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Research Article

Perfect Coloring of Graphs Related to Irreducible Fullerenes in Carbon Structures

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Abstract: Fullerenes are polyhedral molecules composed solely of carbon atoms, available in various sizes and shapes. These structures can also be depicted as graphs, with the vertices symbolizing the atoms and the edges representing the bonds between them. A fullerene graph is defined as a 3-connected, 3-regular planar graph that consists only of pentagonal and hexagonal faces. This paper examines the perfect 2- and 3-coloring of fullerene graphs, with a particular focus on irreducible fullerenes. The proposed approach begins by obtaining the adjacency matrix of the graphs and then comparing its eigenvalues with those of the parameter matrices. If the eigenvalues of a parameter matrix are a subset of the graph's eigenvalues, we retain these matrices for further analysis to determine their suitability for perfect coloring.

Keywords: planar graph, parameter matrices, regular graph, perfect coloring, irreducible fullerenes

MSC: 05C10, 05C50, 05C75, 05C15

1. Introduction

Graphs play a significant role in various fields due to their ability to represent complex relationships between objects. In computer science, they are used in algorithms, data structures, and network analysis. In biology, graphs help model and analyze biological systems, such as protein interaction networks or neural connections. Graphs also find applications in social sciences for studying social networks and in logistics for optimizing routes in transportation networks. Their flexibility makes them essential tools for solving real-world problems across diverse disciplines [1–3].

A perfect coloring of graphs associated with irreducible fullerenes, which are unique carbon-based structures composed entirely of carbon atoms arranged in a polyhedral form, refers to an advanced method of assigning colors to the vertices of these graphs while satisfying strict mathematical conditions. In this context, the coloring process typically involves ensuring that specific constraints are met, such as the number of edges, or connections, between vertices of different colors remaining constant throughout the graph. This constant relationship between colored vertices is governed by a predefined set of rules, often represented by a parameter matrix, which dictates how the graph's vertices should interact in terms of coloring. In the case of fullerenes, these perfect colorings go beyond simple aesthetic arrangements and offer profound insights into the structural, geometric, and chemical properties of the fullerene molecules. Since fullerenes exhibit highly symmetrical and regular patterns, applying perfect coloring can help uncover key characteristics,

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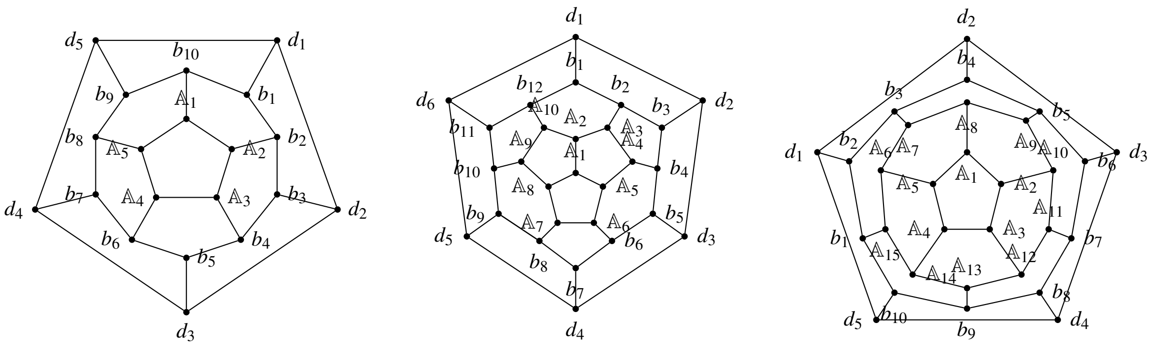
such as stability, symmetry, and even electronic properties of the molecule. For example, analyzing the way the graph is colored can shed light on the molecule's potential reactivity, strength, and the behavior of electrons within the structure. Additionally, perfect colorings can assist in identifying the molecule's suitability for practical applications, such as in nanotechnology, where the precise arrangement of atoms plays a critical role in material performance. This approach also links mathematical theory with real-world chemistry, providing a deeper understanding of molecular interactions and potential uses in developing new materials or enhancing existing ones. Fullerenes can be depicted as graphs, with vertices representing atoms and edges representing the bonds between them. We begin by introducing the concept of fullerene graphs and then examine their perfect coloring. Euler's formula dictates that a fullerene graph always contains twelve pentagonal faces. Motzkin and Grunbaum [4] showed that fullerene graphs exist for any even number of vertices $n \geq 24$ and also for $n = 20$. Although pentagonal faces are fewer than hexagonal ones, their arrangement is crucial in defining the overall shape of a fullerene graph. All icosahedral fullerenes share a common feature: their distinct geometric structure. The simplest graph representing an icosahedral fullerene is the dodecahedron, $\mathbb{C}_{20}$. Fullerenes are carbon allotropes where carbon atoms are linked by single and double bonds, forming a closed or partially closed network with fused rings made up of five to seven atoms. Fullerenes with a closed mesh topology are commonly identified by their empirical formula $\mathbb{C}_n$, where n represents the number of carbon atoms. In a fullerene graph, each carbon atom is treated as a vertex, and each bond between atoms is represented as an edge. A sequence of operations, known as expansion and inversion, along with their inverse, reduction, is sufficient to generate all fullerenes from smaller ones. Figure 1 shows the fundamental graphs used to generate fullerenes include $\mathbb{C}_{20}$, $\mathbb{C}_{28}$, and $\mathbb{C}_{30}$. We will demonstrate that perfect 2- and 3-colorings exist for each of these graphs. A graph is called a regular graph if all vertices have the same degree, and it is termed k-regular if each vertex has a degree of k, where k is a positive integer.



($\mathbb{C}_{20}$) ($\mathbb{C}_{28}$) ($\mathbb{C}_{30}$)

Figure 1. The irreducible fullerenes

Definition 1 A planar graph is a graph that can be represented in the plane such that its edges intersect only at their vertices. In other words, it can be drawn in a way that no two edges overlap except at their endpoints.

Definition 2 A plane graph is a graph that has been drawn on the plane without any overlapping edges. The edges in a plane graph can be depicted as either straight lines or curves.

Creating a planar drawing of a graph $\mathbb{G}$ involves representing $\mathbb{G}$ as a plane graph. In a plane graph, the regions enclosed by edges are referred to as faces. The edges that define the boundary of a face are called the edges incident to that face, and the size of the face corresponds to the number of edges incident to it. If a face is bounded by k edges, it is termed a k-gon. The combinatorial structure of a planar graph can be characterized by the cyclic order of the edges incident to each vertex. An embedding of a planar graph specifies this cyclic order in a plane drawing. In this context, a planar graph is considered one for which such an embedding is provided.

Definition 3 A connected graph is a graph where there is a path between any two vertices. A connected graph $\mathbb{G}$ is termed 3-connected if it remains connected even after the removal of any two vertices from $\mathbb{G}$.

Definition 4 A coloring of the vertex set $\mathbb{V}$ of a graph $\mathbb{G} = (\mathbb{V}, \mathbb{E})$ using n colors is considered perfect if every color is used, and for any pair of colors i and j, the number of neighbors of color j for any vertex v with color i is a constant $\mathbb{A}_{ij}$. The matrix $\mathbb{A} = (\mathbb{A}_{ij})_{i,\, j \in \{1,\, \ldots,\, m\}}$ is referred to as the parameter matrix.

Example 1 Consider the graph $\mathbb{Q}_3$. In this case, if the vertices $(0,\, 0,\, 0)$ and $(1,\, 1,\, 1)$ are assigned the color white, the vertices $(1,\, 0,\, 1)$ and $(0,\, 1,\, 0)$ are colored black, and the rest of the vertices are colored red, this results in a perfect 3-coloring. The corresponding matrix for this 3-coloring reflects the connections between vertices of different colors, where the rows and columns correspond to the white, black, and red vertices. The matrix obtained is:

$$\mathbb{A} = \begin{bmatrix} 0 & 1 & 2 \\ 1 & 0 & 2 \\ 1 & 1 & 1 \end{bmatrix}$$

This paper classifies all perfect 2-colorings and 3-colorings of graphs corresponding to irreducible fullerenes and identifies their associated parameter matrices. We begin by presenting the theorems essential to our research methodology, followed by the main findings from our study. Section 2 demonstrates that the graph $\mathbb{C}_{20}$ has a perfect 2-coloring with parameter matrices $\mathbb{A}_2$ and $\mathbb{A}_6$. Additionally, we show that the graph $\mathbb{C}_{28}$ does not admit a perfect 2-coloring, while the graph $\mathbb{C}_{30}$ has a perfect 2-coloring with the parameter matrix $\mathbb{A}_6$. Section 3 establishes that none of the graphs corresponding to irreducible fullerenes possess a perfect 3-coloring. Section 4 lists application of the graphs corresponding to irreducible fullerenes. Finally, Section 5 highlights the key points and offers concluding remarks.

2. Perfect 2-coloring of the graphs corresponding to irreducible fullerenes

This section first presents the theorems related to perfect 2-coloring. These theorems are then used to determine the possible parameter matrices for all perfect 2-colorings of the graphs under consideration. For further reading on perfect 2-coloring, interested readers are referred to [5–11].

Definition 5 For any graph $\mathbb{G}$ and any integer m, a mapping $\mathbb{T} : \mathbb{V}(\mathbb{G}) \to \{1, \ldots, m\}$ is considered a perfect m-coloring with the matrix $\mathbb{A} = (\mathbb{A}_{ij})_{i,\, j \in \{1,\, \ldots,\, m\}}$ if it is surjective and, for each vertex of color i, the precise number of its neighbors of color j is specified by $\mathbb{A}_{ij}$. The matrix $\mathbb{A}$ is known as the parameter matrix of a perfect coloring. When $m = 2$, the two colors are designated as $\mathbb{W}$ and $\mathbb{B}$, representing white and black, respectively.

The following are important theorems and lemmas regarding perfect 2-coloring; for more detailed information, one can refer to [6].

Theorem 1 Let $\mathbb{G}$ be a k-regular graph, and let $\mathbb{T}$ be a perfect m-coloring of $\mathbb{G}$ with the parameter matrix $\mathbb{A} = (\mathbb{A}_{ij})_{i,\, j \in \{1,\, \ldots,\, m\}}$. Then, the sum of the elements in each row of matrix $\mathbb{A}$ is equal to k.

Theorem 2 If $\mathbb{T}$ is a perfect m-coloring of the graph $\mathbb{G}$, then any eigenvalue of the parameter matrix $\mathbb{A}$ is also an eigenvalue of the adjacency matrix of $\mathbb{G}$.

Theorem 3 Let $\mathbb{A}$ be a perfect 2-coloring of a connected graph $\mathbb{G}$ with the corresponding parameter matrix $\begin{pmatrix} \mathbb{A}_{11} & \mathbb{A}_{12} \\ \mathbb{A}_{21} & \mathbb{A}_{22} \end{pmatrix}$. Then, $\mathbb{A}_{12}$ and $\mathbb{A}_{21}$ are nonzero.

Theorem 4 If $\mathbb{W}$ represents the set of white vertices in a perfect 2-coloring of a graph $\mathbb{G}$ with the parameter matrix $A = (\mathbb{A}_{ij})_{i,\, j=1,\, 2}$, then $|\mathbb{W}| = |\mathbb{V}(\mathbb{G})| \dfrac{\mathbb{A}_{21}}{\mathbb{A}_{12} + \mathbb{A}_{21}}$.

Theorem 5 Suppose the parameter matrix of a perfect 2-coloring of a k-regular graph is $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$. The eigenvalues of this parameter matrix are k and $a - c$, with $a - c \neq k$. According to Theorem 2, we conclude that $a - c$ is an eigenvalue of a k-regular connected graph that is distinct from k.

Lemma 1 If a graph $\mathbb{G}$ has a perfect 2-coloring with the parameter matrix $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$, then it also has a perfect 2-coloring with the parameter matrix $\begin{pmatrix} d & c \\ b & a \end{pmatrix}$.

Given the conditions, the possible parameter matrices for a perfect 2-coloring of cubic graphs can be one of the following:

$$\mathbb{A}_1 = \begin{bmatrix} 0 & 3 \\ 1 & 2 \end{bmatrix}, \quad \mathbb{A}_2 = \begin{bmatrix} 0 & 3 \\ 2 & 1 \end{bmatrix}, \quad \mathbb{A}_3 = \begin{bmatrix} 0 & 3 \\ 3 & 0 \end{bmatrix}, \quad \mathbb{A}_4 = \begin{bmatrix} 1 & 2 \\ 1 & 2 \end{bmatrix}, \quad \mathbb{A}_5 = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}, \quad \mathbb{A}_6 = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}.$$

Theorem 6 The graph $\mathbb{C}_{20}$ admits a perfect 2-coloring with parameter matrices $\mathbb{A}_2$ and $\mathbb{A}_6$.

Proof. According to Theorem 2, the graph $\mathbb{C}_{20}$ can only achieve a perfect 2-coloring with matrices $\mathbb{A}_2$, $\mathbb{A}_4$, and $\mathbb{A}_6$, as the eigenvalues of other matrices, such as $\mathbb{A}_1$ and $\mathbb{A}_3$, do not match the eigenvalues of the adjacency matrix of $\mathbb{C}_{20}$. However, as stated in Theorem 4, matrix $\mathbb{A}_4$ cannot serve as a parameter matrix for a perfect 2-coloring because the resulting number of white vertices is not an integer. Consequently, the graph $\mathbb{C}_{20}$ can have perfect 2-colorings only with matrices $\mathbb{A}_2$ and $\mathbb{A}_6$, as outlined below:

$$T_1(\mathbb{A}_1) = \mathbb{T}_1(\mathbb{A}_3) = \mathbb{T}_1(b_1) = \mathbb{T}_1(b_3) = \mathbb{T}_1(b_6) = \mathbb{T}_1(b_8) = \mathbb{T}_1(d_3) = \mathbb{T}_1(d_5) = \mathbb{W}$$

$$\mathbb{T}_1(\mathbb{A}_2) = \mathbb{T}_1(\mathbb{A}_4) = \mathbb{T}_1(\mathbb{A}_5) = \mathbb{T}_1(b_2) = \mathbb{T}_1(b_4) = \mathbb{T}_1(b_5) = \mathbb{T}_1(b_7) = \mathbb{T}_1(b_9)$$

$$= \mathbb{T}_1(b_{10}) = \mathbb{T}_1(d_1) = \mathbb{T}_1(d_2) = \mathbb{T}_1(d_4) = \mathbb{B}$$

$$\mathbb{T}_2(\mathbb{A}_1) = \mathbb{T}_2(\mathbb{A}_2) = \mathbb{T}_2(\mathbb{A}_3) = \mathbb{T}_2(b_4) = \mathbb{T}_2(b_5) = \mathbb{T}_2(b_9)$$

$$= \mathbb{T}_2(b_{10}) = \mathbb{T}_2(d_3) = \mathbb{T}_2(d_4) = \mathbb{T}_2(d_5) = \mathbb{W}$$

$$\mathbb{T}_2(\mathbb{A}_4) = \mathbb{T}_2(\mathbb{A}_5) = \mathbb{T}_2(b_1) = \mathbb{T}_2(b_2) = \mathbb{T}_2(b_3) = \mathbb{T}_2(b_6) = \mathbb{T}_2(b_7)$$

$$= \mathbb{T}_2(b_8) = \mathbb{T}_2(d_1) = \mathbb{T}_2(d_2) = \mathbb{B}$$

It is clear that $\mathbb{T}_1$ is a perfect 2-coloring with the matrix $\mathbb{A}_2$, and $\mathbb{T}_2$ is a perfect 2-coloring with the matrix $\mathbb{A}_6$. □

Theorem 7 The graph $\mathbb{C}_{28}$ does not admit any perfect 2-coloring.

Proof. According to Theorem 4, and given that the only integer eigenvalue of the adjacency matrix of $\mathbb{C}_{28}$ is 3, none of the parameter matrices are suitable for a perfect 2-coloring of $\mathbb{C}_{28}$. Consequently, the graph $\mathbb{C}_{28}$ does not possess any perfect 2-coloring. □

Theorem 8 The graph $\mathbb{C}_{30}$ admits a perfect 2-coloring with the parameter matrix $\mathbb{A}_6$.

Proof. According to Theorem 2, the graph $\mathbb{C}_{30}$ can only achieve a perfect 2-coloring using the matrix $\mathbb{A}_6$, as the eigenvalues of other matrices, like $\mathbb{A}_1$ and $\mathbb{A}_2$, are not contained within the set of eigenvalues of the adjacency matrix of $\mathbb{C}_{30}$. The mapping T is defined as follows:

$$T(\mathbb{A}_1) = T(\mathbb{A}_2) = T(\mathbb{A}_3) = T(\mathbb{A}_4) = T(\mathbb{A}_5) = T(b_1) = T(b_2) = T(b_3) = T(b_4) = T(b_5)$$

$$= T(b_6) = T(b_7) = T(b_8) = T(b_9) = T(b_{10}) = \mathbb{W}$$

$$T(\mathbb{A}_6) = T(\mathbb{A}_7) = T(\mathbb{A}_8) = T(\mathbb{A}_9) = T(\mathbb{A}_{10}) = T(\mathbb{A}_{11}) = T(\mathbb{A}_{12}) = T(\mathbb{A}_{13}) = T(\mathbb{A}_{14})$$

$$= T(\mathbb{A}_{15}) = T(\mathbb{C}_1) = T(\mathbb{C}_2) = T(\mathbb{C}_3) = T(\mathbb{C}_4) = T(\mathbb{C}_5) = \mathbb{B}$$

This clearly shows that $\mathbb{T}$ is a perfect 2-coloring with matrix $\mathbb{A}_6$. □

3. Perfect 3-coloring of graphs corresponding to irreducible fullerenes

This section examines the limited parameter matrices that can be used for perfect 3-coloring in 3-regular graphs. We then show that none of the graphs associated with irreducible fullerenes possess a perfect 3-coloring. For further information on perfect 3-coloring, you can consult sources [12–14]. Based on the findings in [8], the only viable parameter matrices for 3-regular graphs are as follows:

$$\mathbb{A}_1 = \begin{bmatrix} 0 & 0 & 3 \\ 0 & 0 & 3 \\ 1 & 1 & 1 \end{bmatrix}, \quad \mathbb{A}_2 = \begin{bmatrix} 0 & 0 & 3 \\ 0 & 0 & 3 \\ 1 & 2 & 0 \end{bmatrix}, \quad \mathbb{A}_3 = \begin{bmatrix} 0 & 0 & 3 \\ 0 & 1 & 2 \\ 1 & 1 & 1 \end{bmatrix}, \quad \mathbb{A}_4 = \begin{bmatrix} 0 & 0 & 3 \\ 0 & 1 & 2 \\ 1 & 2 & 0 \end{bmatrix},$$

$$\mathbb{A}_5 = \begin{bmatrix} 0 & 0 & 3 \\ 0 & 2 & 1 \\ 1 & 1 & 1 \end{bmatrix}, \quad \mathbb{A}_6 = \begin{bmatrix} 0 & 0 & 3 \\ 0 & 2 & 1 \\ 1 & 2 & 0 \end{bmatrix}, \quad \mathbb{A}_7 = \begin{bmatrix} 0 & 0 & 3 \\ 1 & 1 & 2 \\ 2 & 1 & 0 \end{bmatrix}, \quad \mathbb{A}_8 = \begin{bmatrix} 0 & 1 & 2 \\ 1 & 1 & 1 \\ 2 & 1 & 0 \end{bmatrix},$$

$$\mathbb{A}_9 = \begin{bmatrix} 0 & 1 & 2 \\ 1 & 2 & 0 \\ 2 & 1 & 0 \end{bmatrix}, \quad \mathbb{A}_{10} = \begin{bmatrix} 0 & 1 & 2 \\ 1 & 2 & 0 \\ 2 & 0 & 1 \end{bmatrix}, \quad \mathbb{A}_{11} = \begin{bmatrix} 0 & 3 & 0 \\ 1 & 0 & 2 \\ 0 & 1 & 2 \end{bmatrix}, \quad \mathbb{A}_{12} = \begin{bmatrix} 1 & 0 & 2 \\ 1 & 2 & 0 \\ 1 & 1 & 1 \end{bmatrix},$$

$$\mathbb{A}_{13} = \begin{bmatrix} 1 & 0 & 2 \\ 1 & 2 & 0 \\ 1 & 1 & 1 \end{bmatrix}, \quad \mathbb{A}_{14} = \begin{bmatrix} 1 & 0 & 2 \\ 1 & 2 & 0 \\ 1 & 1 & 1 \end{bmatrix}, \quad \mathbb{A}_{15} = \begin{bmatrix} 1 & 0 & 2 \\ 1 & 2 & 0 \\ 1 & 1 & 1 \end{bmatrix}, \quad \mathbb{A}_{16} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix},$$

$$\mathbb{A}_{17} = \begin{bmatrix} 1 & 2 & 0 \\ 1 & 0 & 2 \\ 0 & 1 & 2 \end{bmatrix}, \quad \mathbb{A}_{18} = \begin{bmatrix} 1 & 2 & 0 \\ 1 & 0 & 2 \\ 0 & 1 & 2 \end{bmatrix}.$$

In this article, we typically denote a parameter matrix as

$$A = \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix},$$

and utilize the following theorems to support our analysis. The matrix A is considered as a general representation, where the elements a, b, c, d, e, f, g, h, and i are parameters that may vary depending on the context. By applying these theorems, we can explore various properties and behaviors of the matrix, which play a crucial role in deriving key results and conclusions within our study. The structure of the matrix allows for flexibility in its application across different scenarios, enhancing the depth and scope of our analysis.

Theorem 9 Let $\mathbb{T}$ be a perfect 3-coloring with the matrix $\begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}$ in a connected graph $\mathbb{G}$. Then, none of the following conditions can occur:

(1) $c = b = 0$,

(2) $f = d = 0$,

(3) $h = g = 0$,

(4) $d = 0 \leftrightarrow b = 0$, $g = 0 \leftrightarrow c = 0$, $f = 0 \leftrightarrow g = 0$.

Proof. It is evident that having 1, 2, and 3 is not possible because the graph is connected. Additionally, $b = 0$, $c = 0$, and $f = 0$ hold true if $d = 0$, $g = 0$, and $h = 0$ respectively. $\square$

Theorem 10 ([12]) Let $\mathbb{T}$ represent a perfect 3-coloring of a graph $\mathbb{G}$ with the matrix $\mathbb{A} = \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}$.

1. If b, c, $f \neq 0$, then

$$|\mathbb{W}| = \frac{|\mathbb{V}(\mathbb{G})|}{\frac{b}{d} + 1 + \frac{c}{g}}, \quad |\mathbb{B}| = \frac{|\mathbb{V}(\mathbb{G})|}{\frac{d}{b} + 1 + \frac{f}{h}}, \quad |R| = \frac{|\mathbb{V}(\mathbb{G})|}{\frac{h}{f} + 1 + \frac{g}{c}},$$

2. If $b = 0$, then

$$|\mathbb{W}| = \frac{|\mathbb{V}(\mathbb{G})|}{\frac{c}{g} + 1 + \frac{ch}{fg}}, \quad |\mathbb{B}| = \frac{|\mathbb{V}(\mathbb{G})|}{\frac{f}{h} + 1 + \frac{fg}{ch}}, \quad |R| = \frac{|\mathbb{V}(\mathbb{G})|}{\frac{h}{f} + 1 + \frac{g}{c}},$$

3. If $c = 0$, then

$$|\mathbb{W}| = \frac{|\mathbb{V}(\mathbb{G})|}{\frac{b}{d} + 1 + \frac{bf}{dh}}, \quad |\mathbb{B}| = \frac{|\mathbb{V}(\mathbb{G})|}{\frac{d}{b} + 1 + \frac{f}{h}}, \quad |R| = \frac{|\mathbb{V}(\mathbb{G})|}{\frac{h}{f} + 1 + \frac{dh}{bf}},$$

4. If $f = 0$, then

$$|\mathbb{W}| = \frac{|\mathbb{V}(\mathbb{G})|}{\frac{b}{d}+1+\frac{c}{g}}, \quad |\mathbb{B}| = \frac{|\mathbb{V}(\mathbb{G})|}{\frac{d}{b}+1+\frac{cd}{bg}}, \quad |R| = \frac{|\mathbb{V}(\mathbb{G})|}{\frac{g}{c}+1+\frac{bg}{cd}}.$$

Theorem 11 Let

$$\mathbb{A} = \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}$$

be the parameter matrix of a cubic graph. The eigenvalues of $\mathbb{A}$ are given by:

$$\lambda_{\mathbb{A}_{1,2}} = \frac{\operatorname{tr}(\mathbb{A})-k}{2} \pm \sqrt{\left(\frac{\operatorname{tr}(\mathbb{A})-k}{2}\right)^2 - \frac{\det(\mathbb{A})}{k}}, \quad \lambda_{\mathbb{A}_3} = k.$$

Proof. Given the condition $g+h+i = d+e+f = a+b+c = k$, it is clear that k is one of the eigenvalues. Therefore, the determinant of matrix $\mathbb{A}$ can be expressed as $\det(\mathbb{A}) = k\lambda_{\mathbb{A}_1}\lambda_{\mathbb{A}_2}$. Using the relationship $\lambda_{\mathbb{A}_2} = \operatorname{tr}(\mathbb{A}) - \lambda_{\mathbb{A}_1} - k$, we can write:

$$\det(\mathbb{A}) = k\lambda_{\mathbb{A}_1}(\operatorname{tr}(\mathbb{A}) - \lambda_{\mathbb{A}_1} - k) = -k\lambda_{\mathbb{A}_1}^2 + k(\operatorname{tr}(\mathbb{A})-k)\lambda_{\mathbb{A}_1}.$$

By solving the quadratic equation $\lambda^2 + (k - \operatorname{tr}(\mathbb{A}))\lambda + \frac{\det(\mathbb{A})}{k} = 0$, we obtain:

$$\lambda_{\mathbb{A}_{1,2}} = \frac{\operatorname{tr}(\mathbb{A})-k}{2} \pm \sqrt{\left(\frac{\operatorname{tr}(\mathbb{A})-k}{2}\right)^2 - \frac{\det(\mathbb{A})}{k}},$$

as derived above. □

Theorem 12 None of the graphs corresponding to irreducible fullerenes possess a perfect 3-coloring.

Proof. According to Theorem 4, the only possible parameter matrices are those listed in the following table. □

Table 1. Parameter matrices

graphs	$\mathbb{A}_1$	$\mathbb{A}_3$	$\mathbb{A}_4$	$\mathbb{A}_5$	$\mathbb{A}_6$	$\mathbb{A}_8$	$\mathbb{A}_{10}$	$\mathbb{A}_{11}$	$\mathbb{A}_{12}$	$\mathbb{A}_{15}$	$\mathbb{A}_{16}$	$\mathbb{A}_{18}$
$\mathbb{C}_{20}$	√	√	√	√	√	√	√	√	√	√	√	√
$\mathbb{C}_{28}$	×	√	√	√	√	×	√	×	√	√	×	√
$\mathbb{C}_{30}$	×	√	√	√	√	×	√	×	√	√	×	√

Based on Theorem 4, we demonstrate that none of the parameter matrices presented in Table 1 are suitable as parameter matrices for a perfect 3-coloring. This is primarily because, in most instances, the number of vertices assigned to color $\mathbb{W}$ is not an integer. Additionally, for the graph $\mathbb{C}_{28}$ with the parameter matrix $\mathbb{A}_4$, although the number of vertices assigned to color $\mathbb{B}$ is an integer, this also prevents it from being a valid parameter matrix for a perfect 3-coloring.

4. Application of the graphs corresponding to irreducible fullerenes

The graphs corresponding to irreducible fullerenes are mathematical models representing carbon molecules that have a spherical structure and no adjacent pentagons. These graphs possess significant properties and have various applications in fields like chemistry, physics, and computer science. For example:

• Irreducible fullerene graphs can be used to study the stability, symmetry, and electronic properties of fullerene molecules.

• These graphs are crucial for the design of new materials and nanodevices, especially those involving carbon nanotubes.

• Irreducible fullerene graphs serve as a foundation for investigating the combinatorial and algorithmic aspects of planar graphs, such as enumeration, generation, coloring, and Hamiltonian cycles.

Several tools are available for generating fullerene structures. Buckygen, created by Brinkmann, McKay, and Goedgebeur, is a highly efficient program for generating all non-isomorphic fullerenes. It generates triangulations where all vertices have a degree of 5 or 6, or their dual representations as fullerene graphs. Buckygen is also capable of generating isolated pentagon rule (IPR) fullerenes. SaGe utilizes the Buckygen generator to create fullerene graphs. The algorithms used in Buckygen are discussed in references [9, 15]. Other programs designed for generating specific types of graphs include Plantri and Fullgen, both of which were also developed using Brinkmann and McKay, and are based on the research presented in papers [16–18]. GaGe [19] is an open-source software developed in C and Java, capable of generating a diverse array of graph types. It enables users to view selected graphs in different formats or save them in various file types. The House of Graphs offers collections of fullerene graphs, including those without a spiral starting at a pentagon and those without any spiral, all generated using Buckygen and Fullgen.

5. Concluding remarks

Fullerenes are polyhedral molecules made entirely of carbon atoms, available in various sizes and shapes. These structures were also represented as graphs, where the vertices corresponded to atoms and the edges indicated the bonds between them. A fullerene graph was defined as a 3-connected, 3-regular planar graph consisting solely of pentagonal and hexagonal faces. The low solubility of fullerenes in fluids limited their use as medicinal substances; however, their hydrophobicity, three-dimensional structure, and electronic properties made them still relevant for medical applications. For instance, the spherical shape of fullerene molecules allowed them to form and position within hydrophobic solutions of enzymes or cells, giving rise to interesting medicinal properties. Some characteristics and optical properties of fullerenes are discussed in [20]. This paper studied the perfect 2- and 3-coloring of fullerene graphs, focusing on irreducible fullerenes. The method involved first obtaining the adjacency matrix of the graphs, followed by comparing its eigenvalues with those of parameter matrices. If the eigenvalues of the parameter matrix were a subset of the graph's eigenvalues, they were retained for further examination in subsequent steps to determine their suitability for perfect coloring.

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Conflict of interest

The authors declare no competing financial interest.

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