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Efficient Dominating Set in Fullerene Graph

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Abstract

A Fullerene graph is a 3-regular, 3-connected graph such that all of the Faces is pentagonal and hexagonal.A spanning subgraph of a graph G is called a perfect star packing in G if every component of the spanning subgraph G isomorphic with star graph $K_{1,3}$. The set of Efficient dominating set of the graph G are sets of vertices D such that each vertex in $V(G) - D$ is adjacent to exactly one vertex in D. We prove that the perfect star packing in a fullerene graph G on n vertices will exist if and only if G has an efficient dominating set of cardinality $\frac{n}{4}$. Then we show that the size of fullerene graph with an efficient dominating set is 8n.

Keywords: perfect star packing, fullerene, dominating set.

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1. Introduction

Fullerene graphs are that represent known with carbon molecules, a fullerene graph can be defined as a graph whose vertices represent atoms and edges is also a bond between atoms. In the fullerene graph, all faces are pentagons and hexagons, according to Euler's formula, the number of pentagonal faces in fullerene graphs is equal to twelve. In this paper we investigated the relationship between efficient dominating set and perfect star packing in the fullerene graph and some theorems that expression of the relationship between these parameters is investigated in fullerene graphs and we prove it.

Suppose p, h, n and m are the number of pentagons, hexagons, vertices and edges of a fullerene graph F, respectively. Since each vertex lies in exactly three faces and each edge lies in two faces, pay attention to the Figure 1
the number of vertices is $n = (5p + 6h)/3$
the number of edges is $n = (5p + 6h)/2 = 3/2n$
and the number of faces is $f = p + h$.
By the Euler's formula $n - m + f = 2$ and so $(5p + 6h)/3 - (5p + 6h)/2 + p + h = 2$.
Therefore, $p = 12, v = 2h + 20$ and $e = 3h + 30$.

Theorem 1.1. Fullerene graphs with n vertices exist for all even $n \geqslant 24$ and for $= 20$.

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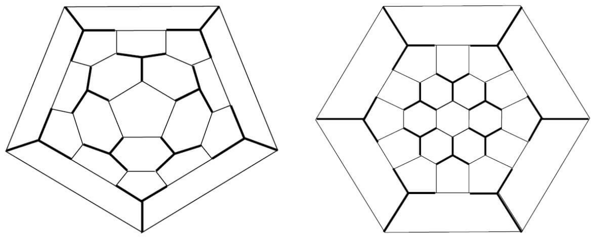

Figure 1: Fullerene graphs.

2. Fullerene graphs

The first fullerene molecule, with a structure like a football, was discovered experimentally in 1985 by Kroto et al. The discovered molecule, C_{60} is comprised only by 60 carbon atoms, and it resembles the Richard Buckminster Fuller's geodetic dome, therefore it was named buckminsterfullerene.

In 1991, the Science magazine pronounced the buckminsterfullerene for the "Molecule of the year", and later in 1996 the discovery of C60 was rewarded with the Nobel prize for chemistry. Each of these all-carbon molecules have polyhedral structure, and all faces of the polyhedron are either pentagons or hexagons. All polyhedral molecules made entirely of carbon atoms are called fullerenes. applying the methods of graph theory to the mathematical models of fullerene molecules called fullerene graphs.

The study from graph theoretical point of view has been motivated by a search for invariants that will correlate with their stability as a chemical compound. A number of graph-theoretical invariants were examined as potential stability predictors with various degrees of success.

As a result of those investigations, achieved a fairly thorough understanding of fullerene graphs and their properties. However, some problems and questions still remain open.

Due to Whitney's Theorem (1933) simple planar 3-connected graphs have a unique planar embedding, and therefore the same holds for fullerene graphs.

Since the discovery of fullerenes in 1985, various types of fullerenes have been identified, which include:
(1) Buckyball: the smallest of which is C_{20} and the most common is C_{60}.
(2) Nanotubical: very small hollow tubes that have excellent performance in the electronics industry.
(3) Megatube: tubes whose diameter is much larger than nanotubes.
(4) Polymers: macromolecules connected by covalent chemical bonds.
(5) Nano-onions: It consists of a solid buckyball shape with spherical particles, which is made based on several layers of carbon.
(6) Dimers ball and chain: these are two buckyball balls that are joined together by a carbon chain are kept.
(7) fullerene rings: they are formed by a ring or rings of fullerene buckyballs.

3. Main Results

In this paper we present a property for a fullerene graph that has perfect star packing and show that If fullerene graph G has a perfect star packing, then the order of G is divisible by 8. We note that star graph $K_{1,3}$ has exactly one center (the vertex of degree 3) and three leaves. A perfect star packing S of a fullerene graph G is a spanning subgraph of G each component of which is a star graph $K_{1,3}$. We call each 1-degree vertex in S being a leaf. In the following, we denote by $C(S)$ the set of all the centers of stars in S.

Remark 3.1. Let S be a perfect star packing of fullerene graph G. Then
1: $C(S)$ is an independent vertex set in G.
2: Any leaf in S has exactly one neighbor belonging to $C(S)$ and has exactly two neighbors being leaves in S.
3: Each cycle in $G - C(S)$ does not have a chord.

Theorem 3.2. Let S be a perfect star packing of fullerene graph G, Then $G - C(S)$ has even number of odd cycles.

Theorem 3.3. If fullerene graph G has a perfect star packing, then the order of G is divisible by 8.

Proof. We suppose that S is a perfect star packing of G and C_0 and C_e are the collections of all the odd cycles and even cycles in $G - C(S)$, respectively. Then we have the following equation.

$$\begin{aligned} |V(G)| &= |C(S)| + \sum_{C \in C_0} |C| + \sum_{C \in C_e} |C| \\ &= \frac{|V(G)|}{4} + \sum_{C \in C_0} |C| + \text{even}. \end{aligned}$$

By Theorem 3.2, C_0 has even number of elements. Combine the above equation, we know that $\frac{|V(G)|}{4} \times 3$ is even. Hence $\frac{|V(G)|}{4}$ is even, that is, the order of G is divisible by 8. □

Proposition 3.4. A fullerene graph G with n vertices has a perfect star packing if and only if G has an efficient dominating set of cardinality $\frac{n}{4}$.

Combine Theorem and Proposition above we get the following theorem.

Theorem 3.5. The order of a fullerene graph with an efficient dominating set is $8n$.

Look at the fullerene graphs Figure 2

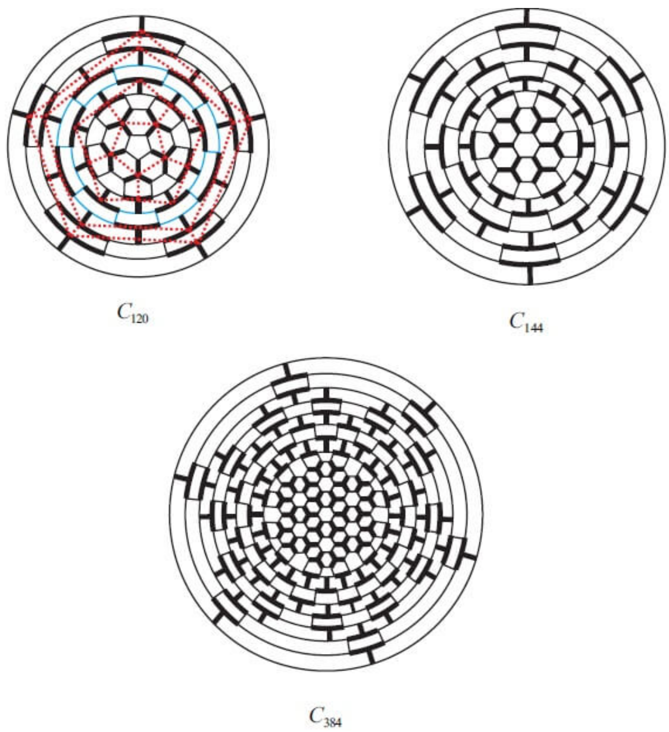

Figure 2: Fullerene graphs

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