Resonance Graphs and Daisy Cubes – Part II

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joint work with

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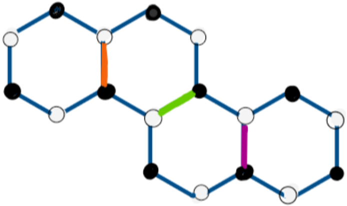
So far... - Part I

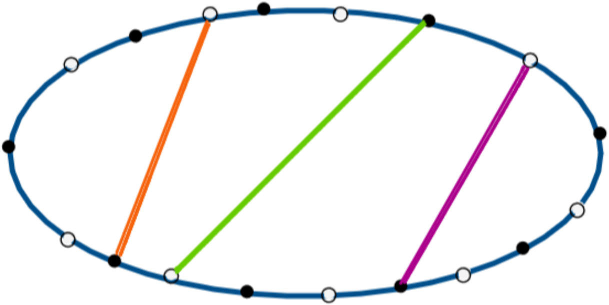
Main result

Let G be a plane elementary bipartite graph other than K_2. Then the following statements are equivalent.
(i) The resonance graph $R(G)$ is a daisy cube.
(ii) The Fries number of G equals the number of finite faces of G.
(iii) G is peripherally 2-colorable.

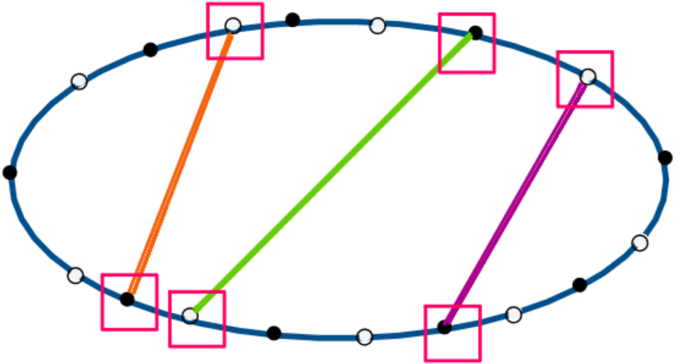
For example- fibonaccene



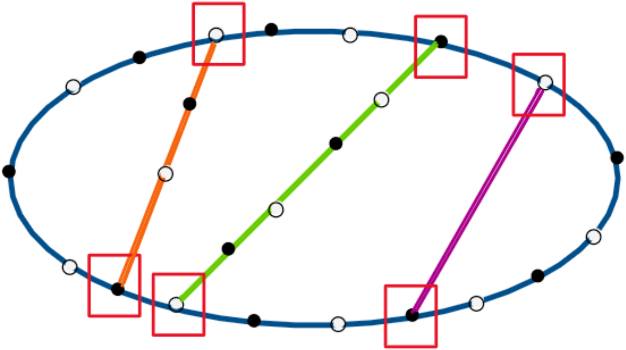
Fibonacene as a bipartite outerplane graph



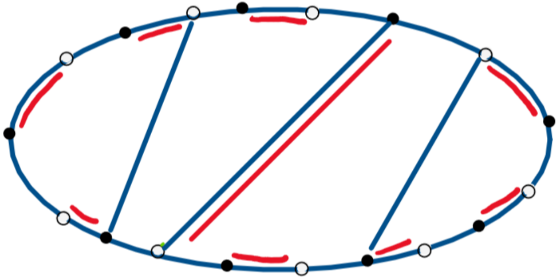
Fibonacene as peripherally 2-colorable (outerplane) graph



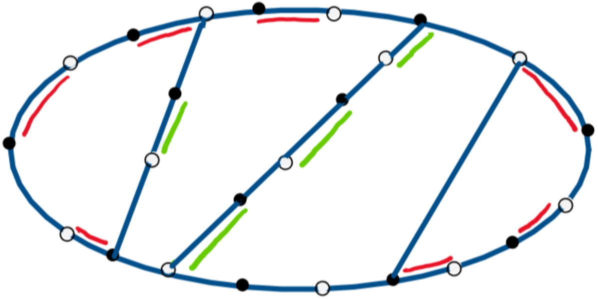
Plane but NOT an outerplane peripherally 2-colorable graph



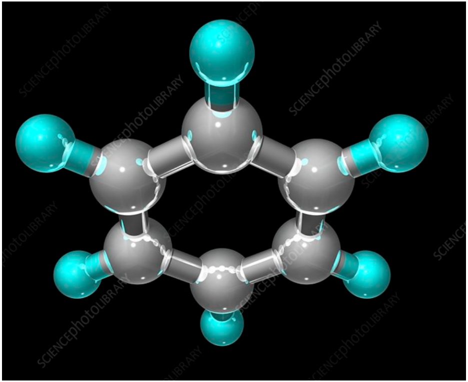
A perfect matching of a peripherally 2-colorable (outerplane) graph...



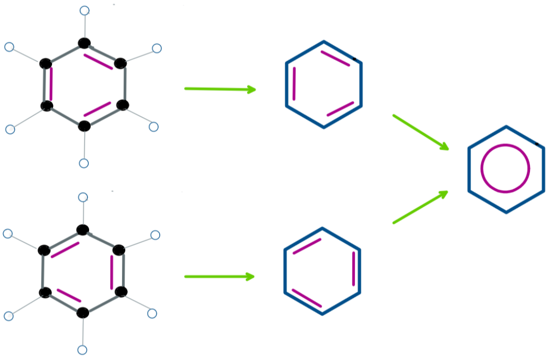
...can be extended in a unique way



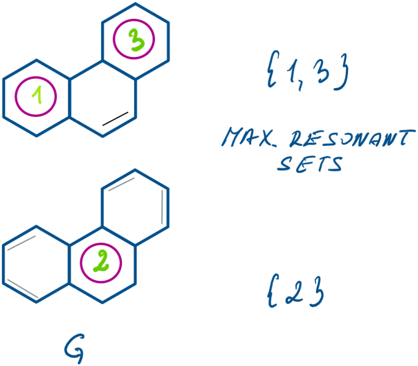
Molecule of benzene



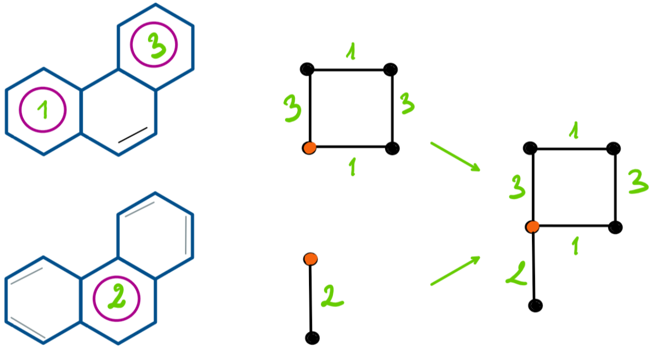
Molecular graph of benzene



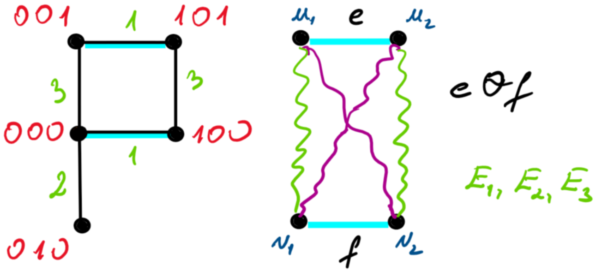
Maximal resonant sets



Resonance graph

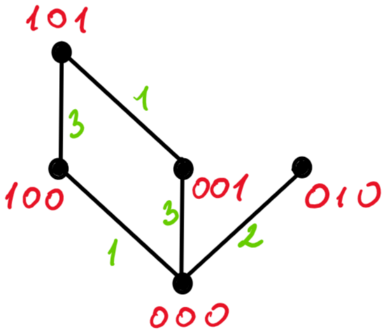


Djoković-Winkler relation Θ

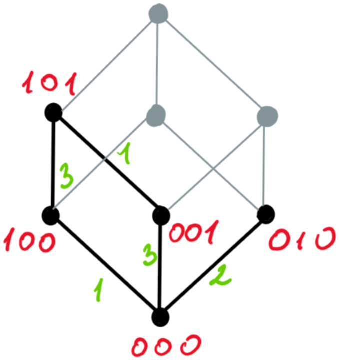


$$e\Theta f \sim d(u_1, v_1) + d(u_2, v_2) \neq d(u_1, v_2) + d(u_2, v_1)$$

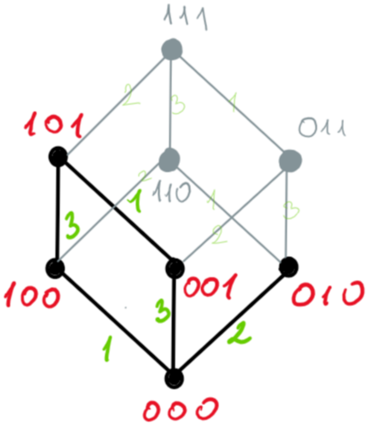
Resonance graphs



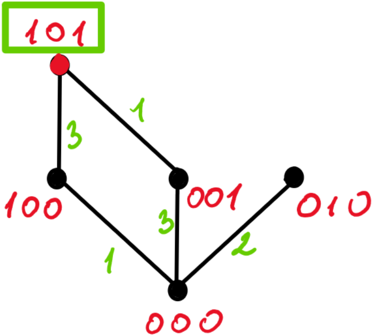
Partial cubes



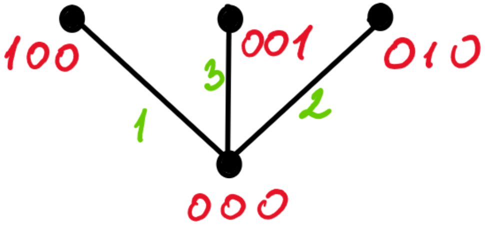
Fibonacci cubes



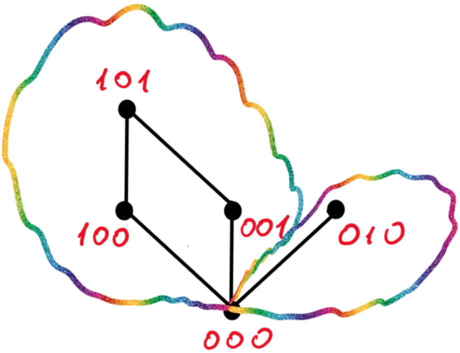
From Fibonacci to Lucas cubes



Lucas cubes



Resonance graphs as a daisy cubes



Lemma

Assume that G is a plane weakly elementary bipartite graph other than K_2. Let $\mathcal{H}(R(G))$ be the set of nontrivial hypercubes of $R(G)$ and $\mathcal{RS}(G)$ be the set of nonempty resonant sets of G. Define $f : \mathcal{H}(R(G)) \to \mathcal{RS}(G)$ such that if Q is a k-dimensional hypercube of $R(G)$ for a positive integer k, then $f(Q) = S_Q$, where S_Q is a cardinality k resonant set of G with the property that each finite face in S_Q is a face-label of a Θ-class of Q. Then f is well-defined and surjective. Moreover, f is a bijection only when $\mathcal{RS}(G)$ is a set of canonical resonant sets of G.

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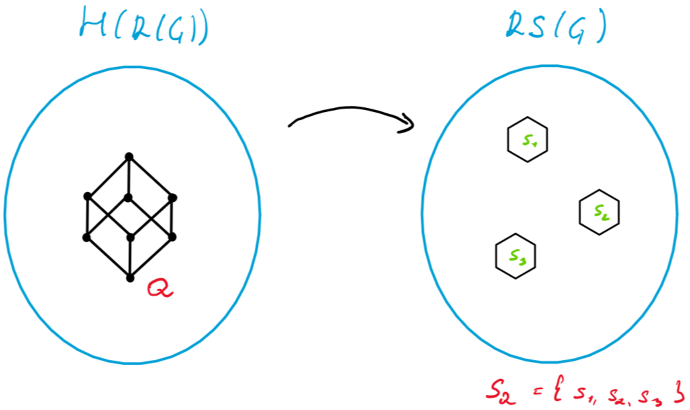
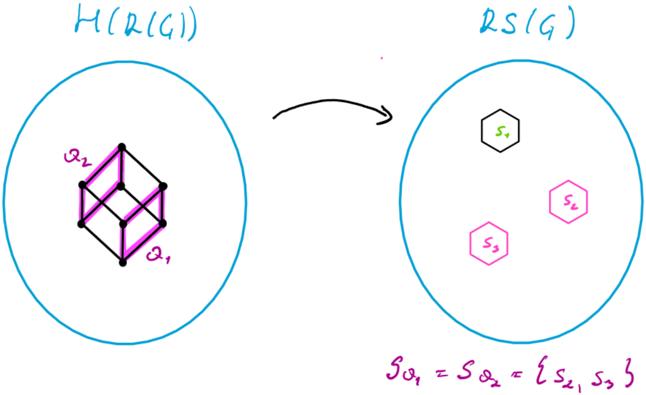
Visualization of lemma



Visualization of lemma



Canonical resonant set

A resonant set S of G is *canonical* if $G - S$ is empty or has a unique perfect matching.

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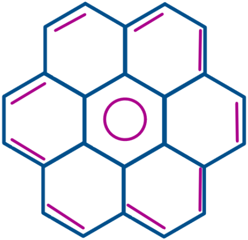

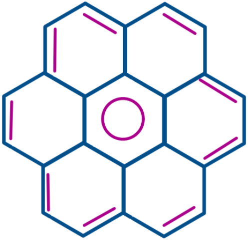

Forcing infinite face

Lemma

Let G be a plane elementary bipartite graph other than K_2. Then the infinite face of G is forcing if and only if any two vertex disjoint cycles C_1 and C_2 such that $C_1 \cup C_2$ is a nice subgraph of G have disjoint interiors.

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Corollary

Let G be an elementary benzenoid system. Then the infinite face of G is forcing if and only if G has no coronenes as nice subgraphs.

Max. hypercubes ONE-TO-ONE max. resonant sets

Lemma

Let G be a plane elementary bipartite graph other than K_2. Assume that the infinite face of G is forcing. Then:

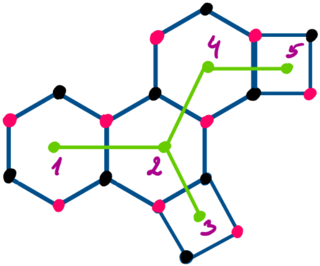
(i) *S is a maximal resonant set of G if and only if S is a canonical resonant set of G.*

(ii) *There is a bijection between the set of maximal hypercubes of $R(G)$ and the set of maximal resonant sets of G which maps a k-dimensional maximal hypercube to a cardinality k maximal resonant set, where k is a positive integer.*

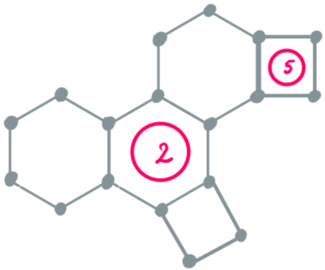
Independent sets

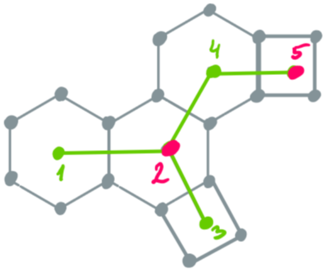
- Independent set ... a set of pairwise nonadjacent vertices of G
- $\mathcal{IS}(G)$... a set of all independendent sets of G

Peripherally 2-colorable graph G and the inner dual of G^*



Resonants sets of G and independent sets of G^*





Connection between (max.) resonant sets and (max.) independent sets

Lemma

Assume that G is a peripherally 2-colorable graph with inner dual G^*. Let $\mathcal{RS}(G)$ be the set of nonempty resonant sets of G and $\mathcal{IS}(G^*)$ be the set of nonempty independent sets of G^*. Define $g : \mathcal{RS}(G) \to \mathcal{IS}(G^*)$ such that $g(S) = S^*$, where S is a resonant set of G and S^* is the corresponding independent set of G^*. Then g is well-defined. Moreover, g induces a bijection between the set of maximal resonant sets of G and the set of maximal independent sets of G^*, which maps a cardinality k maximal resonant set of G to a cardinality k maximal independent set of G^*, where k is a positive integer.

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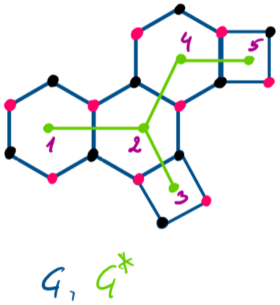
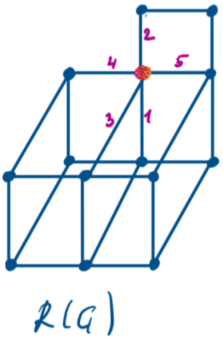
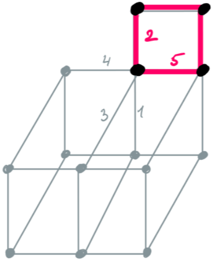
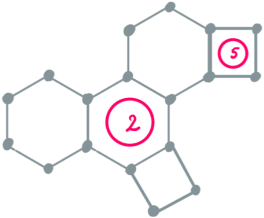
G with inner dual G^* and the resonance graph $R(G)$

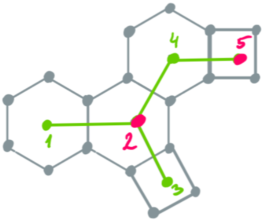




Max. hypercubes of $R(G) \to$ max. resonant sets of $G \to$ max. independent sets of G^*







Corollary

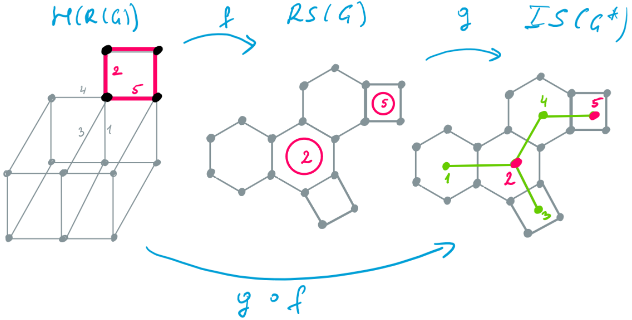
short version

$$f : \mathcal{H}(R(G)) \to \mathcal{RS}(G), \quad g : \mathcal{RS}(G) \to \mathcal{IS}(G^*)$$

Then

$$g \circ f : \mathcal{H}(R(G)) \to \mathcal{IS}(G^*) \text{ is a bijection (all maximal)}$$

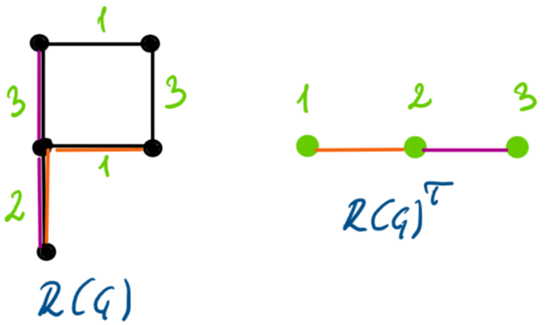
Corollary



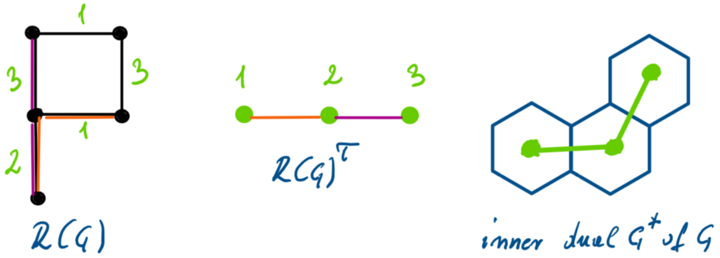
τ-graph

The *τ-graph* H^τ of H is a graph whose vertex set is the set of Θ-classes of H, and two distinct Θ-classes E and F are adjacent in H^τ if H has two edges $e \in E$ and $f \in F$ such that e and f form a convex path on three vertices, that is, $e = uv$, $f = vw$, and v is the only common neighbor of u and w

Resonance graph $R(G)$ and τ-graph $R(G)^\tau$



τ-graph of $R(G)$ and inner dual G^* of G



Finally - when the resonance graph is a daisy cube?

Theorem

Let G be a plane elementary bipartite graph other than K_2. Then its resonance graph $R(G)$ is a daisy cube if and only if there is a bijection ϕ between the set of maximal hypercubes of $R(G)$ and the set of maximal independent sets of the inner dual G^* of G, where $R(G)^\tau$ is a tree and is isomorphic to the inner dual G^* of G, and ϕ maps a k-dimensional maximal hypercube Q of $R(G)$ to a cardinality k maximal independent set S_Q^* of G^* with the property that each vertex of S_Q^* corresponds to a face-label of a Θ-class of Q, where k is a positive integer.

When the daisy cube is a resonance graph?

Lemma

Let A and B be daisy cubes. If their τ-graphs A^τ and B^τ are isomorphic, then A and B are isomorphic.

Main result

Theorem

A daisy cube H with at least one edge is a resonance graph of a plane bipartite graph if and only if its τ-graph H^{τ} is a forest. Moreover, H is a resonance graph of a plane elementary bipartite graphif and only if its τ-graph H^{τ} is a tree.

Two corollaries

Fibonacci cubes

The number of maximal hypercubes of a Fibonacci cube Γ_n equals the Padovan number a_{n+1} for any $n \geq 1$.

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$\Gamma_n^\tau = P_n$ and $|\mathrm{MIS}(P_n)| = a_{n+1}$

$a_n = a_{n-2} + a_{n-3},\ a_0 = a_1 = a_2 = 1$

Two corollaries

Lucas cubes

Let Λ_n be a Lucas cube where $n \geq 3$. Then its τ-graph Λ_n^τ is a cycle C_n.

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Let Λ_n be a Lucas cube where $n \geq 3$. Then its τ-graph Λ_n^τ is a cycle C_n.

Corrolary: Lucas cubes cannot be the resonance graphs of a plane bipartite graph.

Input: $RFD(G_1, G_2, \ldots, G_n)$ of a P2-C G associated with a sequence $s_1, \ldots, s_n$ of finite faces.

Output: Binary codes for all perfect matchings of G.

$B := \{00, 01, 10\}$

for $r = 2, \ldots, n-1$ **do**

    $B' := \emptyset$

    set $j \in \{1, \ldots, r\}$ such that s_j is adjacent to s_{r+1}

    $i = \min\{l \mid s_l \text{ is adjacent to } s_j\}$

    for *each* $x \in B$ **do**

        $B' := B' \cup \{x0\}$

        if $x_j = 0$ **then**

            $B' := B' \cup \{x1\}$

        end

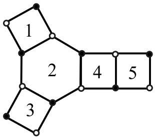
    end

    $B := B'$

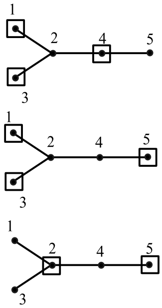
end

return B

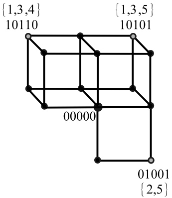
Binary code labelling



G



G^*

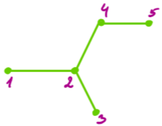


$R(G)$

Input: Inner dual G^* with vertices $s_1, \ldots, s_n$ of a P2-C G.
Output: Binary codes for all perfect matchings of G.

find the maximal independent sets $I_1, \ldots, I_k$ of G^*
$B := \emptyset$
for $r = 1, \ldots, k$ **do**
  for *every subset* X *of* I_r **do**
    $B := B \cup \{x_1 x_2 \ldots x_n\}$, where for every $i \in \{1, \ldots, n\}$, $x_i = 1$ if $s_i \in X$ and $x_i = 0$ if $s_i \notin X$
  end
end
return B

Example

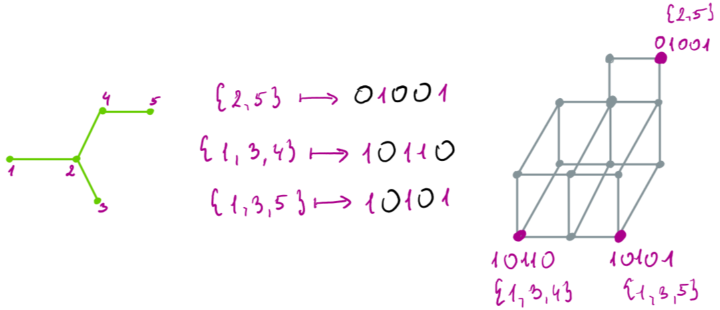


$\{2,5\} \longmapsto 01001$

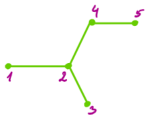
$\{1,3,4\} \longmapsto 10110$

$\{1,3,5\} \longmapsto 10101$

Example


1
2
3
4
5
{2,5} ↦ 01001
{1,3,4} ↦ 10110
{1,3,5} ↦ 10101
{2,5}
01001
10110
{1,3,4}
10101
{1,3,5}

Example

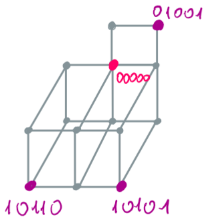


{2, 5} ⟼ 01001

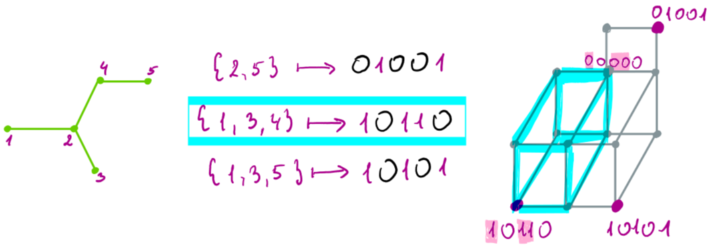
{1, 3, 4} ⟼ 10110

{1, 3, 5} ⟼ 10101

∅ ⟼ 00000



Example



THANKS FOR YOUR TIME