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A RESULT ON TOTAL COLORING OF FULLERENE NANODISCS

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1. Introduction

A *graph* is a mathematical model used to represent relationships between objects. The general characters that both of these objects and their relationships can assume, allowed the construction of the so-called Graph Theory, which has been applied to model problems in several areas, such as Mathematics, Physics, Computer Science, Engineering, Chemistry, Psychology and industry. Most of them are large scale problems.
Fullerene graphs are mathematical models for carbon-based molecules experimentally discovered in the early 1980s by Kroto, Heath, O'Brien, Curl and Smalley. Many parameters associated with these graphs have been discussed to describe the stability of fullerene molecules.
By definition, fullerene graphs are cubic, planar, 3-connected with pentagonal and hexagonal faces.
The motivation of the present study is to find an efficient method to obtain a 4-total coloring of a particular class of fullerene graphs named fullerene nanodiscs, if it exists.

2. Basic Concepts of Graph Theory

This section is based on the reference Bondy and Murty, 2008.

Definition 1. A **graph** $G = (V(G), E(G))$ is an ordered pair, where $V(G)$ is a nonempty finite set of vertices and $E(G)$ is a set of edges disjoint from $V(G)$, formed by unordered pairs of distinct elements from $V(G)$, that is, for every edge $e \in E(G)$ there is u and $v \in V(G)$ such that $e = \{u, v\}$, or simply $e = uv$.

If $uv \in E$, we say that u and v are adjacent or that u is a neighbor of v, and that the edge e is incident to u and v, and u and v are said to be extremes (or ends) of e. Two edges that have the same end are called adjacent.
The degree of a vertex v in G, represented by $d(v)$, is the number of edges incident to v. We denote by $\delta(G)$ and $\Delta(G)$ the minimum and maximum degrees respectively, of the vertices of the graph G.

A graph G is said **connected** when there is a path between each pair of vertices of G. Otherwise, the graph is called disconnected.

A **cubic** graph is one in which all vertices have three incident edges and in this case, all vertices have degree 3. Cubic graphs play a fundamental role in Graph Theory.

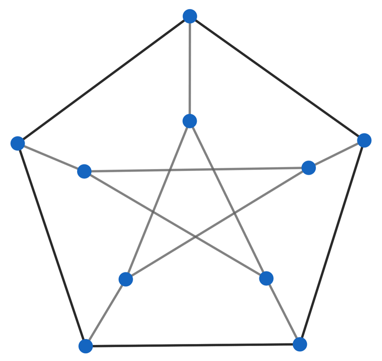

Figure 1: *Cubic Graph.*

A graph G is planar if there is a representation of G in the plane so that the edges meet only at the vertices, that is, the edges do not cross. Such a representation of G is said to be embeddable or planar. A planar representation divides the plane into regions called faces. There is always a single face called external or infinite, which is not limited (has infinite area). The outer boundary or cycle of a connected planar graph face is a closed walk that limits and determines the face.

Two faces are adjacent if they have a common edge between their boundaries. We denote the boundary of f by $\partial(f)$. If f is any face, the degree of f, denoted by $d(f)$, is the number of edges contained in the closed walk that defines it. In a planar connected graph with f faces, n vertices and m edges, we have that $n + f - m = 2$, which is known as Euler's formula.

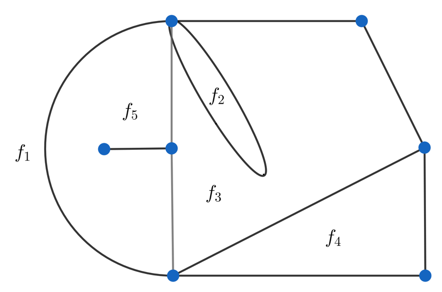

Figure 2: *Planar Graph.*

2.1 Total Coloring

In graph theory, coloring is a color assignment to the graph elements, subject to certain restrictions. The coloring study started with the Four Color Conjecture, which deals with determining the minimum number of colors needed to color a map of real or imaginary countries, so that countries with common borders have different colors. This conjecture was proposed by Francis Guthrie in 1852. After 124 years, the Four Color Conjecture was demonstrated by Kenneth Appel and Wolfgang Haken with the help of a computer. The famous Four Color Theorem is a reference in the area of Graph Theory.

Definition 2. A **total coloring** C^T of a graph G is a color assignment to the set $E \cup V$ in a color set $C = \{c_1, c_2, ..., c_k\}$, $k \in \mathbb{N}$, such that distinct colors are assigned to:

- Every pair of vertices that are adjacent;
- All edges that are adjacent;
- Each vertex and its incident edges.

A k-total coloring of a graph G is a total coloring of G that uses a set of k colors, and a graph is k-total colorable if there is a k-total coloring of G. We define as the **total chromatic number** of a graph G the smallest natural k for which G admits a k-total coloring, and is denoted by $\chi''(G)$.

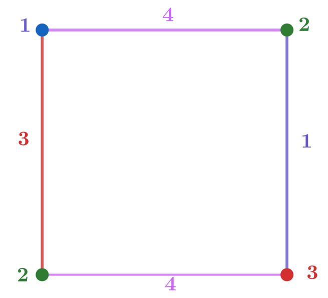

Figure 3: *Graph with 4-total coloring.*

Behzad and Vizing independently conjectured the same upper bound for the total chromatic number.

Conjecture (Total Color Conjecture (TCC))
For every simple graph G,

$$\chi''(G) \leq \Delta(G) + 2.$$

The TCC is an open problem, but has been checked for several classes of graphs. Knowing that $\chi''(G) \geq \Delta(G) + 1$, and from the TCC, we have the following classification: If $\chi''(G) = \Delta(G) + 1$, the graph is **Type** 1; and if $\chi''(G) = \Delta(G) + 2$, the graph is **Type** 2.
For cubic graphs, the TCC has already been demonstrated, which indicates that these graphs have total chromatic number 4 $(\Delta + 1)$ or 5 $(\Delta + 2)$. However, the problem of deciding which are Type 1 or Type 2 is difficult.

3. Fullerene Graphs

3.1 Fullerene: A small history

In 1985 a new carbon allotrope was reported in the scientific community: C_{60}. A group of scientists, led by Englishman Harold Walter Kroto and Americans Richard Errett Smalley and Robert Curl, trying to understand the mechanisms for building long carbon chains observed in interstellar space, discovered a highly symmetrical, stable molecule, composed of 60 carbon atoms different from all the other carbon allotropes.

The C_{60} has a structure similar to a soccer hollow ball (Figure 4), with 32 faces, being 20 hexagonal and 12 pentagonal. They decided to name the C_{60} *buckminster-fullerene*, in honor of American architect Richard Buckminster Fuller, famous for his geodesic dome constructions, which were composed of hexagonal and pentagonal faces.
At the end of the 1980s, other carbon allotrope molecules with similar spatial structure to the C_{60} were reported called fullerene molecules (Kroto et al., 1985).

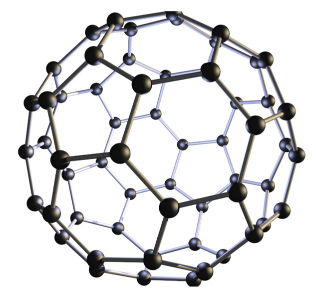

Figure 4: *Molecular structure of C_{60}.*

The buckminsterfullerene was the first new allotropic form discovered in the 20th century, and earned Kroto, Curl and Smalley the Nobel Prize in Chemistry in 1996. Nowadays fullerene molecules are widely studied by different branches of science, from medicine to mathematics. These molecules are supposed to contribute to transport chemotherapy, antibiotics or antioxidant agents and released in contact with deficient cells.

3.2 Fullerene Graphs

Each fullerene molecule can be described by a graph where the atoms and the bonds are represented by the vertices and edges of the graph, respectively. In addition, fullerene graphs preserve the geometric properties of fullerene molecules, i.e., fullerene graphs are planar and connected. Moreover, all vertices have exactly 3 incident edges and all faces are pentagonal or hexagonal (Nicodemos, 2017).

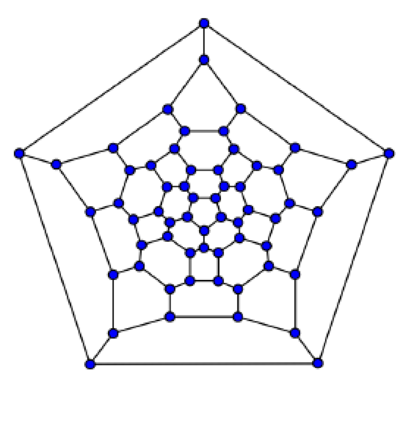

Figure 5: *Fullerene Graph.*

3.3 Fullerene Nanodiscs

The fullerene nanodiscs, or nanodiscs of radius $r \geq 2$ are structures composed of two identical flat covers connected by a strip along their borders. While in the nanodisc lids there are only hexagonal faces, in the connecting strip, 12 pentagonal faces are arranged side by side.
A nanodisc of radius $r \geq 2$, represented by $D_{r,t}$, can be obtained through its flattening. The idea is to arrange the faces in layers around the nearest previous layer starting from a hexagonal face (Nicodemos, 2017).

The sequence

$$\{1, 6, 12, 18, ..., 6(r-1), 6r, 6(r-1), ..., 18, 12, 6, 1\}$$

provides the amount of faces on each layer of nanodisc planning D_r, while $r \geq 2$. In addition, this sequence states that a D_r nanodisc has $(6r^2 + 2)$ faces, $12r^2$ vertices and $(2r + 1)$ layers. The 12 pentagonal faces will always be distributed in the same layer with other $(6r - 12)$ hexagonal faces. This is the key property of fullerene nanodiscs.

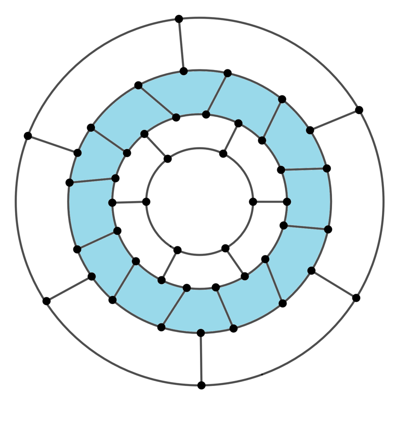

Figure 6: *Nanodisc D_2.*

4. Goals

To prove that a cubic graph is Type 1, it suffices to show a total coloring with 4 colors. However, to demonstrate that a cubic graph is Type 2, we need to show that it has no total coloring with only 4 colors. Thus, finding Type 2 cubic graphs is more complicated.
We define the girth of a graph G as the length of its shortest cycle. Until now, every Type 2 cubic graph we know has squares or triangles. So, we could think that there are no Type 2 cubic graphs with girth at least 5. Thus, we investigate the following question.

Question
(Sasaki, 2013) Does there exist a Type 2 cubic graph with girth at least 5?

Motivated by this question, we analyze the family of fullerene nanodiscs, in search of evidences that can positively or negatively contribute to this question. In this context, we look for an efficient algorithm to find a 4-total coloring of the fullerene nanodisc, if this coloring exists.

5. Results

After a few attempts using the brute force method, we were able to obtain a 4-total coloring of the D_2 nanodisc, with $r = 2$. Therefore, D_2 is Type 1, which contributes to the evidences that the previously proposed question has a negative answer.

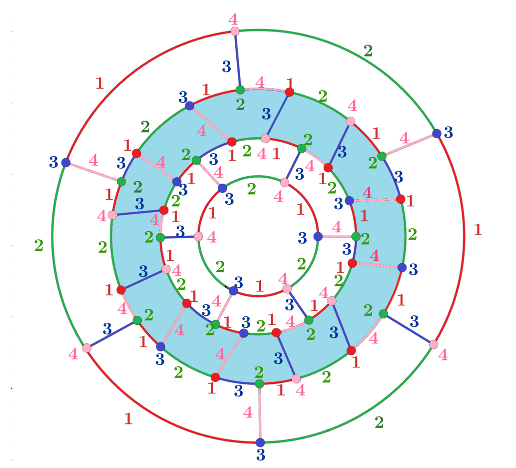

Figure 7: *A 4-total coloring of D_2.*

6. Conclusion

We will continue the study of total coloring of nanodiscs, looking for an algorithm that gives a total coloring of the graphs of the infinite family of fullerene nanodiscs, also seeking to answer the question previously proposed.

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