G. Then C is M-**alternating** if edges of C are alternately in M and out of M.
- Let G be a plane bipartite graph. If the periphery of a face s of G is an M-alternating cycle, then s is called an M-**resonant face** of G.

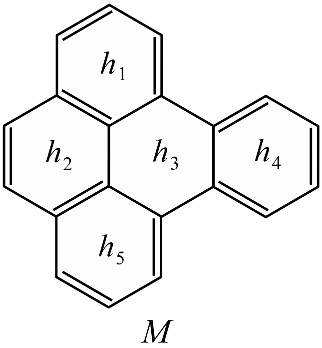


Figure: Hexagons h_1, h_2, h_4, h_5 are M-resonant faces.

The Fries number

The Fries number was initially introduced for benzenoid hydrocarbons (K. Fries; 1927), and naturally extended to plane bipartite graphs (H. Abeledo, G. W. Atkinson; 2007).

Definition

Let G be a plane bipartite graph and S be the set of finite faces of G. The **Fries number** of G is the maximum cardinality of a subset $S' \subseteq S$ satisfying the property that there exists a perfect matching M of G such that each finite face in S' is M-resonant.

Example: the Fries number of the graph on the previous slide equals 4.

If the Fries number of G is the number of finite faces of G, then there exists a perfect matching M of G such that each finite face of G is M-resonant.

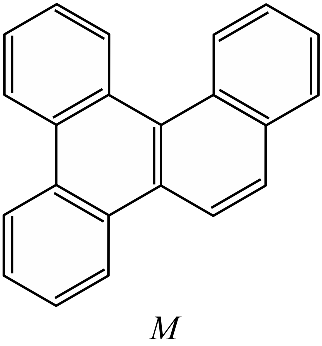


Figure: Catacondensed benzenoid graph with Fries number 5.

Peripherally 2-colorable graphs

We now introduce the following new terminology to describe the structure of plane elementary bipartite graphs whose resonance graphs are daisy cubes.

Definition (Brezovnik, Che, Tratnik, Žigert Pleteršek; 2024)

Let G be a plane elementary bipartite graph with more than two vertices. Then G is called **peripherally 2-colorable** if:

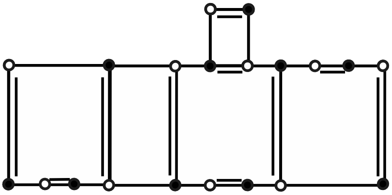
(*i*) every vertex of G has degree 2 or 3,

(*ii*) vertices with degree 3 (if exist) are all exterior vertices of G, and

(*iii*) G can be 2-colored black and white so that:

- two vertices with the same color are nonadjacent, and
- vertices with degree 3 (if exist) are alternately black and white along the clockwise orientation of the periphery of G.

G_1



G_2

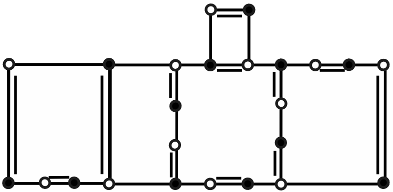


Figure: Peripherally 2-colorable graphs. G_1 is also outerplane.

Lemma (Brezovnik, Che, Tratnik, Žigert Pleteršek; 2024)

Let G be a 2-connected outerplane bipartite graph. The G is peripherally 2-colorable if and only if G does not have any adjacent triple of finite faces that is linearly connected.

Characterization for plane elementary bipartite graphs

Theorem (Brezovnik, Che, Tratnik, Žigert Pleteršek; 2024)

Let G be a plane elementary bipartite graph other than K_2 and n a positive integer. Then the following statements are equivalent.
(i) The resonance graph $R(G)$ is a daisy cube with $\mathrm{idim}(R(G)) = n$.
(ii) The Fries number of G is n, where n is the number of finite faces of G.
(iii) G is peripherally 2-colorable and with n finite faces.

Plane weakly elementary bipartite graphs

Our next goal is to provide an answer for when the resonance graph of a plane bipartite graph is a daisy cube.

- For a plane bipartite graph G with a perfect matching, the **elementary components** of G are the components of the subgraph obtained from G by removing all forbidden edges of G.
- A plane bipartite graph with a perfect matching (not necessarily connected) is called **weakly elementary** if deleting all forbidden edges does not produce any new finite face.

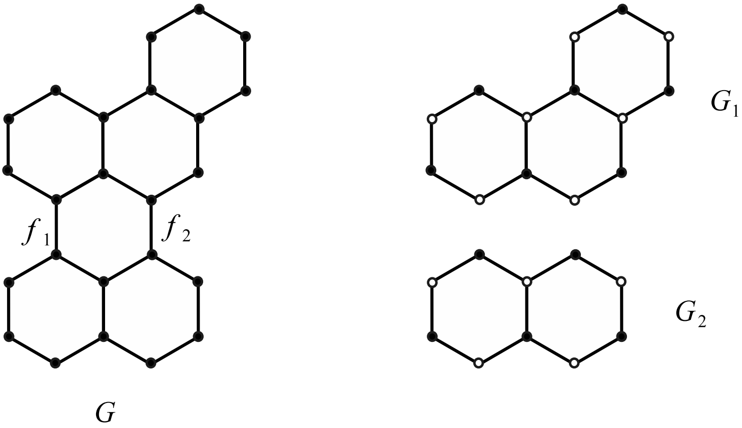


Figure: Plane weakly elementary bipartite graph G with two elementary components.

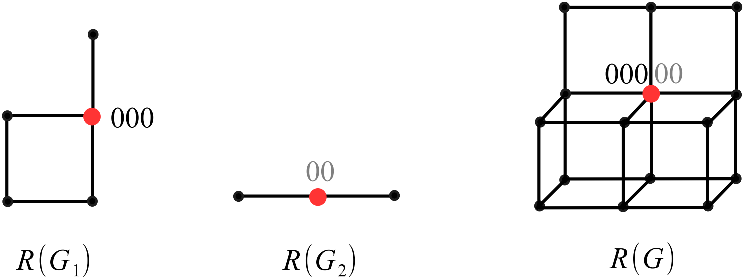


Figure: Resonance graphs $R(G_1)$, $R(G_2)$, and $R(G) = R(G_1) \Box R(G_2)$.

Resonance graph of a plane weakly elementary bipartite graph

Observation

Let G be a plane weakly elementary bipartite graph with elementary components $G_1, G_2, \ldots, G_t$. Then the resonance graph $R(G)$ is a Cartesian product of resonance graphs $R(G_i)$ for all $1 \leq i \leq t$, that is,

$$R(G) = \square_{i=1}^{t} R(G_i).$$

Cartesian product of daisy cubes

Theorem (Brezovnik, Che, Tratnik, Žigert Pleteršek; 2024)

Let $R = R_1 \Box R_2 \Box \cdots \Box R_t$ *be the Cartesian product of nontrivial graphs* $R_1, R_2, \ldots, R_t$*. Then* R *is a daisy cube with* $\mathrm{idim}(R) = n$ *if and only if each* R_i *is a daisy cube with* $\mathrm{idim}(R_i) = n_i$ *for all* $1 \leq i \leq t$*, and* $n = n_1 + n_2 + \cdots + n_t$*.*

Characterization for plane bipartite graphs

Theorem (Brezovnik, Che, Tratnik, Žigert Pleteršek; 2024)

Let G be a plane bipartite graph with a perfect matching and n a positive integer. Then the following statements are equivalent:
(i) $R(G)$ is a daisy cube with $\mathrm{idim}(R(G)) = n$.
(ii) G is plane weakly elementary bipartite, and for each of its elementary components G_i other than K_2, the Fries number of G_i is n_i, where n_i is the number of finite faces of G_i for all $1 \leq i \leq t$, and $n = n_1 + n_2 + \cdots + n_t$.
(iii) G is plane weakly elementary bipartite, and for each of its elementary components G_i other than K_2, G_i is peripherally 2-colorable and with n_i finite faces for all $1 \leq i \leq t$, where $n = n_1 + n_2 + \cdots + n_t$.

THANK YOU!

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