A computer-assisted proof of a Barnette’s conjecture: Not only fullerene graphs are hamiltonian.

František Kardoš
LaBRI, University of Bordeaux, France
frantisek.kardos@labri.fr

September 9, 2014

Abstract

Fullerene graphs, i.e., 3-connected planar cubic graphs with pentagonal and hexagonal faces, are conjectured to be hamiltonian. This is a special case of a conjecture of Barnette, dating back to the 60s, stating that 3-connected planar graphs with faces of size at most 6 are hamiltonian. We prove the conjecture.

1 Introduction

Tait conjectured in 1880 that cubic polyhedral graphs (i.e., 3-connected planar cubic graphs) are hamiltonian. The first counterexample was found by Tutte in 1946; later many others were found, see Figure 1. Had the conjecture been true, it would have implied the Four-Color Theorem.

However, each known non-hamiltonian cubic polyhedral graph has at least one face of size 7 or more [1,10]. Barnette conjectured that all cubic polyhedral graphs with maximum face size at most 6 are hamiltonian. In particular, this conjecture covers the fullerene graphs, 3-connected cubic planar graphs with pentagonal and hexagonal faces only. It was verified for all fullerene graphs with up to 176 vertices [1]. On the other hand, cubic polyhedral graphs having only faces of sizes 3 and 6 or 4 and 6 are known to be hamiltonian [1,5].

Jendroľ and Owens proved that the longest cycle of a fullerene graph of size $n$ covers at least $4n/5$ vertices [6], the bound was later improved to $5n/6 - 2/3$ [7] and $6n/7 + 2/7$ [8]. Marušič [9] proved that the fullerene graph obtained from another fullerene graph with an odd number of faces by the so-called leapfrog operation (truncation; replacing each vertex by a hexagonal face) is hamiltonian. In fact, hamiltonian cycle in the derived graph corresponds to a decomposition of the original graph into an induced forest and a stable set.

In this paper we prove
Theorem 1 Let $G$ be a 3-connected planar cubic graph with faces of size at most 6. Then $G$ is hamiltonian.

The main idea of the proof is the following: First, we find a set of short cycles covering all the vertices of a graph (Section 3). Then, we use hexagonal faces to transform all the cycles into one long cycle (Section 5).

2 Preliminaries

A Barnette graph is a 3-connected planar cubic graph with faces of size at most 6, having no triangles and no two adjacent quadrangles.

We reduce Theorem 1 to the case of Barnette graphs:

Theorem 2 Let $G$ be a Barnette graph. Then $G$ is hamiltonian.

Lemma 1 Theorem 2 implies Theorem 1

Proof. Suppose Theorem 2 true. Let $G$ be a smallest counterexample to Theorem 1. Assume $f = v_1v_2v_3$ is a triangle in $G$. If one of the faces adjacent to $f$ is a triangle, then, by 3-connectivity, $G$ is (isomorphic to) $K_4$, a hamiltonian graph. Hence, all the three faces adjacent to $f$ are of size at least 4. Let $G_1$ be a graph obtained from $G$ by replacing $v_1v_2v_3$ by a single vertex $v$. It is easy to see that every hamiltonian cycle of $G_1$ can be extended to a hamiltonian cycle of $G$, see Figure 2 for illustration.

From this point on we may assume that $G$ contains no triangles. Let $f_1$ and $f_2$ be two adjacent faces of size 4 in $G$. Let $v_1$ and $v_2$ be the vertices they share; let $f_1 = v_1v_2u_3u_4$, let $f_2 = v_1v_2w_3w_4$. We denote by $f_3$ (resp. $f_4$) the face incident to $u_3$ and $w_3$ ($u_4$ and $w_4$, respectively). If both $f_3$ and $f_4$ are quadrangles, then $G$ is the graph of a cube, which is clearly hamiltonian. Suppose $d(f_4) \geq 5$, $d(f_3) = 4$. Let $G_2$ be a graph obtained from $G$ by collapsing the faces $f_1$, $f_2$, $f_3$ to a single vertex. Again, every hamiltonian cycle of $G_2$ can be extended to a hamiltonian cycle of $G$, see Figure 2.
Finally, suppose that both $f_3$ and $f_4$ are of size at most 5. We remove the vertices $v_1$ and $v_2$, identify $u_3$ with $w_3$ and $u_4$ with $w_4$; this way we obtain a graph $G_3$. It is easy to see that $G_3$ is a 3-connected cubic planar graph with all the faces of size at most 6. Moreover, every hamiltonian cycle of $G_3$ can be extended to a hamiltonian cycle of $G$, as seen on Figure 3.

Figure 3: A pair of adjacent quadrangles may be reduced to a single edge.

\[ \square \]

### 2.1 2-factors and resonant hexagons

In the paper we will use a modified definition of a 2-factor. We will call a **2-factor** any spanning subgraph $F$ of a Barnette graph $G$ such that each component of $F$ is a connected regular graph of degree 1 or 2 – an isolated edge or a cycle. We will treat the isolated edges of $F$ as 2-cycles; this way $F$ becomes a 2-regular multigraph.

A hexagonal face $f$ of a Barnette graph is **resonant** with respect to a given 2-factor $F$, if precisely three non-adjacent edges incident with $f$ are in $F$, moreover, the three edges belong to three different cycles.

Different examples of 2-factors of the same Barnette graph are depicted in Figures 15 and 25 where components of the factor are boundaries of grey regions; a hexagonal face is resonant if and only if it is white and has no label.

Let $C_f$ be the boundary cycle of a hexagon $f$ resonant with respect to a 2-factor $F$. Then $F' = F \Delta C_f$ is also a 2-factor of the same graph (for a 2-cycle incident to $f$ we keep a single edge). Note that the number of cycles in $F'$ is two less than in $F$, since the three cycles of $F$ incident to $f$ are transformed into a single cycle.

### 2.2 Patches and clusters

Let $G$ be a Barnette graph. Let $S(G)$ be the set of the *small* faces (faces of size 4 or 5) of $G$. It is straightforward to derive from the Euler’s formula that
Let \( f_4 \) and \( f_5 \) be the numbers of quadrangles and pentagons in \( G \), respectively.

A configuration of small faces in \( G \) is an equivalence class with respect to \( \sim \). Informally, all the configurations of \( G \) are singletons if and only if the small faces of \( G \) are far from each other.

A \textit{patch} is a 2-connected subgraph of a Barnette graph, having at most one face of size different from 4, 5, and 6, and such that all vertices of degree 2 are incident to this special face, often referred to as the outer face of the patch.

A \textit{k-disc} centered at a face \( f \) of a Barnette graph \( G \), denoted by \( B_k(f) \), is a patch composed of facial cycles of faces at (dual) distance at most \( k \) from the face \( f \).

A \textit{cluster} based at a small face \( f \) of a Barnette graph \( G \), denoted by \( C(f) \), is a patch that can be obtained as a union of 2-discs centered at the small faces from the configuration containing \( f \).

It is easy to see that small faces belonging to the same configuration always give the same cluster. Observe that different clusters need not be disjoint.

The graph depicted in Figure 4 has three configurations/clusters:

\[ \{ p_1, p_2, p_3, p_4 \}, \{ p_5, p_6, p_7, p_8, p_9 \}, \{ p_{10}, p_{11}, p_{12} \} \]

The rest of the paper consists of the proof of Theorem 2. Instead of finding a Hamilton cycle directly, we first find a 2-factor with lots of resonant hexagons (Section 3), then we modify the 2-factor in order to have an odd number of cycles if needed (Section 4), and finally we use the resonant hexagons to glue all the cycles into a single cycle (Section 5).

3 Finding a 2-factor of a Barnette graph

The goal of the first part is to find a 2-factor \( F \) of a given Barnette graph with the following properties:

- each 2-cycle of \( F \) is incident to two resonant hexagons;
- each other cycle of \( F \) is incident to at least 3 resonant hexagons;
- no cycle is inside another.
Figure 4: An example of a Barnette graph. Pentagonal faces are denoted $p_1, \ldots, p_{12}$.

If a Barnette graph is large enough, it contains vast areas with no small faces. Locally these parts resemble the hexagonal grid, therefore, one can cover them with sets of disjoint hexagons in the following way: The dual of the hexagonal grid is the 6-regular triangular grid, which has a canonical 3-coloring, which provides a canonical 3-coloring of the faces of the hexagonal grid. One can pick the 6-cycles corresponding to the faces of one color class as a set of cycles covering all the vertices of the grid (possibly except for some boundary vertices).

However, we want to cover all the vertices of the graph, including those incident to small faces. We proceed in three steps:

1. cut the graph in a way that all the pentagonal faces are destroyed;
2. use the 3-coloring argument for the resulting graph containing only even faces;
3. fix the irregularities along the path where the graph has been cut.

Let $G$ be a Barnette graph and $C_0$ be a configuration of $G$. Let $P^*$ be a path in the dual graph $G^*$ with the following properties:

- $P^*$ contains all the 5-vertices of $G^*$;
- if $f_1^*$ and $f_2^*$ belong to the same configuration, then all the 5-vertices on the subpath of $P^*$ between $f_1^*$ and $f_2^*$ belong to this configuration;
- the 5-vertices corresponding to pentagons of $C_0$ are the first 5-vertices of $P^*$;
- $P^*$ is the shortest path among all the paths with the first two properties.
Figure 5: The three grey-and-white colorings of the graph from Figure 4, corresponding to the given order of pentagons.

Clearly \( P^* \) starts and ends in a 5-vertex of \( G^* \). Moreover, \( P^* \) induces an order on the set of the configurations of \( G, C_0 \) being the first one. Observe that 4-vertices of \( G^* \) may, but do not have to be hit by \( P^* \).

The path \( P^* \) can always be decomposed into a sequence of \( \ell \leq 11 \) subpaths \( P^*_1, \ldots, P^*_\ell \) joining consecutive pairs of 5-vertices. Let us call these subpaths segments. Clearly, each segment is a shortest possible path joining two 5-vertices of \( G^* \).

We cut the graph \( G \) along \( P^* \). We replace the face corresponding to the first and the last vertex of \( P^* \) by a hexagon; we replace each face corresponding to the other vertices of \( P^* \) by two hexagons.

This way we obtain a patch \( G' \) with all the faces of even size except for the outer face, hence, there is a canonical face coloring using three colors, say 1, 2, 3 (we do not require a color for the outer face). We choose a color, say 1, and recolor grey all the faces of \( G' \) colored 1; we recolor white the faces of \( G' \) colored 2 and 3. (Later, we will inspect all the three choices of coloring.)

We transform this grey-and-white coloring of \( G' \) into a grey-and-white coloring of \( G \) in the following way: The faces corresponding to the first and the last vertex of \( P^* \) keep their color. A face corresponding to an inner vertex of \( P^* \) is colored grey if at least one of the corresponding hexagons in \( G' \) is grey; otherwise it is colored white, see Figure 5 for illustration.

For each segment \( P^*_i \), its neighborhood is a cubic planar graph with all faces of even size (hexagons and quadrangles), thus, locally, there is a canonical coloring of the cut faces using the colors \( A, B, C \). Along \( P^*_i \) two parts of the graph \( G' \) (together with two possibly different grey-white colorings) meet; let us call them the left and right subgraph (left and right coloring). If grey
corresponds to different color classes amongst $A$, $B$, and $C$ in the two subgraphs, we say that the segment $P_i$ is active; otherwise it is inactive. For example, the segment $p_6p_7$ is active in all the three colorings depicted in Figure 5, the segment $p_4p_5$ is active in all the three colorings, whereas the segment $p_9p_{10}$ is inactive in the first coloring and active in the other two.

Along an inactive segment, either the 3-colorings of the hexagonal grid coincide perfectly (and so it is inactive in all the three colorings), or the colors 2 and 3 are switched (and then it is active in the other two colorings). Along an active segment, either the color 1 is switched with another color (so that it is inactive in some other coloring), or the three colors are permuted in a cyclic manner (which corresponds to two switches; this segment is active in all the three colorings).

It is clear that we may disregard inactive segments, since in their neighborhood the cycles bounding the grey faces cover the vertices of $G$ perfectly.

In the following paragraphs we will analyse the coloring along active segments and inside the clusters of a Barnette graph.

### 3.1 Active segments

Let $P_i^*$ be an active segment, let grey correspond to $B$ in one subgraph and to $C$ in the other. Then only $A$-faces of $P_i^*$ are white, whereas $B$- and $C$-faces of $P_i^*$ are grey. We label $\times$ all $A$-faces adjacent to (at least one) pair of adjacent grey faces – since they are no more resonant. Clearly, for a hexagonal $A$-face labelled $\times$ there has to be exactly two pairs (not necessarily disjoint) of adjacent grey $B$- and $C$-faces. On the other hand, each such pair is adjacent to exactly two $A$-faces labelled $\times$. The dual path $P_i^*$ can thus be transformed into a sequence of $A$-faces labelled $\times$ joined by $B|C$-edges. We will call these sequences $\times$-paths.

If two $B|C$-edges incident with the same $A$-face labelled $\times$ form a 60° angle, we can shorten the $\times$-path by recoloring the ($B$ or $C$) face incident to both $B|C$-edges from grey back to white, and by removing the $\times$ label from the $A$-face, see Figure 6 right. This way we transform one long cycle into three shorter cycles, one of them a 2-cycle, and we re-introduce two new resonant hexagons.

The resulting structure in the neighborhood of $P_i^*$ is the following: All vertices are covered by cycles of length 6 (single faces), 10 (two hexagons sharing a $B|C$-edge in one direction), or 2 ($B|C$-edges in another direction incident to two resonant hexagons). A mixed primal-dual path (with alternating $B|C$-edges and $A$-faces labelled $\times$) separates the two subgraphs of regular coloring.

### 3.2 Trivial clusters

Let $p_i$ be a pentagonal face of $G$ such that the segments $P_{i-1}^*$ and $P_i^*$ meet at $p_i$. For both subgraphs that meet along $P_{i-1}^* \cap P_i^*$, the face corresponding to $p_i$ is either white or grey. Let $A$, $B$, $C$ be the three colors of the canonical coloring of the neighborhood of $P_{i-1}^*$ such that $p_i$ is colored $A$. Then for the neighborhood of $P_i^*$, if in one of the graphs we keep the same coloring, in the other one the
Figure 6: Two hexagonal patterns meeting along a cutting path $P_i^*$ (left). The sequence of $A$-faces labeled $\times$ is drawn with the double lines (middle); we always keep it as short as possible (right).

Figure 7: A pentagon always causes a single switch of colors – the two colors different from its color are switched.

roles of $B$ and $C$ are switched, see Figure 7 for illustration. Therefore, the following claim is indeed true:

Claim 1 Let $p_i$ be a pentagonal face of a Barnette graph $G$ incident with segments $P_{i-1}^*$ and $P_i^*$. Then

(i) both $P_{i-1}^*$ and $P_i^*$ are inactive if and only if $p_i$ is grey in both subgraphs;

(ii) both $P_{i-1}^*$ and $P_i^*$ are active if and only if $p_i$ is grey in one subgraph and white in the other;

(iii) either $P_{i-1}^*$ or $P_i^*$ is active if and only if $p_i$ is white in both subgraphs.

In the words of Figure 7 in the first case, for both subgraphs grey corresponds to $A$. In the second case, grey corresponds to $A$ in one of the subgraphs
Figure 8: All the possibilities (up to symmetry) of the situation in the neighborhood of a pentagonal face where one active paths starts.

Figure 9: Examples of the situation in the neighborhood of a pentagonal face where two active paths meet.

and to B or C in the other. In the third case, grey corresponds to B or C in both subgraphs – it makes precisely one of the segments inactive, since the colors are switched.

If \( P_i^* \) is active and \( P_{i-1}^* \) is not (or vice versa), the faces corresponding to \( p_i \) are white in both graphs, hence, \( p_i \) is the first A-face of the \( \times \)-path leading to \( p_{i+1} \) (or the last A-face of the \( \times \)-path coming from \( p_{i-1} \)), see Figure 8 for illustration. In this case, locally, all the vertices are covered by cycles of length 2, 6, or 10.

If both \( P_i \) and \( P_{i-1} \) are active, the \( \times \)-paths coming from \( p_{i-1} \) and leaving towards \( p_{i+1} \) are chained in a natural way, the pentagon \( p_i \) being part of one of the patterns, see Figure 9 for illustration. In the neighborhood of a pentagonal face, apart from cycles of length 2, 6, or 10, a cycle of length 9 (a pentagon and a hexagon merged) or 13 (a pentagon and two hexagons merged) can be formed.

### 3.2.1 Clusters with two pentagons

Let \( p_i \) and \( p_{i+1} \) be two pentagons at distance at most 2, and let \( P_{i-1}^* \), \( P_i^* \), and \( P_{i+1}^* \) be the corresponding segments. We denote \( C_{(1,0)} \) the cluster with pentagons adjacent, \( C_{(1,1)} \) the cluster where the pentagons share two adjacent hexagons, and \( C_{(2,0)} \) the cluster where the pentagons share only one adjacent
Figure 10: If no segment leaving a cluster with two pentagons is active, then both pentagons are of the same color: either they are both grey or they are both white and joined by a ×-path.

hexagon. We will discuss the number of active segments leaving the clusters.

Since each pentagon corresponds to a single switch of the three colors, the cluster itself corresponds to an even permutation of the colors – an identity or a single cycle of length 3. Therefore, both $P^*_i$ and $P^*_{i+1}$ can be inactive only if the cluster does not permute the colors. This can only happen if $p_i$ and $p_{i+1}$ have the same color, which is the case in $C_{(1,1)}$, see Figure 10 for illustration.

If $P^*_i$ is active and $P^*_{i+1}$ is not (or vice-versa), then the cluster permutes the colors, and so $p_i$ and $p_{i+1}$ are not of the same color. This is the case in $C_{(1,0)}$ and in $C_{(2,0)}$. The corresponding ×-path entering into the cluster either ends in $p_i$ (and then $P^*_i$ is inactive), or it misses $p_i$ and ends in $p_{i+1}$. In some of the cases, by permuting the order of $p_i$ and $p_{i+1}$, we may switch between these two cases, see Figure 11.

If both $P^*_i$ and $P^*_{i+1}$ are active, then either two different ×-paths start at $p_i$ and $p_{i+1}$ (and thus $P^*_i$ is inactive) or $P^*_i$ is active and a single ×-path goes around both pentagons. Again, for $C_{(1,0)}$ and for $C_{(2,0)}$, by changing the order of $p_i$ and $p_{i+1}$ sometimes we may switch between these two cases, see Figure 12.

For $C_{(1,1)}$, since the cluster itself does not permute the colors, we can always reroute the ×-path entering and leaving the cluster in such a way that it does not touch any pentagon, and thus consider the cluster as it did not have any active segments, see Figure 13 for illustration.

3.2.2 Clusters with more than two pentagons

Inside a cluster with more than two pentagons, for each pair of consecutive pentagons the ×-path behaves in the same way as in the clusters with two pentagons. However, applying the rules for active paths between the pentagons does not always lead directly to a 2-factor with desired properties, see Figure 14 for illustration. Nonetheless, a ×-path respecting the coloring of the pentagons can always be reconstituted. Using local modifications concerning pairs of pentagons (depicted in Figures 11(c-d), 12(c-d) and 13), which either change the
Figure 11: Examples of clusters with two pentagons with one active segment leaving. There is always one grey and one white pentagon. First line: pentagons adjacent, second line: pentagons at distance 2. The \( \times \)-path either ends at the closest pentagon (a) or at the furthest one (b); sometimes we may choose at which pentagon the \( \times \)-path would end (c) and (d).

Figure 12: Examples of clusters with two pentagons with two active segments leaving. First line: pentagons adjacent, second line: pentagons at distance 2. Either a \( \times \)-path starts at each pentagon (a) or a single \( \times \)-path cuts the cluster (b); sometimes we may switch between the two options (c-d).
Figure 13: In the cluster $C(1,1)$, we can always reroute the $\times$-path in a way to avoid the pentagons.

Figure 14: Even if the grey-and-white coloring (a) seems to yield a 2-factor having some cycles inside others (b), a $\times$-path respecting the coloring of the pentagons can always be reconstituted (c).

order of the pentagons inside a cluster, or put a pair of pentagons of the same color aside, the set of $\times$-paths can be simplified.

To check that the grey-and-white coloring of $G'$ may be extended to a coloring of $G$ with desired properties inside any possible cluster of a Barnette graph, we wrote a computer program.

To generate all the possible clusters of Barnette graphs containing at least one pentagon, we applied the procedure ADD described in Algorithm 1 to a patch $P_0$ consisting of a single pentagon. Initially, the database of clusters contains a single cluster $\nabla(P_0)$ — the 2-disc centered at a pentagon; the database of graphs is empty.

Having the clusters generated, we analysed them using a second program. The analysis of the clusters depends of their curvature.

For each cluster of curvature at most 5, we checked the following: For each possible position of two segments leaving the cluster and for every pair of colorings, there is always a way to extend the 2-factor from the boundary of the
Algorithm 1 Generation of clusters containing a given patch

1: procedure Add(patch P)
2: if δ(P) ≤ 3 then
3: complete the graph and add it to the database of graphs
4: else if P ≠ ∇(P) or (μ(P) ≥ 7 and δ(P) ≤ μ(P)) then
5: find the least convex face f₀ of the boundary of P
6: if f₀ is not adjacent to a 4-face then
7: P₄ ← P with f₀ ← 4-face
8: if ∇(P₄) is not in the database of clusters then
9: Add ∇(P₄) to the database
10: ADD(P₄)
11: P₅ ← P with f₀ ← 5-face
12: if ∇(P₅) is not in the database of clusters then
13: Add ∇(P₅) to the database
14: ADD(P₅)
15: P₆ ← P with f₀ ← 6-face
16: ADD(P₆)

cluster towards its inside. Depending on the choice of colorings, there can be 0, 1, or 2 active segments leaving the cluster.

If a Barnette graph contains a cluster C of curvature 6, then either all the other clusters have curvature at most 5, or there are exactly two clusters of curvature 6 (recall that the total curvature is 12). However, in both cases, for C we only need to check that for every possible position of one segment leaving the cluster and for each of the three possible colorings, there is always a way to extend the 2-factor from the boundary of the cluster towards its inside.

If a Barnette graph contains a cluster C of curvature at least 7, then it has exactly one such cluster. Moreover, the rest of the graph has bounded size, since adding a layer of hexagons to a patch with curvature bigger that 6 decreases its perimeter \[2\]. It means there is only a finite number of Barnette graphs containing C. We decided to generate these graphs and check their hamiltonicity directly if δ(C) ≤ μ(C) (this explains lines 2–4 of the algorithm). The largest graph to check this way has 202 vertices. The smallest Barnette graph that cannot be obtained this way has 28 vertices; it has two clusters with two 4-faces and two 5-faces each, separated by two layers of four 6-faces.

If μ(C) ≥ 7 and δ(C) > μ(C), we use the general procedure. Again, we only need to check one segment leaving the cluster.

In Table 1 we provide numbers of clusters analysed.

For some of the clusters containing vertices incident to three pentagons, it can happen that a pentagonal face is at the same time the first face of a ×-path and an internal face of another ×-path, similarly to what is depicted in Figure 24.

For the graph from Figure 4 the three colorings from Figure 5 lead to the 2-factors depicted in Figure 15.
Table 1: Numbers of clusters to analyse, given number of pentagons and quadrangles. Amongst the clusters of curvature greater than 6, only those with \(\delta(C) > \mu(C)\) are counted.

| \(f_4\) \(f_5\) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|-------------------|---|---|---|---|---|---|---|---|---|
| 0                 | 1 | 3 | 11| 67| 408|3015|18360|24521|980|
| 1                 | 3 | 22|167|1408|6452|5229|609 |
| 2                 | 16| 183|401|218 |54  |

Figure 15: Three different 2-factors corresponding to the three grey-and-white colorings from Figure 5.
4 Changing the parity of the number of cycles

We want to use resonant hexagons to glue the cycles of a 2-factor. Since at each step three different cycles are glued into a single cycle, the parity of the number of components of the 2-factor remains invariant. Therefore, before any attempt to glue all the small cycles together into one long cycle, sometimes we need to change the parity of the number of the cycles.

**Lemma 2** Let $F$ be a 2-factor of a Barnette graph $G$ obtained by the procedure described in the previous section. Let $f_k$ be the number of all the faces of size $k$ in $G$ ($k = 4, 5, 6$), let $x_k$ be the number of grey faces of size $k$ in $G$ ($k = 4, 5, 6$), let $c$ be the number of cycles in $F$, and finally let $q$ be the number of $\times$-paths in $G$. Then $f_6 + f_5 + x_4 + q + c \equiv 0 \ (\text{mod} \ 2)$.

Proof. Let $n$ be the number of vertices of $G$. Euler’s formula yields $n = 8 + f_5 + 2f_6$. If a cycle covers $c_4$ quadrangles, $c_5$ pentagons, and $c_6$ hexagons, its length is $2 + 2c_4 + 3c_5 + 4c_6$. Since each $\times$-path starts and ends in a (white) pentagon, $x_5 = f_5 - 2q$.

Clearly, each vertex is covered by exactly one cycle, thus we have

$$8 + f_5 + 2f_6 = n = 2c + 2x_4 + 3x_5 + 4x_6$$

which is equivalent to

$$4 + f_5 + f_6 = c + q + x_4 + 2x_5 + 2x_6,$$

the claim immediately follows.

It follows from Lemma [2] that in order to change the parity of the number of cycles, it suffices to increase or decrease the number of grey quadrangles by 1, or to increase or decrease the number of grey pentagons by 2, or, in other words, change the number of $\times$-paths by 1.

4.1 Changing the color of a quadrangle

Let $f$ be a 4-face of a Barnette graph $G$. If a $\times$-path passes by a face adjacent to $f$ but not directly by $f$, we can change the color of $f$ by rerouting the path, see Figure [16] (a) for illustration. We can do the same any time some $\times$-path can be rerouted this way.

If there is no $\times$-path that can be rerouted around $f$ and the face $f$ is white, then it suffices to recolor it grey directly, see Figure [16] (b). If $f$ is grey, we switch its color and the color of two adjacent faces at opposite position (we may choose which two), see Figure [16] (c). In both cases we introduce a new $\times$-cycle.

If a $\times$-path passes directly by a quadrangle $f$, it is always possible to reroute it in a way that the path avoids $f$, and then apply the operation from the previous paragraph, see Figure [16] (d).

To be sure that there can be no conflict with other $\times$-paths, the program checked all the clusters containing at least one 4-face. We know that we can
choose any cluster to be the first cluster of the cut. Therefore, it suffices to check that for every cluster containing a 4-face, for every possible position of a segment leaving the cluster, there exists a coloring such that (at least) one of the operations can be applied to change the parity of the number of cycles locally inside the cluster.

Out of all clusters containing a 4-face, there is only one that does not allow us to change the parity of the number of cycles inside the cluster: it is a cluster of curvature 6, containing a 4-face adjacent to four 5-faces. Barnette graphs containing this cluster can easily be characterized: Such a graph either contains two clusters of this type, or it contains one cluster of this type and another cluster of curvature 6, having two adjacent 5-faces, both adjacent to two 4-faces. In both cases a Hamiltonian cycle can be found easily.

4.2 Changing the color of a pair of pentagons

From this point on we only need to consider Barnette graphs having no 4-faces, i.e., the fullerene graphs.

The four basic operations $O_1$, $O_2$, $O_3$, $O_4$ that can be used to change the parity of the number of cycles using two pentagons are depicted schematically in Figure 17.

If the number of $\times$-paths is zero, the graph $G$ is a leapfrog fullerene and all the pentagons are of the same color. We could choose a different color class of
$G'$ to be the grey color and then each $\times$-path would be a simple path joining $p_i$ and $p_{i+1}$ for some $i$. However, it suffices to pick a pair of grey pentagons and apply $O_1$: we separate them from the rest of the graph by a $\times$-cycle, the two pentagons becoming the ends of a new $\times$-path, see Figure 18.

We deal now with different $\times$-paths, regarding the number of segments they correspond to.

Let a $\times$-path $\tau$ correspond to a single segment $P_i$, i.e., it begins at $p_i$ and ends at $p_{i+1}$. In this case we apply $O_2$: we increase the number of grey pentagons by 2 in the following way: We color the $A$-faces along $\tau$ labelled $\times$; for each $B|C$-edge incident with two white faces we label them both $\times$; for each $B|C$-edge incident with two grey faces we recolor them white; finally, for each white face adjacent to an old grey face and a new grey we add the label $\times$ to it. This way the $\times$-path $\tau$ becomes a $\times$-cycle, see Figure 19 for illustration. We can use this operation any time a $\times$-path can be rerouted so that it does not touch any other pentagon.

Let a $\times$-path $\tau$ correspond to at least three segments, i.e., let $\tau$ begin at $p_i$ and end at $p_{i'}$, where $i' - i \geq 3$. It means $\tau$ meets at least two grey pentagons. In this case, we decrease the number of grey pentagons in the following way: We change the labels along the subpath from $p_{i+1}$ to $p_{i+2}$ in a similar way as in the previous paragraph, creating two parallel $\times$-paths. If $p_{i+1}$ and $p_{i+2}$ are on the same side of $\tau$, we apply $O_3$: a new path from $p_{i+1}$ to $p_{i+2}$ is created, see...
Figure 19: The parity of the number of cycles can be changed by modifying a $\times$-path into a $\times$-cycle.

Figure 20 for illustration. If $p_{i+1}$ and $p_{i+2}$ are on different sides of $\tau$, we apply $O_4$: $\tau$ is divided into two different paths: one from $p_i$ to $p_{i+2}$ and the other from $p_{i+1}$ to $p_{i'}$, see Figure 20 for illustration. Observe that the operations depicted in Figure 12 (c-d) are special cases of operation $O_4$.

We let the computer check if these operations are sufficient to change the parity of the number of cycles inside clusters containing only pentagons. Since for each cluster $C$, we can choose this cluster to be the first one of the cut, and as we can choose the coloring, it suffices to check that for each possible position of (at most) one segment leaving the cluster, there is a choice of coloring such that at least one of the operations (or its inverse) may be applied inside the cluster.

The program identified 10 clusters for which it is not true: the trivial cluster $C_0$ having 1 pentagon, the clusters $C_1 = C_{(1,0)}$ and $C_2 = C_{(2,0)}$ containing 2 pentagons of different colors, the cluster $C_3$ with three pentagons sharing a common vertex, two clusters $C_4$ and $C_5$ with 4 pentagons and four clusters $C_6$, $C_7$, $C_8$, $C_9$ with 6 pentagons, depicted in Figure 21. There is a combinatorial reason for this: if three pentagons share a vertex, either one or two of them have to be grey, so we do not have the freedom to change their colors independently.

For some of the other clusters the local change is quite complicated, see for example Figure 22.

If a fullerene graph contains $C_6$, it is a nanotube of type $(5,0)$, and it is known to be hamiltonian [8]. If a fullerene graph contains $C_7$ ($C_8$, $C_9$, respectively), then it is a nanotube of type $(4,2)$ (of type $(6,2)$, $(8,0)$). Out of all the possible clusters (caps) to close the other end of the tube, $C_7$ ($C_8$, $C_9$) is the only that does not allow us to change the parity of the number of cycles. However, if both caps of a nanotube are $C_7$ ($C_8$, $C_9$), then it has an even number of hexagons and exactly 6 grey and 6 white pentagons, so by Lemma 2 the number of cycles in the 2-factor is odd.

It remains to consider fullerene graphs only having clusters $C_0$, $C_1$, $C_2$, $C_3$, $C_4$, and $C_5$.

By inspecting all the six clusters, we argue that for each active segment leaving a cluster, the $\times$-path can be transformed into a pair of $\times$-paths (interconnected inside the cluster or not) – it is nothing else than applying a half of
Figure 20: The parity of the number of cycles can be changed by ‘pushing’ a $\times$-path through two grey pentagons. If the two pentagons are on the same side of the $\times$-path, this operation creates a new $\times$-path joining them. If the two pentagons are on different sides of the $\times$-path, this operation cuts the path into two.

Figure 21: Clusters with 4 and 6 pentagons for which it is not possible to increase or decrease the number of grey pentagons by 2.
one of the operations $O_2$, $O_3$ and $O_4$ inside the cluster and the other half inside another. In each of the clusters this modification corresponds to increasing or decreasing the number of grey pentagons by one. It suffices to find a pair of clusters joined by a $\times$-path such that performing some operation either increases or decreases the number of grey pentagons for both clusters.

If a cluster containing two pentagons ($C_1$ or $C_2$) is the first cluster of the cut, the segment leaving the cluster has to be active. We may choose the coloring in such a way that the $\times$-path begins at the furthest pentagon. This coloring can be modified both in order to decrease (by $O_3$ or $O_4$) and to increase (by $O_2$, after rerouting the path in a way not to touch the other pentagon) the number of grey pentagons inside this cluster, so no matter how this modification affects the next cluster, there is always a way to change the parity of the number of cycles.

For the two clusters with four pentagons ($C_4$ and $C_5$), since they do not permute the colors, either there are two active segments of the same color, or there are no active segments. In the second case we find the closest $\times$-path and reroute it in the way that it enters the cluster twice (if there are not $\times$-paths, then all the other pentagons are grey and isolated, we may apply $O_1$ to a pair of them). In any case, there are always two grey and two white pentagons inside the cluster. We can change one of the $\times$-paths leaving the cluster into two $\times$-paths in two different ways, leaving the cluster either with one or with three grey pentagons, see Figure 23 for illustration.

It remains to consider fullerene graphs having only clusters $C_0$ and $C_3$.

Let there be at most two $C_3$s. It means there are at least six $C_0$s – isolated pentagons. If none of the operations above can be applied, then each $\times$-path among the isolated pentagons consists of exactly two segments. Let $\tau$ join $p_i$ with $p_{i+2}$. If $\tau$ may be rerouted in such a way that it does not touch $p_{i+1}$, we change it into a cycle in the same way as for the $\times$-paths consisting of a single segment. Assume that $\tau$ touches $p_{i+1}$. Each of the three pentagons $p_i$, $p_{i+1}$, $p_{i+2}$ corresponds to a single shift of the three colors 1, 2, 3 of the canonical 3-coloring of the graph $G'$. Hence, by parity argument, for exactly one of the
Figure 23: Two ways to modify the 2-factor in the neighborhood of a cluster $C_4$, when one of the ×-paths is doubled. We can both decrease and increase the number of grey pentagons.

segments $P_{i-1}$ and $P_{i+2}$ (which are both inactive) there is no switch in the coloring, and for the other one the colors 2 and 3 are switched. Without loss of generality let $P_{i-1}$ be the segment without a switch; let $p_i$ be colored 2. Then along $P_i$ the colors 1 and 3 are switched; along $P_{i+1}$ all the three colors are permuted. It means that if we choose the color 3 to correspond to grey, then the segment $P_{i-1}$ will remain inactive, but all the three segments $P_i$, $P_{i+1}$ and $P_{i+2}$ will be active, so we can change the parity of the number of the cycles for the ×-path starting at $p_i$ going around $p_{i+1}$ and $p_{i+2}$ as described above.

It remains to consider fullerene graphs having only clusters $C_0$ and $C_3$, having at least three $C_3$s. If there are four $C_3$s and no $C_0$s, then by replacing the vertex incident to three pentagons inside each $C_3$ by a triangle we obtain a graph having only faces of size 3 and 6. These graph are known to be hamiltonian \[4\], and clearly the reduction preserves hamiltonicity.

It remains to consider fullerene graphs having exactly three $C_3$s and three $C_0$s. Let $T_1$, $T_2$, $T_3$ be the clusters of type $C_3$, and let $p_1$, $p_2$, $p_3$ be the isolated pentagons.

Let $P^*$ be a dual path starting at a cluster $T_j$ for some $j = 1, 2, 3$. Since $T_j$ is a cluster with an odd number of pentagons, it corresponds to a single shift of colors. If we replace the central vertex of $T$ by a triangle, the three pentagons become hexagons. Let 1 be the color of the triangle of the 3-coloring along $P^*$, If we choose 1 to be grey, then the segment joining $T_j$ and $p_i$ is inactive; there has to be exactly one grey pentagon inside $T_j$ and we may choose which one. On the other hand, if we choose 2 or 3 to be grey, then the ×-path starting at $T_j$ uses faces colored 1; there are two grey pentagons inside $T_j$.

Suppose the second cluster that meets $P^*$ is an isolated pentagon $p_i$ for some $i = 1, 2, 3$. If $p_i$ is not of color 1, then it is grey, and the ×-path continues towards the next cluster. By doubling the ×-path between $T_j$ and $p_i$ the number of grey pentagons can be decreased by two. In fact, this is a special case of one of the operations $O_3$ or $O_4$.

It means that we may suppose that for each cluster $T_j$, each pentagon $p_i$ is
of the same color as the triangle corresponding to $T_j$ (of a local 3-coloring along a shortest path joining them). Globally, all the odd faces (the three isolated pentagons and the three triangles) have to be of the same color. Therefore, if we choose this color to be grey, there will be no active segments joining the clusters. We obtain a 2-factor such that $p_i$ is grey for $i = 1, 2, 3$, moreover, for each cluster $T_j$, there is one grey pentagon (we can choose which one), two white pentagons labelled $\times$, joined by a $\times$-path of length two. If we need to change the parity of the number of cycles, we choose a pair of grey pentagons, we find a path joining them, and we apply operation $O_1$. If the blown-up $\times$-path meets $T_j$ for some $j = 1, 2, 3$, we can always choose a grey pentagon inside $T_j$ in such a way that the $\times$-paths are merged, see Figure 24 for an example.

For the graph from Figure 4, all the three factors in Figure 15 are of even size. We can change it to odd easily by operations $O_1 - O_4$ at several places, for example as depicted in Figure 26.

5 Putting the cycles together

We use similar ideas as were used in [3]. We start with the 2-factor $F_0$ of $G$ composed of an odd number of short cycles (possibly including 2-cycles) such that no cycle is inside another. For each resonant hexagon $h$ we introduce a
new vertex $v_h$; we delete the three edges of $F_0$ incident with $h$ and replace them by six new edges joining $v_h$ to all the six vertices incident with $h$. This way we obtain a new graph $F$, with vertices of degree 2 and 6. Vertices of $F$ of degree 2 correspond to vertices of $G$; vertices of $F$ of degree 6 correspond to hexagons resonant with respect to $F_0$. Edges of $F$ are either the new edges joining $v_h$ to one of the vertices incident with $h$ for some resonant hexagon $h$, or edges incident with a grey face and a white face labelled $\times$.

If $h_1$ and $h_2$ are resonant hexagons adjacent in $G$, then $v_{h_1}$ and $v_{h_2}$ are joined by two paths of length 2 in $F$. Besides these pairs of paths of length 2, all the remaining edges of $F$ can be decomposed into edge-disjoint cycles, each corresponding to a sequence of $\times$-labelled faces (along $\times$-paths), where two consecutive $\times$-labelled faces are either adjacent, or sub-adjacent via a 2-cycle (i.e. they are not adjacent, but each shares a vertex with a common 2-cycle). If such a cycle is incident with just two resonant hexagons, we treat it as a pair of two paths of length 2. All other such cycles will be called special.

Finally, we suppress all the vertices of degree 2. This way we obtain a 6-regular plane multigraph $H$, with vertices corresponding to the resonant hexagons of $G$. Since it is a plane (multi)graph of even degree, it is eulerian, hence, it has a face-coloring using two colors, say black and white, such that the black faces of $H$ are those containing the grey faces of $G$, and the white faces of $H$ are those containing the white faces of $G$ labelled $\times$. We color the faces of $F$ with black and white correspondingly.

A 2-gon between parallel edges of $H$ is black only if it corresponds to 2-cycle of $F_0$, otherwise it is white. Exceptionally, a black 2-gon may correspond to a grey cycle incident to two resonant hexagons inside clusters of big curvature,

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure25.png}
\caption{Three different 2-factors with an odd number of cycles derived from those from Figure 14.}
\end{figure}
Figure 26: Inside clusters of big curvature containing triples of pentagons sharing a vertex, multiplicity of edges of the multigraph \( H \) may exceed two. Two examples with one active segment and one with two active segments leaving the same cluster.

see Figure [26] left and center. The first example shows that the graph \( H \) does not have to be 3-connected.

Each special cycle contains a certain number, say \( k \), black 2-gons, \( k-1 \) white 4-gons separating them, and two white triangles at the ends. These triangles may be collapsed to 2-cycles again inside clusters of big curvature, see Figure [26] right.

We now introduce an algorithm, which changes back sequentially the 6-vertices of \( F \) into triples of edges of \( G \), finally arriving back to a 2-factor of \( G \) containing just one cycle. We will modify \( F \) at the same time as we will delete parts of \( H \). The goal is to glue the white parts together as much as possible, without separating a black face from the rest of the graph. If there were no special cycles in \( H \), each edge would be of multiplicity two, and the algorithm would in fact find a decomposition of \( H \) into an induced tree and a stable set, just as Marušič did for leaprog fullerenes [9].

We start with an arbitrary 6-vertex \( v_h \) of \( H \) (as of \( F \)). In \( F \), we replace \( v_h \) and the six edges incident with it by a triple of non-adjacent edges incident with \( h \), in such a way that the three white faces become one face. We recolor this face red. In \( H \), we remove \( v_h \) and all the six incident edges. We color the corresponding new face of \( H \) red as well.
At each moment of the procedure, \( H \) is a 2-connected multigraph with vertices corresponding to hexagons resonant with respect to \( F \). Precisely one face of \( H \) is colored red; all other faces are white or black. In the coloring with black and white, the red face counts as a black face. Some of the vertices of \( H \) are of incident to three different white faces (let us call them solid), some of them are incident to two different white faces (let us call them fragile). There are no vertices incident to just one white face (so-called unstable vertices). All the fragile vertices are incident with the red face of \( H \).

On the other hand, in \( F \), all the vertices corresponding to resonant hexagons always have degree 6 (once we replace all of them by triples of edges, we will get a 2-factor of \( G \)); the other vertices have degree 2. There is precisely one face of \( F \) colored red (counting as a special white face), some faces still have their original white or black color; however, there can be some faces colored with other colors than white, black, or red, but for each color there is a unique face with this color; they all count as white faces.

In each step of the algorithm, we look at the fragile vertices on the boundary of the red face of \( H \). For each fragile vertex of \( H \), its removal from \( H \) causes that some other fragile vertices become unstable, and some stable vertices become fragile, or even unstable. After removing a fragile vertex, we keep removing unstable vertices until there are just stable and fragile vertices.

It is always possible to choose a fragile vertex such that after removing it and all the unstable vertices subsequently, the resulting graph remains 2-connected or empty: If all the vertices incident to the red face of \( H \) are fragile, we choose any of them. If there are fragile and stable vertices, we choose a fragile vertex adjacent to a stable one.

This operation usually corresponds to dropping a black face (if it is surrounded by doubled edges) or a sequence of black faces incident to a special cycle. The sequence of reductions of the multigraph \( H \) emulates the ear-decomposition of the underlying simple graph.

What does deleting a fragile/unstable vertex correspond to in \( F \)?

Let \( v_h \) be a fragile vertex of \( F \) corresponding to a resonant hexagon \( h \). Since it is fragile, it is incident with three black faces (not necessarily different), two white faces, and exactly one face, which has a color different from black and white, say red. We replace \( v_h \) and all the six incident edges with a triple of edges of \( G \) in such a way that the red face is united with the two white faces. Observe that \( h \) is colored red now.

Let \( v_h \) be an unstable vertex of \( F \). It means that it is incident with three black faces (not necessarily different), a white face, and precisely two faces with colors different from black and white (unless it is the last vertex of \( H \); we will deal with this case later).

If both faces have the same color, say red, it means there is a path in \( F \) from \( h \) to itself. In order not to create a short cycle bounding a black face, we replace \( v_h \) and all the six incident edges with a triple of edges of \( G \) in such a way that the three black faces are merged, we color \( h \) black; for the white face we introduce a new unique color.

If the two faces which are neither black nor white have distinct colors, say
red and blue, we replace \( v_h \) and all the six incident edges with a triple of edges of \( G \) in such a way that the red, blue, and white faces are merged; we keep just one of the two colors for the new face including \( h \). (If one of the colors is red, we keep it; if none is red, we keep an arbitrary one.)

Finally, if \( H \) consists of a single cycle, we start with any of its (fragile) vertices, and we apply the same procedure for all the other vertices (which become unstable gradually) but the last.

When there is just one resonant hexagon in \( F \), either it is incident with the same red face three times and three different black faces, or it is incident with three faces of different colors and the same black face three times (because of the parity argument). In the former case, we glue the black faces, in the latter, we glue the colorful faces.

Altogether, there is a single black and a single red face at the end of the algorithm, hence, the corresponding 2-factor consists of a single cycle, as desired.

6 Concluding remarks

The proof of Theorem 1 is constructive – it allows to implement a linear time algorithm to find a Hamilton cycle in a cubic polyhedral graph with faces of size at most 6.

One could extend the results towards classes of graphs embedded in other surfaces than plane/sphere, such that the faces of size different than 6 are far from each other.

References

[1] R. E. L. Aldred, S. Bau, D. A. Holton, and B. D. McKay, Nonhamiltonian 3-Connected Cubic Planar Graphs, SIAM J. Discrete Math. 13 (1) (2000), 25–32.

[2] G. Brinkmann and A. W. M. Dress, A Constructive Enumeration of Fullerenes, J. Algorithm. 23 (2) (1997), 345–358.

[3] R. Erman, F. Kardos, and J. Mislof, Long cycles in fullerene graphs, J. Math. Chem. 46 (4) (2009), 1103–1111.

[4] P. R. Goodey, A class of hamiltonian polytopes, (special issue dedicated to Paul Turán) J. Graph Theory 1 (1977) 181-185.

[5] P. R. Goodey, Hamiltonian circuits in polytopes with even sided faces, Israel J. Math. 22 (1975) 52-56.

[6] S. Jendrof and P. J. Owens, Longest cycles in generalized Buckminster-fullerene graphs, J. Math. Chem. 18 (1995) 83–90.

[7] D. Krif, O. Pangrác, J.-S. Sereni, and R. Škrekovski, Long cycles in fullerene graphs, J. Math. Chem. 45 (4) (2009), 1021–1031.
[8] K. Kutnar and D. Marušić, On cyclic edge-connectivity of fullerenes, Discrete Appl. Math. 156 (10) (2008), 1661–1669.

[9] D. Marušić, Hamilton Cycles and Paths in Fullerenes, J. Chem. Inf. Model., 47 (3) (2007), 732–736.

[10] J. Zaks, Non-hamiltonian simple 3-polytopes having just two types of faces, Discrete Math. 29 (1980) 87-101.
Appendix

In the following series of figures, a Hamilton cycle is found starting from the 2-factor depicted in Figure 25 middle. Stable vertices of $H$ are white, fragile vertices are marked with a dot; unstable vertices are marked with a cross. If there is an unstable vertex, we process it first. If there is no unstable vertex, the vertex chosen to be processed next is marked with an arrow.
