

# Forcing matching number of non-bipartite graphs

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# Introduction

$C_{60}$  was synthesized by Kroto et al. in 1985. Kroto et al. won the 1996's Nobel Chemistry Prize.

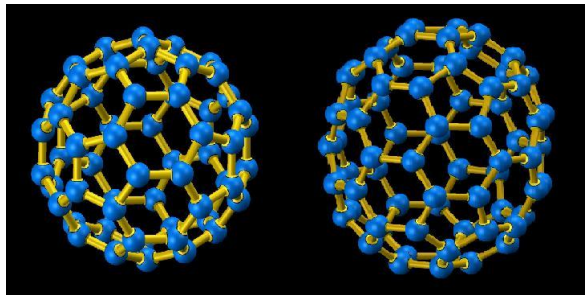


Figure:  $C_{60}$  (left) and  $C_{70}$  (right).

A **fullerene graph**, the molecular graph of a spherical fullerene, is a finite trivalent graph embedded on the surface of a sphere with only hexagonal and (exactly 12) pentagonal faces, using  $F_n$  denote a fullerene graph with  $n$  vertices.

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- A fullerene graph  $F_n$  exists for even  $n \geq 20$  and except 22.
- $C_{60}$  has 1812 fullerene isomers.

# Introductions

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- $C_{60}$  has 1812 fullerene isomers.

Fullerene displays excellent properties such as superconductivity, magnetism, and has extensive applications in materials and biology etc. These properties and applications stimulate many theoretical researches on fullerene graphs such as isomer count, spectrum, perfect matching count, Hamilton cycles and symmetry. We refer to a book of Fowler and Manolopoulos.

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

# Introduction

A **perfect matching**  $M$  (or Kekulé structure, 1-factor) of a graph  $G$  is a set of independent edges such that every vertex of  $G$  is incident with exactly one edge in  $M$ . Perfect matchings of a molecule graph play a key role in the resonance energy of the molecule.

For a benzenoid system  $H$ , the number  $\Phi(H)$  of perfect matchings of  $H$  is closely related to its stability: for example, see the following simple computation model (1975)

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However, Austin et al. found that there is no direct connections between the Kekulé structure count and fullerene's stability.

S.J. Austin, P.W. Fowler, P. Hansen, D.E. Manolopoulos and M. Zheng, Fullerene isomers of  $C_{60}$  · Kekulé counts versus stability, Chem. Phys. Lett. 228 (1994) 478-484.

Flocke et al. founded that Kekulé structures of a fullerene do not contribute to the resonance energy equally.

N. Flocke, T.G. Schmalz and D.J. Klein, Variational resonance valence bond study on the ground state of  $C_{60}$  using the Heisenberg model, J. Chem. Phys. 109 (1998) 873-880.

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Recent works show that the Kekulé structures of a fullerene with large innate degree of freedom are more important than the ones with smaller innate degree of freedom in resonance theory.

D. Vukičević and M. Randić, On Kekulé structures of buckminsterfullerene, Chem. Phys. Lett. 401 (4-6) (2005) 446-450.

The concept of innate degree of freedom of a Kekulé structure was first introduced by Randić and Klein in 1985. The same idea was proposed by Harary et al. in 1991 in term of “forcing number” of a perfect matching of a graph.

M. Randić and D.J. Klein, In: *Mathematical and Computational Concepts in Chemistry*, N. Trinajstić eds., (Wiley, New York, 1985), pp. 274-282.

F. Harary, D.J. Klein and T.P. Živković, Graphical properties of polyhexes: perfect matching vector and forcing, *J. Math. Chem.* 6 (1991) 295-306.

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# Forcing number of graphs

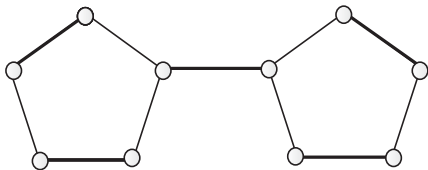
Let  $G$  be a graph with a perfect matching  $M$ . A subset  $S \subseteq M$  is called a **forcing set** of  $M$  if  $S$  is contained in only one perfect matching  $M$  of  $G$ .

The **minimum forcing set** of  $M$  is a forcing set of  $M$  with minimum cardinality and its cardinality is called the **forcing number** (innate degree of freedom) of  $M$ , denoted by  $f(G, M)$ .

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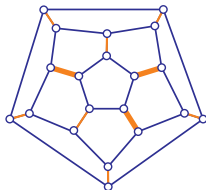
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**Figure:** A graph with a unique perfect matching, and  $f(G, M) = 0$ .

# Forcing number of graphs



**Figure:** Three thick orange edges can determine a unique perfect matching of Dodecahedron.

# Forcing number of graphs

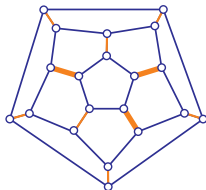


Figure: Three thick orange edges can determine a unique perfect matching of Dodecahedron.

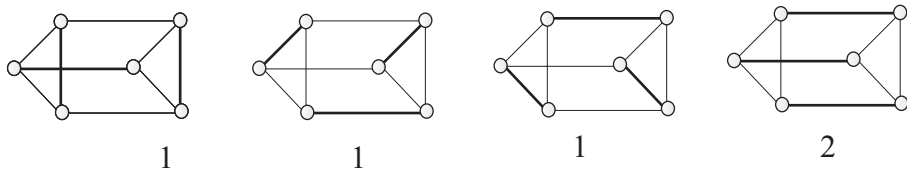


Figure: The four perfect matchings of the triangle prism and their forcing numbers.

# Spectrum of Forcing numbers of graphs

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- $\text{Spec}(\text{Triangle Prism}) = \{1, 2\}$ ,
- $\text{Spec}(\text{Dodecahedron}) = \{3\}$ .

Theorem 2.1 (Vukičević, Kroto and Randić, 2005)

$$\text{Spec}(C_{60}) = \{5, 6, 7, 8, 9, 10\}.$$

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Theorem 2.3 (Li Chunmei, 2008)

$$\text{Spec}(K_3 \times P_{2n}) = \{n - \lfloor \frac{n}{3} \rfloor, n - \lfloor \frac{n}{3} \rfloor + 1, \dots, 2n - 1, 2n\}.$$

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## Theorem 3.1 (Pachter and Kim, 1998)

*Let  $G$  be a plane bipartite graph with a perfect matching  $M$ . Then  $f(G, M) = c(M)$ , where  $c(M)$  is the maximum number of disjoint  $M$ -alternating cycles.*

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**Note:** For non-bipartite graphs, the above result is not necessarily holds. For a general bipartite graph, Adams, Mahdian and Mahmoodian obtained the following result.

## Theorem 3.2 (Adams, Mahadian and Mahmoodian, 2004)

*Let  $G$  be a bipartite graph with maximum degree 3. Then it is NP-Complete to determine a minimum forcing set of a perfect matching of  $G$ .*

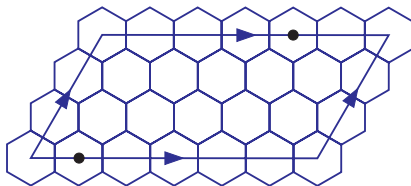
# Forcing number of bipartite graphs

In 2002, Riddle [The minimum forcing number for the torus and hypercube, Discrete Math. 245 (2002) 283-292.] provided the trailing vertex method to determine the minimum forcing set of a bipartite graph. His idea is based on the fact that **a bipartite graph with a unique perfect matching must contain a 1-degree vertex.**

By improving Riddle's trailing vertex method, Wang et al. computed the forcing number of toroidal fullerene graphs, and presented a linear time algorithm determining the minimum forcing number of toroidal fullerene graphs.

# Forcing number of bipartite graphs

A toroidal fullerene  $G$  is a cubic bipartite graph embedded on the torus such that each face of  $G$  is bounded by a cycle of size 6. It can be produced by a parallelogram identification. For example,



## Theorem 3.3 (Wang, Ye and Zhang, 2008)

*Let  $G$  be a toroidal fullerene graph. Then  $f(G)$  equals to the side length of a maximum equilateral triangle.*

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## Theorem 3.4 (Wang, Ye and Zhang, 2008)

*Let  $G$  be a toroidal fullerene graph. Then  $f(G)$  can be computed in  $O(n)$  times where  $n$  is the vertex number of  $G$ .*

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# Forcing number of fullerene graphs

Fullerene graphs are non-bipartite. As we known, there is few work done for forcing numbers of non-bipartite graphs. For general fullerene graphs, we have the following main result.

## Theorem 4.1 (Zhang, Ye and Shiu, 2008)

*Let  $F$  be a fullerene graph. Then  $f(G) \geq 3$  and the bound can be achieved by infinite many fullerene graphs.*

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## Theorem 4.2 (Kotzig, 1959)

*Let  $G$  be connected and have a unique perfect matching. Then  $G$  has a bridge belonging to the perfect matching.*

# Cyclic edge-connectivity of fullerene graphs

A graph  $G$  is **cyclically  $k$ -edge connected** if at least  $k$ -edges must be removed to disconnect  $G$  into two components that each contains a cycle.

The **cyclic edge-connectivity** of  $G$ , denoted by  $c\lambda(G)$ , is the maximum integer  $k$  such that  $G$  is cyclically  $k$ -edge connected.

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A set of  $k$  edges whose elimination disconnects a graph into two components, each containing a cycle, is called a **cyclic  $k$ -edge-cutset**. A cyclical  $k$ -edge-cutset is **trivial** if at least one component is a single cycle of size  $k$ .

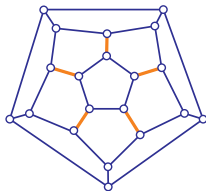


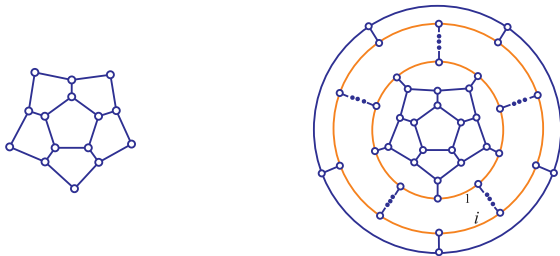
Figure: The orange edges form a trivial 5-edge-cutset.

# Cyclic edge-connectivity of fullerene graphs

Theorem 4.3 (Došlić, 2003)

*The cyclic edge-connectivity of a fullerene graph is 5.*

Construction for fullerene graphs with non-trivial cyclic 5-edge-cutset:



**Figure:** Pentacap (left) and fullerene graphs  $F_p^i$  ( $i = 1, 2, \dots$ ) with nontrivial cyclic 5-edge cutsets.

## Theorem 4.4 (Kutnar, Marušič, 2007; Kardoš, Škrekovski, 2008)

*Let  $F$  be a fullerene admitting a nontrivial cyclic 5-edge-cut. Then  $F$  contains a pentacap, and more precisely,  $F$  contains two disjoint antipodal pentacaps.*

In fact, in the proof of Theorem 4.4, Kutnar and Marušič showed that removing edges in a non-trivial cyclic edge-cutset separates  $F$  into two 2-connected graphs each of which has a face of size 10 on which the 2-degree vertices and 3-degree vertices appear alternately along some direction, and the edges in  $S$  are not incident with any pentagon of  $F$ . Hence a fullerene graph with a nontrivial cyclic 5-edge cut is isomorphic to a  $F_P^i$  for some number  $i$ .

# Extendability of fullerene graphs

A graph  $G$  with a perfect matching is  $k$ -extendable if  $|G| \geq 2k + 2$  and any  $k$  independent edges can be extended to a perfect matching of  $G$ .

## Theorem 4.5 (Holton and Plummer, 1988)

*If  $G$  is a cubic 3-connected planar graph which is cyclically 4-edge-connected and has no faces of size 4, then  $G$  is 2-extendable.*

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By the result of Holton and Plummer together with the cyclic edge-connectivity of fullerene graphs, H. Zhang and F. Zhang obtained the following result.

## Theorem 4.6 (H. Zhang and F. Zhang, 2001)

*Every fullerene graph is 2-extendable.*

# An outline to the Proof of Theorem 4.1

Our method is to prove that any two independent edges  $e_1$  and  $e_2$  can not determine a unique perfect matching of a fullerene graph.

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Let  $F' := F \ominus \{e_1, e_2\}$  be the subgraph from  $F$  by deleting edges  $e_1$  and  $e_2$  together with their incident vertices.

# Proof of Theorem 4.1

If  $F'$  has no vertices of degree one, then  $F'$  is either 2-connected or  $F'$  has a subgraph isomorphic to the graph  $G$ .

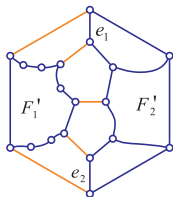


Figure: The graph  $G$ .

$G$  has a nontrivial cyclic 5-edge-cutset  $S$ . As one component of removing the edges of  $S$  from  $F'$ ,  $F'_1$  has a face  $f$  of size 10. However, 2-degree vertices and 3-degree vertices of  $F'_1$  do not appear alternately on the boundary of  $f$ , a contradiction. So  $F'$  is 2-connected.

# Proof of Theorem 4.1

If  $F'$  has a 1-degree vertex, then repeatedly deleting the resulting 1-degree vertices and their neighbors we arrive at a 2-connected nonempty subgraph  $F''$  of the fullerene graph  $F$ .

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By Kotzig's unique factor theorem,  $F'$  has at least two different perfect matchings  $M_1$  and  $M_2$ . So, for any two independent edges  $e_1$  and  $e_2$ ,  $F$  has at least two perfect matchings  $M_1 \cup \{e_1, e_2\}$  and  $M_2 \cup \{e_1, e_2\}$  both of which contain  $e_1$  and  $e_2$ .

So we have  $f(M; F) \geq 3$ . Immediately,  $f(F) \geq 3$ . This complete the proof of Theorem 3.3.

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# Sharpness of the lower bound

The bound given in Theorem 4.1 is sharp for infinite many fullerene graphs.

Construction of the fullerene graphs attaining the bound:

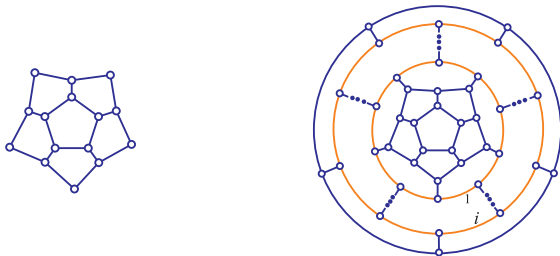


Figure: Hexacap (left) and fullerene graphs  $F_H^i$  ( $i = 1, 2, \dots$ ).

# Sharpness of the lower bound

## Proposition 5.1 (Zhang, Ye and Shiu, 2008)

The forcing numbers of fullerene graphs  $F_P^i$  and  $F_H^i$  satisfy  $f(F_P^i) = 3$  and  $f(F_H^i) = 3$ .

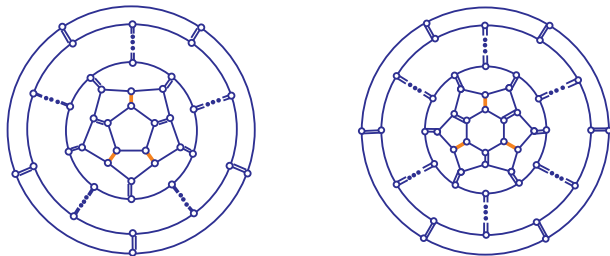


Figure: Three origin edges determine a unique perfect matching of  $F_P^i$  (left) and  $F_H^i$  (right).

# Sharpness of the lower bound

By Proposition 5.1, there are infinite many fullerene graphs attaining the bound 3 in Theorem 4.1.

As a direct corollary of Proposition 5.1 and Theorem 4.4, we have following result,

## Corollary 5.2 (Zhang, Ye and Shiu, 2008)

*Let  $F$  be a fullerene graph with nontrivial cyclic 5-edge cutset. Then  $f(F) = 3$ .*

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# Problems on forcing matching number

There are many interesting open problems on forcing matching number of bipartite graphs such as:  $n$ -dimensional hypercube  $Q_n$ , square grid  $P_{2n} \times P_m$ .

Pachter and Kim proposed the following conjecture:

**Conjecture 1.** (Pachter and Kim, 1998)  $f(Q_n) = 2^{n-2}$ .

Riddle (2002) showed that Conjecture 1 holds for even  $n$ . Kleinerman (2006) showed that  $f(Q_n) \geq \frac{2n-2}{2n-1} 2^{n-2}$  for odd  $n$ . The conjecture for odd  $n$  still remains open.

# Problems on forcing matching number

By the Van der Waerden's Conjecture, Riddle (2002) showed that for sufficiently large  $n$ , there exist matchings of hypercube  $Q_n$  with forcing number greater than  $c2^{n-1}$  for any constant  $c < 1$ .

**Problem 2.** (Riddle, 2002) Determine the maximum forcing number for perfect matchings  $F(Q_n)$ .

**Problem 3.** Determine the minimum forcing number  $f(P_{2n} \times P_m)$ .

Pachter and Lam (1998) showed that  $n \leq f(P_{2n} \times P_{2n}) \leq n^2$ . Afshani, Hatami and Mahmoodian (2004) obtained the spectrum of forcing number of  $P_{2n} \times P_{2n}$ :  $Spec(P_{2n} \times P_{2n}) = \{n, n+1, \dots, n+i, \dots, n^2\}$ . Other cases still remain open.

# Problems on forcing matching number

For fullerene graphs, we are interested in the following problems.






**Problem 4.** Determine all fullerene graphs for which the minimum forcing number is equal to 3.

**Problem 5.** Give a sharp upper bound for forcing number of perfect matchings of fullerene graphs.






**Problem 6.** Determine all fullerene graphs for which all perfect matchings have the same forcing number.

**Problem 7.** Seek an effect algorithm to compute the forcing number of a fullerene graph.

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THANK YOU!