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Exact square coloring of subcubic planar graphs *

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Abstract

We study the exact square chromatic number of subcubic planar graphs. An exact square coloring of a graph G is a vertex-coloring in which any two vertices at distance exactly 2 receive distinct colors. The smallest number of colors used in such a coloring of G is its exact square chromatic number, denoted $\chi^{[\sharp^2]}(G)$. This notion is related to other types of distance-based colorings, as well as to injective coloring. Indeed, for triangle-free graphs, exact square coloring and injective coloring coincide. We prove tight bounds on special subclasses of planar graphs: subcubic bipartite planar graphs and subcubic K_4 -minor-free graphs have exact square chromatic number at most 4. We then turn our attention to the class of fullerene graphs, which are cubic planar graphs with face sizes 5 and 6. We characterize fullerene graphs with exact square chromatic number 3. Furthermore, supporting a conjecture of Chen, Hahn, Raspaud and Wang (that all subcubic planar graphs are injectively 5-colorable) we prove that any induced subgraph of a fullerene graph has exact square chromatic number at most 5. This is done by first proving that a minimum counterexample has to be on at most 80 vertices and then computationally verifying the claim for all such graphs.

1 Introduction

In this paper, we study exact distance coloring problems for graphs. The celebrated Hadwiger-Nelson problem asking for the "chromatic number of the plane" falls into this category of problems: there, one wishes to assign a color to each point of the Euclidean plane, such that two points at distance exactly 1 receive distinct colors. A recent breakthrough result on this problem, showing that at least five colors are necessary, appeared in [22] (it is long known that seven colors suffice [24]). Similar problems are studied for other metric spaces, see [30]. In the graph setting, for a positive integer p, an exact p-distance coloring of a graph G is an assignment of colors to the vertices of G, such that two vertices at distance exactly p receive distinct colors [37, Section 11.9]. The exact p-distance chromatic number of G, denoted $\chi^{[\sharp p]}(G)$, is the smallest number of colors in an exact p-distance coloring of G and the study of this parameter is gaining growing attention, see [8, 28, 30, 40]. Denote $G^{[\sharp p]}$, the exact distance-p-power of G, which is a graph obtained by taking vertices of G and adding an edge between any two distinct vertices at distance exactly p.

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We have $\chi^{[\sharp p]}(G) = \chi(G^{[\sharp p]})$. Thus, for p = 1 this notion coincides with the usual chromatic number. Similarly denote $\omega^{[\sharp p]}(G)$ and $\alpha^{[\sharp p]}(G)$, respectively the maximum clique and the maximum independent set in $G^{[\sharp p]}$, that is $\omega^{[\sharp p]}(G) = \omega(G^{[\sharp p]})$ and $\alpha^{[\sharp p]}(G) = \alpha(G^{[\sharp p]})$.

Exact distance p-powers of graphs were first studied by Simić [42], see also [4, 9] for more recent works. Exact p-distance colorings have first been studied for graphs of bounded expansion. For a fixed graph class C of bounded expansion (for example, the class of planar graphs), the exact p-distance chromatic number is bounded by an absolute constant for graphs in C when p is odd [28, 37], and by a linear function of the maximum degree when p is even [28]. Exact p-distance colorings have been studied in specific graph classes: trees [8], graphs of bounded tree-width [28], chordal graphs [40], graphs of bounded genus [28, 40].

Distance-based colorings of graphs have been extensively studied since the first papers on the subject were published in the 1960s by Kramer and Kramer [32, 33]. In their setting, for a positive integer p, a p-distance coloring of a graph G is an assignment of colors to the vertices of G, such that two vertices at distance at most p receive distinct colors. The smallest possible number of colors of such a coloring is denoted by $\chi^p(G)$ (see [1, 27, 43, 44] for some important results). The problem of 2-distance coloring subcubic and cubic planar graphs is already far from trivial, and the focus of many research works: see [7, 20, 26, 27, 43]. Notably, a special case of a conjecture by Wegner [44], recently solved in [43], states that $\chi^2(G) \leq 7$ for every subcubic planar graph G.

The goal of the present paper is to study exact p-distance colorings with a focus on the special case p=2 and for subclasses of planar graphs. Given a graph G, the graph $G^{[\sharp 2]}$ is called the exact square of G. Similarly, an exact 2-distance coloring of G is called an exact square coloring of G, and $\chi^{[\sharp 2]}(G)$ is the exact square chromatic number of G.

What makes the study of exact distance coloring rather more difficult, is that $\chi^{[\sharp p]}$ is not necessarily monotone with respect to taking subgraphs. Indeed K_n is exact p-distance 1-colorable for every $p \geq 2$. However, if restricted to exact square coloring (p=2), then $\chi^{[\sharp 2]}$ is monotone with respect to taking induced subgraphs. On the other hand, the parameter $\chi^{[\sharp 2]}$ is unbounded even for trees, indeed for the star $K_{1,t}$ with t leaves, $(K_{1,t})^{[\sharp 2]}$ is isomorphic to the disjoint union of the complete graphs K_t and K_1 , and hence $\chi^{[\sharp 2]}(K_{1,t}) = t$. Thus, it is natural to restrict the study of exact square colorings to graphs with no induced $K_{1,t}$. For triangle-free graphs, this turns out to be the same as bounding the maximum degree. Thus, the class of subcubic graphs will be a focus of this study.

A related notion is the one of *injective coloring*, introduced in [25] and well-studied since then, see for example [10, 15, 35]. An injective coloring of a graph G is a vertex-coloring where any two vertices receive distinct colors whenever they are joined by a path of length 2. The smallest number of colors of an injective coloring of G is its *injective chromatic number*, denoted $\chi_i(G)$.

From these definitions, we have for any graph G:

$$\chi^{[\sharp 2]}(G) \le \chi_i(G) \le \chi^2(G).$$

Moreover, whenever G is triangle-free, we have $\chi^{[\sharp 2]}(G) = \chi_i(G)$, since in G, vertices joined by a path of length 2 must also be at distance 2. Since many of our results are for triangle-free graphs, they can be re-interepreted as results on injective colorings. For a subcubic graph G, the maximum degree of $G^{[\sharp 2]}$ is at most 6 and thus $\chi^{[\sharp 2]}(G) \leq 7$. In fact, the bound $\chi_i(G) \leq 7$ is also true [25]. Equality in the latter is shown to hold if and only if G is the Heawood graph [15, 25], and using the arguments of [15, 25], the same holds for the exact square chromatic number. Thus, for every subcubic planar graph G, we have $\chi_i(G) \leq 6$. A stronger bound was conjectured as follows.

Conjecture 1 ([15]). If G is a subcubic planar graph, then $\chi_i(G) \leq 5$.

Note that there is a subcubic planar graph G (with triangles) satisfying $\chi_i(G) = 5$ [15], so if true, the conjectured bound would be tight. However, we do not know of any subcubic planar

graph with exact square chromatic number 5. Conjecture 1 was generalized to arbitrary values of the maximum degree [15, 34], in the spirit of a well-studied conjecture by Wegner [44] on the (non-exact) square chromatic number. Conjecture 1 was proved for K_4 -minor-free graphs [15] (and it follows from [6] that $\chi^{[\sharp 2]}(G) \leq 5$ for any K_4 -minor-free graph G). Furthermore, the bound was improved to four colors for outerplanar subcubic graphs [36]. If G is a subcubic graph with girth at least 19 (resp. 10) then $\chi_i(G) \leq 3$ (resp. $\chi_i(G) \leq 4$) [35]. If G has girth at least 6, then $\chi_i(G) \leq 5$ [10]. Similar (but larger) bounds are known for $\chi^2(G)$, see [7, 20].

Exact square colorings also appear in another, more general, context: the one of L(p,q)-labelings. Given two non-negative integers p and q, an L(p,q)-labeling of a graph G is an assignment ℓ of non-negative integers to the vertices of G, such that for any two vertices u and v, we have $|\ell(u)-\ell(v)| \geq p$ if u and v are adjacent, and $|\ell(u)-\ell(v)| \geq q$ if they are at distance 2. The first (and most) studied case is when p=2 and q=1 [23]; see the survey [14]. Thus, for any graph G, there is a 1-to-1 correspondence between: (a) L(1,0)-labelings and classic vertex-colorings of G, (b) L(1,1)-labelings and (non-exact) square colorings of G, and (c) L(0,1)-labelings and exact square colorings of G. However, it seems that L(0,1)-labelings are rarely studied, see [6, 14] for a few references.

We first prove some results for specific classes of subcubic planar graphs in Section 2, filling some gaps from the literature. Let G be a subcubic graph. We show that $\chi^{[\sharp 2]}(G) \leq 4$ if G is K_4 -minor-free. We also show that if G is planar and bipartite, then its exact square is planar, thus $\chi_i(G) = \chi^{[\sharp 2]}(G) \leq 4$. Moreover these bounds are tight: there exist bipartite subcubic K_4 -minor-free graphs with exact square chromatic number 4. In passing we also show that the exact square of every subcubic bipartite outerplanar graph G is outerplanar, thus $\chi_i(G) = \chi^{[\sharp 2]}(G) \leq 3$. This is tight since for every tree T with a vertex of degree 3, $\chi^{[\sharp 2]}(T) \geq 3$.

The main focus of our paper (Section 3) is on fullerene graphs, which are cubic planar graphs where every face has length 5 or 6. They form an important and interesting class of cubic graphs, whose definition arises from chemistry: indeed they correspond to the structure of fullerene molecules. Their graph-theoretic properties are well-studied, in particular, in relation with colorings. See the survey [3]. For instance since it is known that fullerene graphs have girth 5, any exact square coloring of a fullerene graph is also an injective coloring, and so our results for this class apply to both settings. We first characterize in Section 3.1 those fullerene graphs with exact square chromatic number 3. It turns out that these fullerene graphs are a special class of so-called (6,0)-nanotubes [2, 29] which we call drums. Then, in Section 3.2, we prove Conjecture 1 for fullerene graphs. The proof is computer-assisted: we first consider a potential minimum counterexample, and prove that it cannot have more than 80 vertices. We then use a computer program to check the list of fullerene graphs of order up to 80, which is available online and certified complete [11, 12, 21].

We conclude in Section 4.

2 Generalities

We now recall some facts from the literature and prove a few new results.

2.1 Preliminaries

Given a vertex v, we denote by d(v) the degree of v and we say that v is a k-vertex if d(v) = k. For a planar graph with a given planar embedding, we call a k-face a face of length k.

A thread in a graph G is a path all of whose internal vertices are 2-vertices. We will use the following lemma.

Lemma 2 ([38]). Any planar graph G of girth at least 5d+1 ($d \ge 1$) contains a vertex of degree 1 or a thread with at least d internal vertices.

Observation 3. For any graph G, $G^{[\sharp 2]}$ is a subgraph of \overline{G} (the complement of G). If G has diameter 2, then $G^{[\sharp 2]}$ is isomorphic to \overline{G} .

The two following results were formulated in the context of injective coloring [15, 25], but the same arguments hold for exact squares.

Theorem 4 ([15, 25]). If G is a connected graph of maximum degree $\Delta = k + 1$, then $\omega^{[\sharp 2]}(G) \leq k^2 + k + 1$. Moreover, equality may only happen if G is the incidence graph of a projective geometry of order k, in which case $G^{[\sharp 2]}$ is isomorphic to two copies of K_{k^2+k+1} .

Using Brook's theorem, the following can be deduced for the special case k=2.

Corollary 5 ([15]). Let G be a connected subcubic graph. Then, $\chi^{[\sharp 2]}(G) \leq 6$, unless G is the Heawood graph (in which case $G^{[\sharp 2]}$ is isomorphic to two disjoint copies of K_7).

It is not difficult to find general subcubic graphs whose exact square contains a 5-clique (e.g. the Petersen graph¹) or a 6-clique (e.g. the triplex graph, a cubic graph of girth 5 and order 12, depicted in Figure 1a).

Another interesting graph G with $\chi^{[\sharp 2]}(G) = 6$ is the subcubic bipartite graph of order 22 built in a similar fashion as the Heawood graph, see Figure 1c. This graph is also the incidence graph of the 11_3 geometric configuration number 31 described in [39]. Each connected component of its exact square is isomorphic to the (non-exact) 3-distance power of the 11-cycle C_{11} . It has maximum degree 6, clique number 4, chromatic number 6 and is thus an extremal example for Reed's conjecture stating that $\chi(G) \leq \left\lceil \frac{\omega(G) + \Delta(G) + 1}{2} \right\rceil$, for every graph G [41].

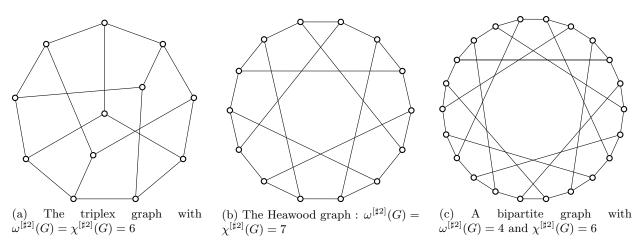


Figure 1: Some extremal examples of cubic graphs having high exact square chromatic number.

The following lemma is interesting to observe.

Lemma 6. Let G be a subcubic planar graph and let I be an independent set of G. Then, $G^{[\sharp 2]}[I]$ is planar.

Proof. Let G' be the graph build on I as follows: for each vertex $x \in V(G) \setminus I$, delete x and join all its neighbors in I. Observe that, as x has at most three neighbors in G, and by considering

If G has diameter 2, then $G^{[\sharp^2]}$ is isomorphic to \overline{G} and if G has girth 5, then $\alpha(G^{[\sharp^2]}) = 2$.

a plane embedding of G, the new graph G' is planar. However this graph may have multiedges (when two vertices of I are in a 4-cycle). By removing all but one edge from any group of parallel edges we get $G^{[\sharp 2]}[I]$.

We deduce the following from Lemma 6.

Proposition 7. For any subcubic planar graph G, we have $\omega^{[\sharp 2]}(G) \leq 4$.

Proof. Let K be a clique in $G^{[\sharp 2]}$. In G, K is an independent set. Thus, by Lemma 6, $G^{[\sharp 2]}[K]$ is a planar complete graph, which implies that $|K| \leq 4$, as desired.

The bound of Proposition 7 is sharp, as we see next.

Proposition 8. There exist bipartite subcubic K_4 -minor-free graphs G of girth 6 with $\omega^{[\sharp 2]}(G) = 4$.

Proof. Consider the graph G consisting of two vertices connected with three vertex-disjoint paths of length 3. Then $G^{[\sharp 2]}$ contains two disjoint copies of K_4 .

2.2 Bipartite planar graphs

We deduce the following from Lemma 6.

Theorem 9. Let G be a connected bipartite planar subcubic graph. Then, $G^{[\sharp^2]}$ consists of two planar connected components, each induced by one part of the bipartition of G. Moreover, if G is outerplanar, then these two components are outerplanar.

Proof. The first part of the statement directly follows from Lemma 6.

For the second part, suppose that G is outerplanar with bipartition (X, Y). Recall that $G^{[\sharp 2]}$ consists of two connected components: the one induced by X and the one induced by Y. It suffices to prove that each biconnected component of $G^{[\sharp 2]}$ is outerplanar.

If G has a bridge, then the two vertices of this bridge are cut-vertices in $G^{[\sharp 2]}$. Since they belong to two different connected components of $G^{[\sharp 2]}$, each component contains a cut-vertex. Since we consider biconnected components of $G^{[\sharp 2]}$, we may assume in the following that G has no bridge.

Since G is cubic, we conclude that G is biconnected. Consider an outerplanar embedding of G and let G be the facial cycle of this embedding. Consider any part of the bipartition of G, say X, ordered in the same way as in G; it suffices to show that $G^{[\sharp 2]}[X]$ is outerplanar. In $G^{[\sharp 2]}$, the order of X induced by G also induces a cycle G_X . We claim that the natural embedding of G_X induces an outerplanar embedding of $G^{[\sharp 2]}[X]$. Indeed, the only edges of $G^{[\sharp 2]}[X]$ not in G_X are created along edges that are chords of G in G. Let G be such a chord, and assume that G in the component of G in G of G and G in G in the edges G in the edges G in the edges G in the edges G in the coordinates of the vertices stay the same. The edges of G follow the embedding of G in the edge G in the edges of G in the edge G in the

Clearly, Theorem 9 implies that the square of bipartite subcubic outerplanar graphs can be colored with four colors (by using the Four Color Theorem).

2.3 K_4 -minor-free graphs

A nested ear decomposition of a graph G is a partition of E(G) into paths E_1, \ldots, E_k of G (the ears), such that the following conditions hold.

- (i) For every ear E_i , only the two end-vertices might be the same (thus E_i induces a path or a cycle).
- (ii) For every ear E_i with i > 1, there is an ear E_j with j < i such that the two endpoints of E_i belong to E_j (we say that E_i is nested in E_j , and the sub-path of E_j between the two endpoints of E_i is the nest interval of E_i).
- (iii) Apart from the endpoints of E_i , for every j < i, no other vertex of E_i belongs to E_j .
- (iv) If two ears E_i and $E_{i'}$ are both nested in E_j , then their nest intervals are either disjoint or one is contained in the other.

This concept was defined in [19]. It is known that in any K_4 -minor-free graph, every biconnected component has a nested ear decomposition. Indeed, a graph is K_4 -minor-free if and only if every biconnected component is two-terminal series-parallel [5], and every biconnected two-terminal series-parallel graph has a nested ear decomposition [19].

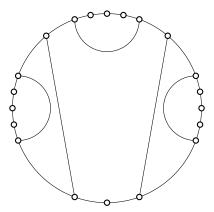


Figure 2: An outerplanar graph with $\Delta = 3$ and $\chi^{[\sharp 2]}(G) = 4$ [36].

Theorem 10. If G is a subcubic K_4 -minor-free graph, then $\chi^{[\sharp 2]}(G) \leq 4$. Furthermore, this bound is tight on subcubic bipartite K_4 -minor free graphs of girth at least 6, and on outerplanar graphs.

Proof. Let G be a minimum counterexample, that is, G is subcubic and K_4 -minor-free, $\chi^{[\sharp 2]}(G) > 4$ and the exact square of every smaller subcubic K_4 -minor-free graph is 4-colorable.

Claim 10.A. G is 2-connected.

Proof of claim. Suppose that G has a cut-vertex v. Since G is subcubic, then it has a bridge xy. The case where one of the two vertices (say x) has degree 1 is easy, since any exact square 4-coloring of G - x would extend to G.

So assume that both x and y are vertices of degree at least 2. We remove the edge xy from G: this creates two components. We add a degree 1 neighbor y' to x and a degree 1 neighbor x' to y. Let G_x and G_y be the components containing x and y, respectively. Now, let ϕ be a k-coloring of $G_x^{[\sharp 2]}$ and $G_y^{[\sharp 2]}$.

Suppose first that we have $\phi(x) = \phi(y')$ and $\phi(x') = \phi(y)$. Then, we interchange the colors $\phi(x)$ and $\phi(y)$ in G_y . This new coloring induces a valid k-coloring of $G^{[\sharp 2]}$.

Similarly, if $\phi(x) \neq \phi(y')$ and $\phi(x') \neq \phi(y)$, we permute the colors of vertices of G_y so that $\phi(x) = \phi(x')$ and $\phi(y) = \phi(y')$. Again this yields a valid k-coloring of $G^{[\sharp 2]}$.

Finally, suppose that $\phi(x) = \phi(y')$ but $\phi(x') \neq \phi(y)$ (the symmetric case is handled similarly). Since $k \geq 4$, there is one free color c_f among the neighbors of x (in G). We now permute the colors in G_y such that $\phi(x') = \phi(x)$ and $\phi(y) = c_f$. Again this yields a valid k-coloring of $G^{[\sharp 2]}$.

Claim 10.B. G contains no 2-vertex lying on a k-cycle, with $k \in \{3, 4\}$.

Proof of claim. Suppose v is a 2-vertex in G lying on a k-cycle $(k \in \{3,4\})$ and consider G' = G - v. Then $\chi^{[\sharp 2]}(G') \leq 4$ by minimality of G. Now, since v is part of a k-cycle in G, it is easy to see that the distance in G' between any pair of vertices x, y is the same as their distance in G. Thus an exact square coloring of G' is valid in G. Since G is subcubic and v is lying on k-cycle, we conclude that v has degree at most 3 in $G^{[\sharp 2]}$. Therefore v can be colored and we are done.

Claim 10.C. G contains no pair of adjacent 2-vertices.

Proof of claim. The proof is similar to the one of the previous claim. Suppose u, v are two adjacent 2-vertices in G and consider $G' = G - \{u, v\}$. Then $\chi^{[\sharp 2]}(G') \leq 4$ by minimality of G. It is easy to see that if the exact distance between two vertices of V(G') in G is 2, then this distance is preserved in G'. Thus an exact square coloring of G' is valid in G and since u, v have degree at most 3 in $G^{[\sharp 2]}$, we are done.

By Claim 10.A, G is 2-connected. Thus, as seen above, G has a nested ear decomposition E_1, \ldots, E_k . Moreover, by Claim 10.C, G has no pair of adjacent 2-vertices. Thus, there must be at least two ears in the decomposition. Consider the last ear E_k , and let E_i be the ear such that E_k is nested in E_i . Moreover, among all ears nested in E_i , let E_j be an ear whose nest interval does not contain any other nest interval. Again by Claim 10.C, the length of E_j is at most 2. But then the vertices of E_j , together with the vertices of E_i that belong to the nest interval of E_j , form either a triangle or a 4-cycle, one of whose vertices has degree 2. By Claim 10.B this contradicts the minimality of G.

For the tightness of the bound, in Proposition 8 we have presented a bipartite K_4 -minor-free graph of girth 6 whose exact square is the disjoint union of two K_4 's. For the class of outerplanar graphs we have the example of Figure 2, given in [36] in the context of injective coloring of outerplanar graphs.

3 Fullerene graphs

We now turn our attention to a special class of cubic planar graphs, namely fullerene graphs. They are the skeletons of cubic 3-dimensional convex polyhedra, each of whose faces is either a pentagon or a hexagon. As the skeleton of a convex polyhedron, a fullerene graph must be 3-connected and most authors consider this condition as part of the definition. However, we rather define a fullerene graph as a "cubic plane graph each of whose faces is of size either 5 or 6". The following can then be proved as an exercise.

Proposition 11 (Folklore). Every fullerene graph has girth 5 and is 3-connected.

As any 3-connected graph admits a unique plane embedding, we may refer to a fullerene graph as a planar graph rather than a plane graph. Further results on their structure were proved, and we give here a few of them which we will use in the proofs of this section. Recall that a graph G is cyclically k-edge-connected if any edge-cut separating two cycles of G has at least k edges. Došlić proved the following.

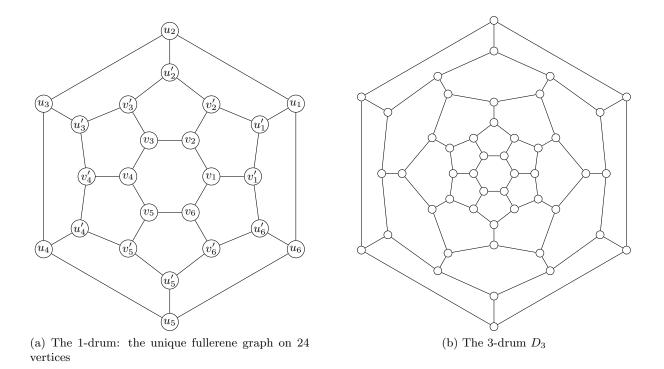


Figure 3: Examples of drums.

Theorem 12 ([18]). Every fullerene graph is cyclically 5-edge-connected.

Using this theorem, one can easily classify all possible small cycles of fullerene graphs. More precisley, we have the following (perhaps folklore) fact; we refer to [31, Lemma 4.1] for a proof.

Lemma 13. Given a fullerene graph G, every non-facial cycle of G is of length at least 9. Moreover, the only cycles of length 9, if any, are the cycles around a vertex incident with 5-faces only.

Note that $\chi^{[\sharp^2]}(G) \geq 3$ for any fullerene graph G. We first characterize those fullerene graphs whose exact square is 3-colorable. Then, we prove $\chi^{[\sharp^2]}(G) \leq 5$ for any fullerene graph G, thus proving Conjecture 1 for this class of graphs.

3.1 Characterizing exact square 3-colorable fullerene graphs

We first need to define a special class of fullerene graphs, that we call drums.

Definition 14. A drum is a fullerene graph with two specific 6-faces F and F', each of which is a neighbor with six 5-faces such that all these twelve 5-faces are distinct. A drum where F and F' are at facial distance k+1 is called a k-drum.

For an example, the 1-drum and 3-drum are depicted in Figure 3. In the literature, drums are known as a specific type of so-called nanotubes, more precisely, following the terminology from [2, 29], they are exactly one of the five types of (6,0)-nanotubes.

We will show next that there exists a unique k-drum up to isomorphism.

Proposition 15. Given a k-drum G, all faces at distance $\ell \leq k$ from F are of a same length.

Proof. We consider a planar embedding of G. Let v_1, v_2, \ldots, v_6 be the six vertices of F in the cyclic order of vertices, and let u_1, u_2, \ldots, u_6 be the six vertices of F' in the cyclic order of vertices, see Figure 3a for the labeling of the 1-drum.

Observe that, since G is cubic, each vertex v_i has a unique neighbor in $G \setminus F$, we call it v'_i . Similarly, each neighbor of u_i not in F' is called u'_i . Observe that each pair of edges $v_i v'_i$ and $v_{i+1}v'_{i+1}$ (addition in indices here and in the rest of the proof are taken modulo 6) is a pair of parallel edges of a 5-cycle.

To prove the claim of the proposition, for $\ell=1$, by the definition, all faces at distance 1 from F are 5-faces. For $\ell=2$ we show that if one of the faces is a 5-face, then they are all 5-faces. So assume a face f at distance 2 from F is a 5-face. Then, as there are only twelve 5-faces, f must be incident to F' and since the 5-faces incident to F' are distinct from those of F, the vertices of f furthest away from F form an edge of F'. Thus, we may label the vertices of f, without loss of generality, $u_1u_1'v_2'u_2'u_2$. But then, the two faces incident to u_1u_1' and u_2u_2' are 5-faces next to F'; by continuing this process, we conclude that all faces at distance 2 from F are the 5-faces incident to F'.

This completes the proof for $\ell=1,2$ with any value of k, which is exhaustive for $k\leq 2$. For the remaining cases, we apply induction on k. Assume that the claim is true for k and all values of ℓ , $\ell\leq k$. Consider a (k+1)-drum $(k\geq 2)$. Thus, all faces at distance 2 from F are 6-faces. In each of these 6-faces, one of the vertices is already labeled v_i' , noting that different faces correspond to different v_i' 's. Label x_i the common neighbor of v_i' and v_{i+1}' (see Figure 4). Thus, $x_{i-1}v_i'x_i$ form part of a 6-face. On this face, label the neighbor of x_i by y_i . Finally, label the common neighbor of y_i and y_{i-1} by z_i . Let G' be the graph obtained from G by deleting all the edges y_iz_{i+1} and then contracting edges z_iy_i and y_ix_i . We claim that G' is a (k-1)-drum where faces at distance ℓ from F in G are at distance $\ell-1$ from F in G'. This would complete the proof by induction. To see that G' is a fullerene graph, observe that from the construction it is 3-regular. Each face of G containing a path $z_iy_iz_{i+1}$ becomes a face of the same size on the path $x_iv_{i+1}'x_{i+1}$, and all other faces remain the same. Hence, we only have 5-faces and 6-faces in G', so we are done.

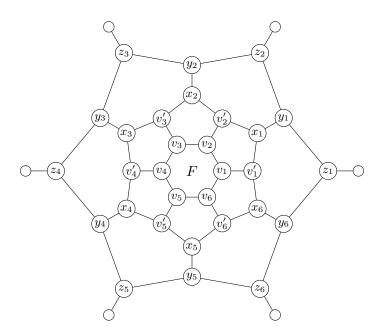


Figure 4: The neighborhood of face F in a drum.

Our goal in this section is to characterize drums as the only fullerene graphs which are exact square 3-colorable. To this end, in the next lemma, we present two planar subcubic graphs that are not exact square 3-colorable, thus they cannot be induced subgraphs of an exact square 3-colorable graph.

Lemma 16. Neither of the two graphs of Figure 5 admits an exact square 3-coloring.

Proof. We will repeatedly use the fact that in a proper 3-coloring of a K_4^- (that is, the complete graph on four vertices minus one edge), the nonadjacent vertices must receive a same color. Applying this observation to the exact square of the graphs of Figure 5, we conclude that in a hypothetical 3-coloring of each of them, vertices v_5 , t_2 , u_3 and w_4 must receive a same color (red in the figure). This is already a contradiction in the graph of Figure 5a, as vertices w_4 and v_5 are at distance 2.

To complete the proof for the graph of Figure 5b, observe that for the same reason, vertices u_1 , t_3 and v_4 must also get a same color, and this color must be distinct from red because u_3 and v_4 are at distance 2. We suppose this color to be green. Furthermore, vertices v_2 and t_6 are colored by the third color (blue), because each of them sees both other colors at distance 2. Moreover, since w_5 must receive the same color as t_6 , we conclude that w_5 must be colored blue.

Now, we know that v_1 sees both blue and green at distance 2, and thus it must be colored red. Repeating the K_4^- argument, we conclude that t_4 and then u_4 must be colored red as well. This is a contradiction, as u_4 is at distance 2 from the vertex v_5 , colored red.

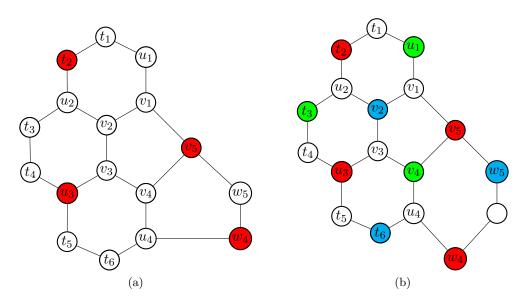


Figure 5: The forced precolorings from the proof of Lemma 16.

Similarly, we show in the next lemma, that the graph of Figure 6, while admitting an exact square 3-coloring, has limits on its possible 3-colorings.

Lemma 17. In an exact square 3-coloring of the graph G of Figure 6, vertices x and y must receive distinct colors.

Proof. By contradiction, suppose ϕ is an exact square 3-coloring of G with $\phi(x) = \phi(y) = 1$. Then, without loss of generality, we can assume that $\phi(v_1) = 2$ and $\phi(v_3) = 3$. Therefore, we have $\phi(v_5) = 2$. But then, $\phi(u_2) = 2$ because u_2 sees v_1 and v_2 at distance 2. Similarly, $\phi(u_4) = 2$. This is a contradiction since v_2 and v_2 see each other at distance 2.

Lemma 18. If G is a fullerene graph which is not the 1-drum and contains the graph of Figure 6 as a subgraph, then $\chi^{[\sharp 2]}(G) \geq 4$.

Proof. Let G be an exact square 3-colorable fullerene graph which contains the graph of Figure 6 as a subgraph. Moreover, let ϕ be its exact square 3-coloring. By Lemma 17 and without loss

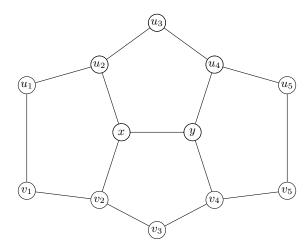


Figure 6: A 5-cycle surrounded by three consecutive 5-cycles.

of generality, we may assume that $\phi(x) = 1$ and $\phi(y) = 2$. Hence, $\phi(u_3) = \phi(v_3) = 3$ and $\{\phi(u_2), \phi(v_2)\} = \{1, 3\}$ and $\{\phi(u_4), \phi(v_4)\} = \{2, 3\}$. By the symmetry along the edge xy, we may assume that $\phi(u_2) = 3$, which then implies $\phi(v_2) = 1$, $\phi(u_4) = 2$ and $\phi(v_4) = 3$. Therefore, we have $\phi(u_1) = \phi(v_1) = 2$ and $\phi(u_5) = \phi(v_5) = 1$.

In summary, starting from the graph of Figure 6, with xy being the central edge, we concluded that the neighboring structure is forced. But we now have other isomorphic copies of the graph of Figure 6 inside G, for example one centered around u_1u_2 and another one centered around v_4v_5 . Thus, the same local neighborhood structures should exist around these edges. The 6-faces in these structures are already given (F and F'). Thus, we conclude that e', e, d, c' are lying on a 5-face. Similarly, a', a, b, b' are lying on a 5-face as well. This forces a graph where all but two vertices have degree 3, the other two vertices being of degree 2. To complete this to a 3-connected cubic graph, we then join these two vertices and obtain the 1-drum.

Lemma 19. The graph of Figure 7 does not admit an exact square 3-coloring.

Proof. To prove the lemma, we claim that in any possible exact square 3-coloring of this graph, vertices x and y must receive a same color. Considering the symmetry of edges xy and xz, the same argument then would apply to x and z. This would lead to a contradiction, since y and z cannot be colored the same.

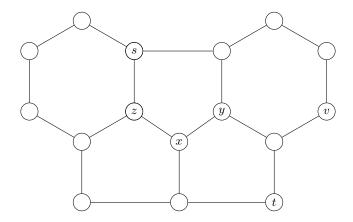


Figure 7: The graph of Lemma 19.

To prove the claim, assume ϕ is an exact square 3-coloring of the graph of Figure 7, and without loss of generality, assume that $\phi(y) = 1$, $\phi(u) = 2$ and $\phi(v) = 3$. Then, $\phi(s) = 3$ and $\phi(t) = 2$. This in turn implies $\phi(x) = 1$, which is the color of y.

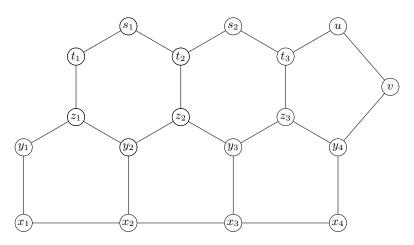


Figure 8: The graph of Lemma 20.

Lemma 20. The graph of Figure 8 does not admit an exact square 3-coloring.

Proof. By contradiction, suppose ϕ is a 3-coloring of the exact-square of this graph. We first claim that $\phi(x_2) = \phi(y_2)$. If not, then we may assume $\phi(x_2) = 1$ and $\phi(y_2) = 2$, then $\phi(y_1) = \phi(y_3) = 3$, which in turn implies that $\phi(t_1) = \phi(t_2) = 1$ but t_1 and t_2 are at distance 2. Note that this proof is based solely on the three faces around y_2 , so similarly, if a vertex has two 5-faces and one 6-face around it, then its color must be the same as the color of its neighbor on the 5-faces. Applying this to our graph we have: $\phi(x_3) = \phi(y_3)$, $\phi(z_3) = \phi(y_4)$.

Suppose $\phi(x_2) = \phi(y_2) = 2$, then as y_3 is at distance 2 from y_2 , and by the symmetry of other colors, we have $\phi(x_3) = \phi(y_3) = 3$, then $\phi(z_2) = 1$ and since z_3 is at distance 2 from both z_2 and x_3 we have $\phi(z_3) = \phi(y_4) = 2$. This in turn implies that $\phi(t_3) = 1$, but then t_2 sees all three colors at distance 2, that is y_2 for color 2, y_3 for color 3 and t_3 for color 1.

We can now state the main theorem of this section.

Theorem 21. A fullerene graph is exact square 3-colorable if and only if it is a k-drum, for a positive integer k.

Proof. First, we show that every drum is exact square 3-colorable. Given a k-drum, consider its 6-face F surrounded by six 5-faces. Color the vertices of F with 1, 2, 3, 1, 2, 3 in a clockwise orientation of F. Observe that, by Proposition 15, for $2 \le l \le k$, there are six faces of the same length at distance l from F. If we consider the subgraph G_l induced by faces at distance at most l from F, its outer face is a 12-cycle. The 3-coloring of F is then uniquely extended to a 3-coloring of G_l , where the 12 vertices of the outer face are colored consecutively 1, 2, 3 in the counterclockwise orientation with respect to F.

Similarly, if we start from the face F' of the k-drum, and color the vertices of F' with 1, 2, 3 in the counterclockwise orientation (of F'), then the coloring extends uniquely to any subgraph obtained by faces at distance at most k-l from F'. In such a coloring, vertices of the outer 12-face are colored consecutively 1, 2, 3 with clockwise orientation with respect to F'. As this orientation of the outer 12-face matches its counterclockwise orientation with respect to F, we can choose a proper rotation of colors on F', so that we can merge the colorings of both parts of the drum. Notice that, except the vertices of the 12-cycle, all the vertices of one part of the drum are at distance at least 3 from vertices of the other part.

It remains to show that if a fullerene graph admits an exact square 3-coloring, then it must be a drum. Let G be an exact square 3-colorable fullerene graph. By Lemma 16, a 5-face cannot have three consecutive 6-faces. By Lemmas 18 and 19, a vertex cannot be incident to three 5-faces. This leaves us with one possibility: each 5-face C is neighbor with two other 5-faces through two non-adjacent edges of C. Labelling the vertices of one of the 5-faces, in the cyclic order, x_2, y_2, z_2, y_3, x_3 , we may assume that each of the edges x_2y_2 and x_3y_3 is incident to another 5-face, thus so far we have the subgraph of Figure 8 induced by vertices x_i 's, y_i 's and z_i 's, for $1 \le i \le 3$. Using the labeling of this figure, the claim of Lemma 20 implies that the second 5-face neighbor of the face $x_3y_3z_3y_4x_4$ cannot be on the edge z_3y_4 , thus it must be on y_4x_4 . Completing this sequence of 5-faces, we conclude that vertices x_i form a face of G as they are already of full degree. This face then can only be a 6-face which is the face F of the drum. The face F' of drum is found the same way by considering the remaining 5-faces.

3.2 Fullerene graphs are exact square 5-colorable

To prove the main result of this section, we first give two lemmas on proper coloring of some graphs. Specifically, we show that the precoloring extension of two graphs (where vertices take colors from lists of given sizes) can always be done when the lists are subsets of $\{1, 2, 3, 4, 5\}$.

Lemma 22. Let abcdef be a 6-cycle and x be a vertex such that $N(x) = \{a, b, c, d, e, f\}$. Suppose these vertices have lists of available colors from the set $\{1, 2, 3, 4, 5\}$ satisfying the following: $|L(a)| \ge 2$, $|L(b)| \ge 2$, $|L(c)| \ge 2$, $|L(d)| \ge 2$, $|L(e)| \ge 2$, $|L(f)| \ge 3$ and |L(x)| = 5 (see Figure 9). Then there exists a proper L-coloring of this graph.

Proof. Assume to the contrary that there is no such coloring.

Suppose that $L(a) \cap L(c) \neq \emptyset$ and without loss of generality let $1 \in L(a) \cap L(c)$. We color $\phi(a) = \phi(c) = 1$. We then greedily color vertices b, d, e, f in this order by observing that at each step there is an available color for the current vertex. Now, if there is an available color from L(x) left for x, we are done. If not, then it is easy to see that b, d, e, f have each been colored with a distinct color from $\{2, 3, 4, 5\}$, say $\phi(b) = 2, \phi(d) = 3, \phi(e) = 4, \phi(f) = 5$ and $L(x) = \{1, 2, 3, 4, 5\}$. Moreover, observe that $L(b) = \{1, 2\}$, $L(d) = \{1, 3\}$, $L(e) = \{3, 4\}$ and $L(f) = \{1, 4, 5\}$, as otherwise one of these vertices could be recolored in order to gain a free color for vertex x. But then we uncolor all the vertices and give the following coloring procedure: assign color 1 to b, d and f, color vertices a, c, e independently, and finish by coloring vertex x. A contradiction.

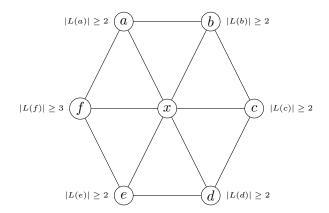


Figure 9: Graph of Lemma 22, where $L(x) = \{1, 2, 3, 4, 5\}$.

We conclude that $L(a) \cap L(c) = \emptyset$ and therefore, by symmetry we have $L(c) \cap L(e) = \emptyset$. Since the colors are taken from the set $\{1, 2, 3, 4, 5\}$, we conclude that $L(a) \cap L(e) \neq \emptyset$, and we fix without loss of generality $\phi(a) = \phi(e) = 1$. Then observe that $1 \in L(b)$, as otherwise we could color greedily the remaining vertices d, c, b, x, f in this order. Symmetrically, we have $1 \in L(d)$. Therefore, we uncolor vertices a, e and fix $\phi(b) = \phi(d) = 1$. Since $L(a) \cap L(c) = \emptyset$, we know that $1 \notin L(c)$. Thus we color greedily the remaining vertices in the following order: a, e, f, x, c. Note that at each step, there exists an available color for the current vertex.

Lemma 23. The graph of Figure 10 with the given lower bounds on the sizes of lists of colors from the set $\{1, 2, 3, 4, 5\}$ is L-colorable.

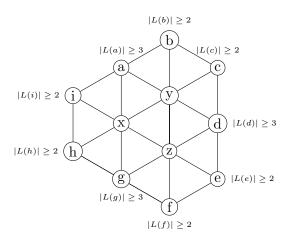


Figure 10: Graph of Lemma 23, where $L(x) = L(y) = L(z) = \{1, 2, 3, 4, 5\}.$

Proof. Let G be the graph from the statement of the lemma. We distinguish three cases:

- 1. Suppose $L(f) \cap L(d) \neq \emptyset$ and let $\alpha \in L(f) \cap L(d)$. Then we give the following partial coloring of G: we color both f and d with color α and then greedily color e, c, b, in this order (at each step, there is at least one available color with respect to L). Now the remaining uncolored vertices a, y, z, g, h, i, x form the configuration of Lemma 22, so we are done.
- 2. We have $L(f) \cap L(d) = \emptyset$. Now, suppose $L(f) \cap L(e) \neq \emptyset$. Then we color e with some color $\alpha \in L(f) \cap L(e)$ and thus we still have $|L(d)| \geq 3$. We then color greedily f, g, h, i, in this order. The remaining uncolored vertices z, x, a, b, c, d, y form the configuration of Lemma 22, so we are done.

3. We have $L(f) \cap L(d) = \emptyset$ and $L(f) \cap L(e) = \emptyset$. We claim that this case is impossible. Indeed, since the colors used by L are taken from the set $\{1,2,3,4,5\}$, without loss of generality we can assume that $L(f) = \{1,2\}$, $\{3,4\} \subseteq L(e)$ and $L(d) = \{3,4,5\}$. Moreover, by symmetry we have $L(g) \cap L(e) = \emptyset$ and thus $L(g) = \{1,2,5\}$. Therefore $|L(g) \cap L(d)| = 1$. Now note that vertex a is symmetric to vertex d and to vertex g and thus must satisfy $|L(a) \cap L(d)| = 1$ and $|L(a) \cap L(g)| = 1$, which is impossible since the colors are taken from a set of five elements.

Let \mathcal{C} be the class of induced subgraphs of fullerene graphs. In order to show that every fullerene graph is exact square 5-colorable, we will prove a stronger statement: that every graph in \mathcal{C} is exact square 5-colorable.

The main result of this section is the following theorem.

Theorem 24. Every graph $G \in \mathcal{C}$ is exact square 5-colorable.

Proof. Let G be a graph of C that is a minimum counterexample to our claim, that is, it is of smallest order among those that are not exact square 5-colorable. Let H be a fullerene graph that contains G as an induced subgraph. In the remainder of the proof, G will be a regarded as a plane graph whose embedding is induced by the unique embedding of H. By Lemma 13, we know that every 5-cycle or 6-cycle of G is a face of both G and G. Furthermore, G has no other cycle of length less than 9, and all cycles of length 9 are obtained from the symmetric differences of three 5-faces sharing a common vertex. Further properties of G are as follows.

Claim 24.A. G is 2-connected.

Proof of claim. Note that the proof could be done in the same lines as for Claim 10.A for exact square 4-colorability of K_4 -minor-free graphs. However, having five colors, we give a simpler proof here.

Suppose that G has a cut-vertex v. Since G is subcubic, it has a bridge uv. If one of u or v is of degree at most 2 (say, it is u), then an exact square 5-coloring of G' = G - u extends to G by using a proper permutation of colors in one of the connected components of G'.

Therefore, both u and v are 3-vertices and the graph G' = G - uv has exactly two connected components G_u and G_v , containing u and v respectively. Let u_1 and u_2 (resp. v_1 and v_2) be the neighbors of u (resp. v) in G_u (resp. G_v). By minimality of G, graphs G_u and G_v are exact square 5-colorable independently. Take such a coloring ϕ^1 of G_u and let $\phi^1(u_1) = 1$, $\phi^1(u_2) = 2$ and $\phi^1(u) = \alpha$. We show that an exact square 5-coloring ϕ^2 of G_v can be chosen to be compatible with ϕ^1 in G. Without loss of generality we can fix $\phi^2(v) = 3 \neq \alpha$. Then by applying a proper permutation of colors of ϕ^2 on G_v , one can choose $\phi^2(v_1)$ and $\phi^2(v_2)$ such that $\alpha \notin \{\phi^2(v_1), \phi^2(v_2)\}$ and we are done.

Claim 24.B. Any two 2-vertices of G are at distance at least 4.

Proof of claim. The configurations of Figure 11 are reducible. Indeed, if one of these configurations occurs, then we remove from G vertices y, v (resp. y, z, v and y, z, t, v) in the case of Configuration 11a (resp. 11b and 11c), in order to obtain a graph G'. The graph G' is in C and therefore has an exact square 5-coloring which can be easily extended to G.

Claim 24.C. G has no 9-face.

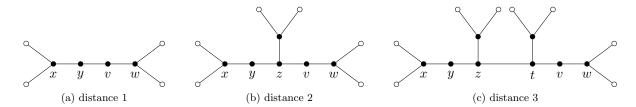


Figure 11: Configurations where two 2-vertices are at distance at most 3. The neighborhood of the black vertices is exactly the one depicted in the figure.

Proof of claim. By Lemma 13, every 9-face of G must contain three 2-vertices pairwise at distance at most 3, contradicting Claim 24.B.

For a face f of G, let $\ell(f)$ denote the length of f, and $n_2(f)$ the number of 2-vertices on the boundary of f.

Claim 24.D. For every face f of G, we have then $n_2(f) \leq \left| \frac{\ell(f)}{4} \right|$.

Proof of claim. This follows directly from Claim 24.B.

Claim 24.E. G is a fullerene graph.

Proof of claim. Let F(G) denote the set of faces of G in its planar embedding. By Euler's Formula we have the following:

$$\sum_{v \in V(G)} (2d(v) - 6) + \sum_{f \in F(G)} (\ell(f) - 6) = -12$$
 (1)

(□)

We assign to each vertex v the charge $\omega(v) = 2d(v) - 6$ and to each face f the charge $\omega(f) = \ell(f) - 6$. We redistribute the charges by applying the following rule: every face f gives 1 to each 2-vertex lying on its boundary.

Note that after this redistribution of charges, the initial sum of charges is preserved. We analyse the new amount of charges of vertices and faces of G:

- every 3-vertex has charge 0,
- every 2-vertex has charge 0 since by Claim 24.A it lies on two faces,
- every face f with $\ell(f) \geq 10$ has strictly positive charge by Claim 24.D,
- every face f with $\ell(f) = 6$ has charge 0 by Claim 24.D,
- every face f with $\ell(f) = 5$ has charge -1 by Claim 24.D.

Therefore, in order to obtain a total charge of -12 after the redistribution of charges, we conclude that G contains exactly twelve 5-faces and no other face of length at least 10. On the other hand, by definition of C, we know that G has no 7-faces, nor 8-faces. Also by Claim 24.C, G has no 9-faces. Thus we conclude that G is a fullerene graph.

Claim 24.F. Every 6-face of G is adjacent to at least one 5-face.

Proof of claim. Suppose to the contrary that G contains a 6-face adjacent to six 6-faces, as in Figure 12a. The graph $G_1 = G - \{a, b, c, ..., x\}$ belongs to C and is exact square 5-colorable. By applying such a coloring to G, we get a valid partial exact square coloring of G. Observe that the remaining uncolored vertices induce two isomorphic connected components in $G^{[\sharp 2]}$ (see Figure 12b). Thus, each can be (properly) colored independently. By counting the number of remaining colors for each of the vertices of each of these connected components we obtain the configuration of Lemma 23, so we are done.

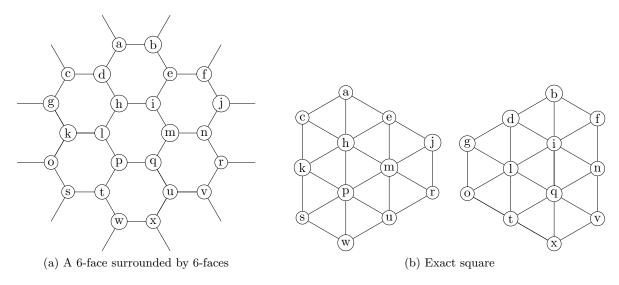


Figure 12: A 6-face surrounded only by 6-faces and its exact square.

Claim 24.G. Every 6-face of G is adjacent to at least two 5-faces.

Proof of claim. Suppose to the contrary that G contains a 6-face adjacent to at least five 6-faces. By Claim 24.F, this 6-face has exactly five adjacent 6-faces and one 5-face, as depicted in Figure 13a. The graph $G_1 = G - \{a, b, c, \ldots, q, s, \ldots, x\}$ belongs to C and is exact square 5-colorable. By applying such a coloring of G_1 to G, we get a valid partial exact square coloring. Observe that the remaining uncolored vertices induce in $G^{[\sharp 2]}$ the graph depicted in Figure 13b. After counting the number of available colors for each uncolored vertex, we properly color this graph using Lemma 22:

1. since $|L(v)| \geq 3$ and $|L(t)| \geq 3$, by the pigeonhole principle assign to v and t the same color,

 (\Box)

- 2. color vertices j, e, a, c in this order,
- 3. color vertices m, h, k, s, w, u, p by Lemma 22,
- 4. color vertices x, o, g in this order,
- 5. color vertices n, q, l, d, b, f, i by Lemma 22.

Thus, the claim is proved.

We can now deduce our last claim.

Claim 24.H. G has at most 80 vertices.

Proof of claim. Since there are exactly twelve 5-faces in G and each can be adjacent to at most five 6-faces, there are at most sixty 6-faces in G. By Claims 24.F and 24.G, every 6-face is adjacent to at least two 5-faces. Thus there can be at most thirty 6-faces in G. Since each vertex belongs to three faces, we conclude that G has at most $\frac{30\cdot6+12\cdot5}{3}=80$ vertices.

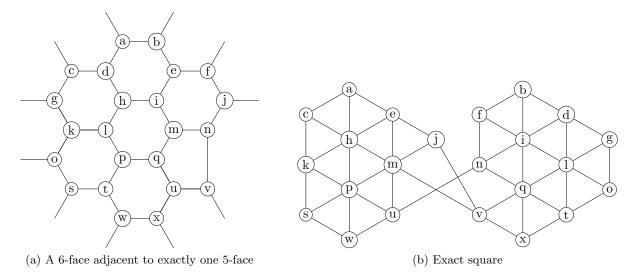


Figure 13: A 6-face surrounded only by one 5-face and its exact square.

To finish the proof, we have verified by computer using SageMath [45] that all fullerene graphs with up to 80 vertices are exact square 5-colorable (in fact they are exact square 4-colorable). Thus G does not exist, and our theorem is proved. The list of these fullerene graphs is available online² and was generated independently using the two computer programs fullgen [11] and buckygen [12, 21] (these two different programs use two different methods, and thus this list is trusted to be complete).

4 Conclusion

We have studied the notion of coloring of exact square on some families of subcubic graphs. This fits into a larger frame of studying the chromatic number of exact distance d-power of graphs, which has recently got attention. However, this special case is also closely related to the well studied notion of injective coloring. While in exact square coloring the pair of vertices of an edge are allowed to have a same color, in injective coloring this is only allowed for those edges that are not in a triangle.

A main question studied here is the maximum possible exact square chromatic number of the class of subcubic planar graphs. Conjecture 1 would imply that this is at most 5. There are examples of subcubic planar graphs which need five colors in any injective coloring, but all known such examples contain triangles and are exact square 4-colorable. These examples are built using K_4^- whose vertices must receive four different colors in an injective coloring, however the exact square of this graph has only one edge and can be colored by two colors only. Thus 4 is also a possible answer for our question.

It can be easily checked that a minimum counterexample to the conjecture has no triangle. Thus, as a natural class, we considered cubic planar graphs each of whose faces is either a 5-cycle or 6-cycle. These are are the duals of planar triangulations having only vertices with degree 5 or 6. Known as fullerene graphs they are well studied. For this class of graphs we characterized the ones admitting an exact square 3-coloring, and we proved that they all admit an exact square 5-coloring.

Further evidence that the upper bound of 5 might be replaced by 4 is the fact that the exact square of any bipartite subcubic planar graph is 4-colorable. Our proof of this fact uses the Four

²https://hog.grinvin.org/Fullerenes

Color Theorem. It would be interesting to give an independent proof. On the other hand, the example of an outerplanar subcubic graph whose exact square is 4-chromatic has a fair number of degree 2 vertices. This suggests that one might be able to build examples of subcubic planar graphs whose exact square is not 4-colorable.

We would like to ask if Theorem 10 can be strengthened by proving the same upper bound of 4 for the injective coloring of K_4 -minor-free graphs. The upper bound of 5 is proved in [15] and the upper bound of 4 on the class of triangle-free K_4 -minor-free graphs follows from Theorem 10.

Acknowledgements

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