Perfect Matchings and Resonant Patterns of Fullerenes

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November · 2 · 2011

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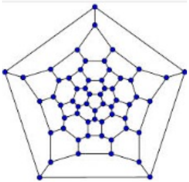

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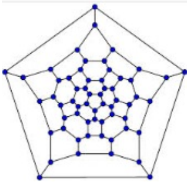

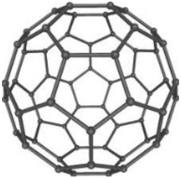

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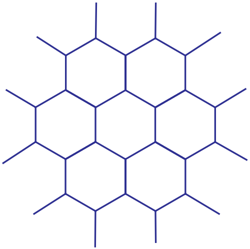
P.W. Fowler and D.E. Manolopoulos, *An Atlas of Fullerenes*, Oxford Unvi. Press, Oxford, 1995.

Leapfrog fullerenes

For any given graph G embedding on a surface, the dual transformation is defined to the operation obtaining the geometric dual of graph G, the truncation transformation is the operation to truncate every vertex of G.

The leapfrog transformation is the operation of the truncation transformation on the geometric dual of the graph G.



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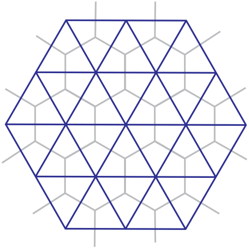

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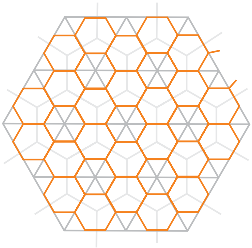

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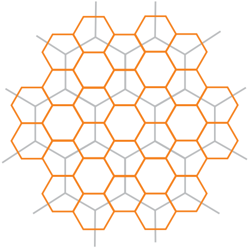

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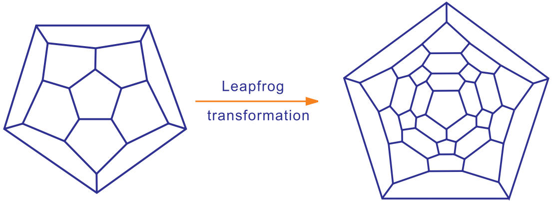
A leapfrog fullerene is a fullerene obtained by applying leapfrog transformation on some fullerene. A leapfrog fullerene is also called Clar sextet fullerene.



Perfect matchings and resonant cycles

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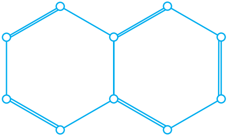

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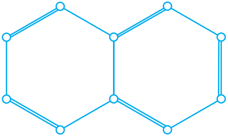

A cycle C is resonant if there is a perfect matching M such that the edges of C alternate between M and $E(G)\setminus M$. In other words, $G - V(C)$ still has a perfect matching.

Resonant pattern

A set $\mathcal{H}$ of disjoint hexagons of a fullerene F is called a resonant pattern if $F - V(\mathcal{H})$ has a perfect matching M (i.e., every hexagon in $\mathcal{H}$ is resonant with respect to M).

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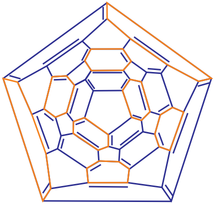

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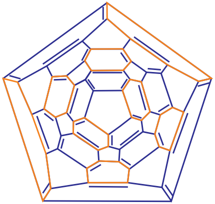

Figure : C_{60} with a resonant pattern.

Let F be a fullerene with a resonant pattern $\mathcal{H}$. Denote the number of perfect matchings of F by $\Phi(F)$. Then $\Phi(F) \geq 2^{|\mathcal{H}|}$.

The number of perfect matchings

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- (ESPERET, KARDOŠ, KING, KRÁL, AND NORINE, 2011, ADV. MATH.) Let G be a bridgeless cubic graph on n vertices. Then $\Phi(G) \geq 2^{n/3656}$.

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- (KUTNAR AND MARUŠIČ, 2008, DAM) Let F be a fullerene with n vertices admitting a non-trivial cyclic 5-edge-cut. Then $\Phi(F) \geq 15 \cdot 2^{\lfloor \frac{n}{20} \rfloor}$.

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- (Kardoš, D. Král, J. Miškuf and J. Sereni, 2009, JMC)
  Let F be a fullerene with n vertices. Then $\Phi(F) \geq 2^{\frac{n-380}{61}}$.

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Remark. The number of perfect matchings of a plane graph can be computed in polynomial-time.

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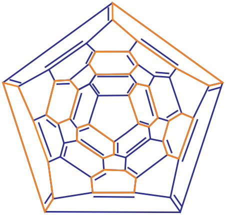

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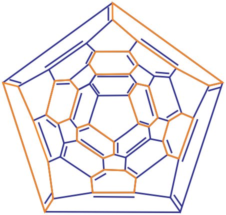

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- (El-Basil, 2000, JMS) The Clar number of C_{60} is 8.

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Let F be a fullerene. Let Q be its vertex-edge incident matrix and R be its vertex-hexagon incident matrix.

$$\begin{array}{ll} \text{maximize} & \mathbf{1}^t\mathbf{y} \\ \text{subject to} & Q\mathbf{x} + R\mathbf{y} = \mathbf{1} \\ \text{and} & \mathbf{x} \text{ and } \mathbf{y} \text{ are integer vectors.} \end{array}$$

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For the Clar problem of plane bipartite graphs, Hansen and Zheng [JMC, 1994] relaxed the integer linear programming into the following linear programming

$$\max\{\mathbf{1}^t\mathbf{y} : Q\mathbf{x} + R\mathbf{y} = 1; \mathbf{x} \geq 0 \text{ and } \mathbf{y} \geq 0\}$$

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- Open Problem: Is there a polynomial-time algorithm to compute Clar number of fullerenes?

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- (Y. and Zhang, 2009, DAM) Let F be a fullerene such that $\text{cl}(F) \leq \lfloor \frac{n-12}{6} \rfloor$. Then subgraphs induced by pentagons of a Clar-extremal fullerene must be generated by the following three basic graphs.

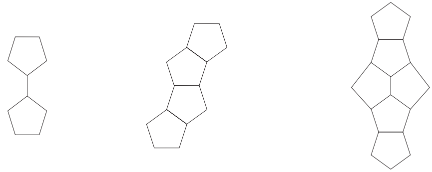

Figure : Three basic graphs.

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The minimum cardinality of forcing sets of M is called the forcing number (or degree of freedom) of M, and is denoted by $f(F; M)$.

The forcing number of a fullerene graph F is defined by

$$f(F) := \min\{f(F; M) | M \text{ is a perfect matching of } F\}.$$

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  The bound is sharp and there are infinitely many fullerenes reaching the bound.

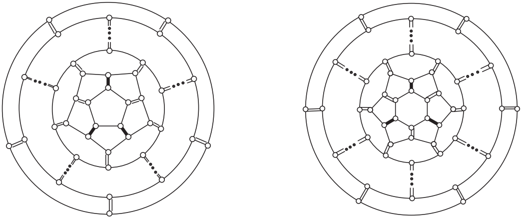

Figure : Fullerenes with forcing number three.

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  From forcing a perfect matching to forcing a 3-edge-coloring:

- CONJECTURE (CQ) Let G be a cubic Petersen-minor-free graph with a unique 3-edge-coloring. Then G contains a triangle.

THANK YOU!