Longest cycles in generalized Buckminsterfullerene graphs

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It is shown that every regular 3-valent polyhedral graph whose faces are all 5-gons and 6-gons contains a cycle through at least 4/5 of its vertices.

1. Introduction

Let $G_3(p,q)$ denote the family of 3-connected regular 3-valent planar graphs whose faces are all p-gons and q-gons, $p<q, p\geqslant 3$. Steinitz's famous theorem (see [5, p. 235]) guarantees the existence of convex polyhedra that are combinatorially equivalent to the graphs from $G_3(p,q)$. It follows from Euler's formula for polyhedra that $p\in\{3,4,5\}$ and that, if $p=3$, then $q\leqslant 10$.

There are many papers devoted to the study of longest cycles in graphs from the families $G_3(p,q)$. For example, Goodey [3,4] has proved that all graphs from $G_3(3,6)$ and $G_3(4,6)$ are Hamiltonian. The families $G_3(3,q)$ for $7\leqslant q\leqslant 10$, $G_3(4,2k+1)$ for $k\geqslant 3$ and $G_3(5,q)$ for $q\geqslant 7$ contain non-Hamiltonian graphs. The longest cycles and, particularly, the shortness exponents and shortness coefficients of these families have been investigated. See, for example, Owens [8–10], Tkáč [11], Walther [12] and Zaks [13].

In this paper we consider graphs from $G_3(5,6)$. By Euler's formula every such graph has exactly twelve 5-gons. A result of Ewald [2, lemma 3.1] implies that there is a cycle through at least 1/3 of the vertices of any graph from $G_3(5,6)$. Nothing further seems to have been published about longest cycles in graphs from this family apart from the conjecture that all these graphs are Hamiltonian (see e.g. Zaks [13]).

Besides pure mathematical interest there is another reason for investigating the structural properties of graphs from $G_3(5,6)$. In chemistry, following the synthesis by Kroto et al. [7] of Buckminsterfullerene (also known as icosahedral C_{60}, soccerballene, footballene, etc.) there has been considerable interest in pure carbon molecules or carbon clusters. All clusters are convex polyhedra, have 3-valent graphs and contain only 5-gons and 6-gons (and, possibly, 7-gons), see Bakowies and Thiel [1]. Provided that there are not actually any 7-gons, the graphs are from $G_3(5,6)$. We may call them generalized Buckminsterfullerene graphs. For an example of recent work on the properties of graphs from $G_3(5,6)$, see John and Mallion [6].

The main aim of the present paper is to prove the following:

THEOREM

Let G be an n-vertex graph from $G_3(5,6)$. Then G contains a cycle of length at least $4n/5$.

2. *Proof of the theorem*

Let C be a maximum cycle in G and let $|C|$ denote its length. We call a vertex or edge *black* if it is in C and *white* if it is not in C. In diagrams, black vertices and edges are represented by large black dots and thick lines, white vertices and edges by white dots and marked thin lines. Unmarked vertices and unmarked thin lines represent vertices and edges whose membership of C has not yet been decided.

We prove a sequence of lemmas from which the theorem follows. Most of the proofs are by contradiction.

LEMMA 1

Every white vertex is adjacent to a black vertex.

Proof

Suppose that not every white vertex is adjacent to a black vertex. Then there exists a white vertex x at distance exactly 2 from C and a minimum white path xyz from x to C. Since y has valency 3 only, xyz is part of the boundary of some face F of G. This face may be a 5-gon $xyztv$ or a 6-gon $xyztuv$, as shown in fig. 1, but in either case zt is black and v is white.

When F is a 5-gon, the operation of replacing the edge tz of C by the path $tvxyz$, which we denote by $tz \to tvxyz$, lengthens C. When F is a 6-gon and u is white, $tz \to tuvxyz$ lengthens C. When F is a 6-gon and u is black, $utz \to uvxyz$ lengthens C. In each case the maximum property of C is contradicted, so the lemma is proved. □

Every black vertex has at least two black neighbours and, therefore, at most one white neighbour. Hence $|C| \geqslant n/2$.

By lemma 1, every white vertex has at least one black neighbour and at most

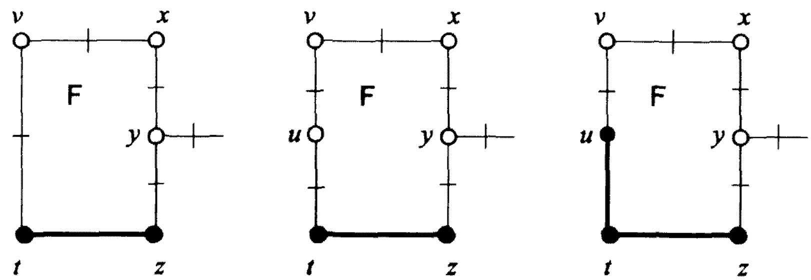

Fig. 1. Proof of lemma 1.

two white neighbours, so $G-C$ has maximum valency two and is a set of paths and cycles. The next two lemmas give further information on the structure of $G-C$.

LEMMA 2

No component of $G-C$ is a cycle (compare [2, lemma 3.1]).

Proof

Suppose that, contrary to the lemma, $G-C$ has a component H that is a cycle. By lemma 1, H is a facial cycle. Figure 2 shows the case where H is a 6-cycle $xyzuvw$.

Now bc is white since otherwise $abcd \to axyzuvwd$ would lengthen C. Hence ch is black. Similarly ef is black. At least one of the edges fg, hg is white, otherwise a 6-cycle $cdefgh$ is formed. By symmetry, we may assume that hg is white. Now use $hcdef \to hgf$ if fg is white (or $hcdefg \to hg$ if fg is black) followed by $ab \to axyzuvwdcb$ and C is lengthened, a contradiction.

When the faces shown in fig. 2 include 5-gons the argument is similar or simpler. We omit the details. □

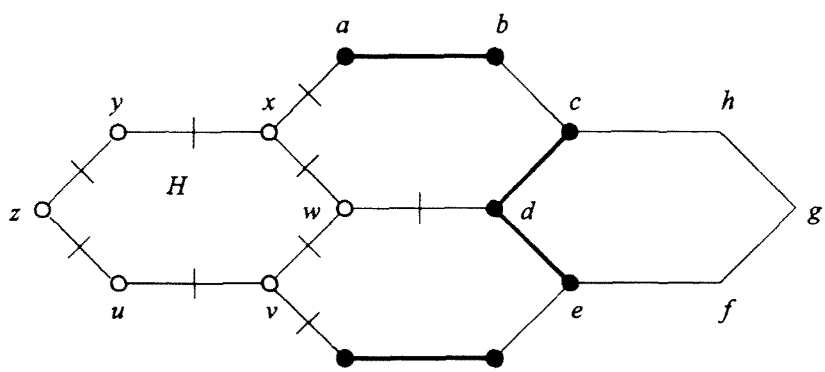

Fig. 2. A white cycle.

LEMMA 3

No component of $G - C$ is a path of length greater than one.

Proof

Suppose that, contrary to the lemma, $G - C$ has a component that is a path of length at least 2, say $xyz\ldots$, where x is one end vertex. Then the white path xyz is part of the boundary of a face of G. The whole boundary is of the form $uwxyz$ or $uwxyzt$, where u, w and uw are black. In the former case, $wu \to wxyzu$, lengthens C. In the latter case C is lengthened by $wu \to wxyztu$ (if t is white) or $wut \to wxyzt$ (if is black, in which case ut is black). Thus we always have a contradiction. □

By lemmas 2 and 3, every component of $G - C$ is either an isolated vertex or a path of length one. Hence every white vertex has at least two black neighbours and so $|C| \geqslant 2n/3$.

We omit the easy proof of the next lemma.

LEMMA 4

Let F be any face of G. If F is a 5-gon, then there is at most one white vertex on F. If F is a 6-gon, then there are at most two white vertices on F and, when there are two, they are in either adjacent or opposite positions.

In order to compare the numbers of black and white vertices we shall now use the concept of *charge*. Initially every black vertex has charge 1 and there is no charge on white vertices. A black vertex has at most one white neighbour. If it has one, that neighbour is given charge 1 and, if not, the charge is shared between the white 2-neighbours (that is, white vertices at distance 2). If there are no white 2-neighbours either, then the charge is shared between the white 3-neighbours, and so on. However, we shall not need to go further than 2-neighbours.

Let $q(x)$ denote the final charge on a white vertex x and $q(x, z)$ the charge given to x by a black vertex z.

LEMMA 5

Let z be a black vertex with no white neighbours. Then z has at most two white 2-neighbours.

Proof

In fig. 3, suffixes indicate distances from z. By symmetry we may assume that a_1z is the white edge incident at z. Then b_1zc_1 and $d_2a_1e_2$ are black paths. By lemma 4 at most one of the two vertices f_2, g_2 is white. Similarly, at most one of h_2, i_2 is white. The result follows. □

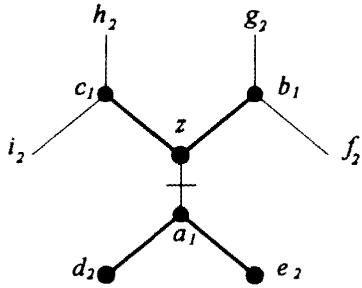

Fig. 3.

Let x be a white vertex and z a black 2-neighbour of x with no white neighbours. Then $q(x,z) = 1/2$ if z has another white 2-neighbour besides x and otherwise $q(x,z) = 1$.

LEMMA 6

Let x be an isolated white vertex. Then $q(x) \geqslant 9/2$.

Proof

At first we assume that the six faces nearest to x are all 6-gons. In fig. 4, suffixes indicate distances from x.

Evidently $q(z,a_1) = q(z,b_1) = q(x,c_1) = 1$. We shall show that x has at least three black 2-neighbours whose neighbours are all black. There are two cases.

Case 1 (a_3, b_3, c_3 black). By lemma 4, d_3 and e_3 are not both white, so at least one of the vertices d_2, e_2 has black neighbours only. Similarly for f_2, g_2 and h_2, i_2.

Case 2 (at least one of a_3, b_3, c_3 white). By symmetry we may assume that a_3 is white. Then g_2g_3, h_2h_3 are black edges.

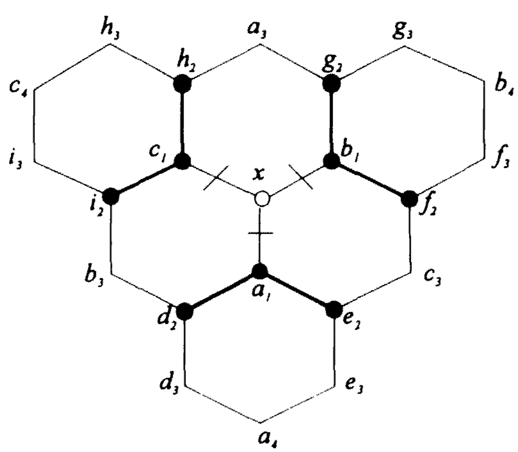

Fig. 4.

(a) We claim that b_3 and c_3 are black. For suppose that b_3 is white. Then i_2i_3 is black and hence c_4 is black since, otherwise, $h_3h_2c_1i_2i_3 \to h_3c_4i_3$ and $g_2b_1 \to g_2a_3h_2c_1xb_1$ would lengthen C. Since c_4 is black, one of the edges h_3c_4, i_3c_4 is black. The other one is white, since otherwise a black 6-cycle would be completed. By symmetry we may assume that i_3c_4 is black. Then $h_3h_2c_1i_2i_3c_4 \to h_3c_4$ and $g_2b_1 \to g_2a_3h_2c_1xb_1$ leave $|C|$ unaltered but produce a white path $b_3i_2i_3$, contrary to lemma 3. Hence b_3 is black. Similarly, c_3 is black.

(b) We claim that i_3 and f_3 are black. For suppose that i_3 is white. Then c_4 is black, since otherwise $h_3h_2c_1i_2 \to h_3c_4i_3i_2$ leaves $|C|$ unaltered but produces a white path $a_3h_2c_1$, contrary to lemma 3. Since c_4 is black i_3 is white, c_4h_3 is black. Then $c_4h_3h_2c_1i_2 \to c_4i_3i_2$ and $g_2b_1 \to g_2a_3h_2c_1xb_1$ lengthen C, another contradiction. Hence i_3 is black. Similarly f_3 is black.

All neighbours of i_2 and f_2 are black, so $q(x, i_2) \geqslant 1/2$ and $q(x, f_2) \geqslant 1/2$. As in Case 1, $q(x, d_2) \geqslant 1/2$ or $q(x, e_2) \geqslant 1/2$.

In both Case 1 and Case 2, $q(x) \geqslant 3 + 3 \times 1/2 = 9/2$, as required.

Now consider how the proof must be modified when some of the six faces nearest to x become 5-gons. In fig. 4, any one of these faces may be converted into a 5-gon by removing one of the vertices $a_3, b_3, c_3, a_4, b_4, c_4$, where to *remove* the vertex a_4 (for instance) means to replace the path $d_3a_4e_3$ by a single edge d_3e_3.

First, suppose that we remove a_3, b_3 or c_3. Each of these vertices is adjacent, in fig. 4, to two black 2-neighbours of x which become adjacent to one another when the vertex is removed. Thus, as far as our proof is concerned, the removal of a_3, b_3 or c_3 is equivalent to asserting that this vertex is black and hence any part of the proof where we suppose it to be white must simply be deleted.

Now suppose that we remove a_4, b_4 or c_4. In Case 1, the proof is unaffected. In Case 2, the removal of c_4 simplifies the proof that b_3 and i_3 are black. In fact, when c_4 is removed, b_3 is black since otherwise $h_3h_2c_1i_2i_3 \to h_3i_3$ and $g_2b_1 \to g_2a_3h_2c_1xb_1$ would lengthen C and i_3 is black since otherwise $h_3h_2c_1i_2 \to h_3i_3i_2$ and $g_2b_1 \to g_2a_3h_2c_1xb_1$ would lengthen C. Similarly, the removal of b_4 simplifies the proof that c_3 and f_3 are black. The removal of a_4 does not affect the proof.

The removal of two or more of the vertices $a_3, b_3, c_3, a_4, b_4, c_4$ can be dealt with by combining the corresponding changes to the proof suggested above. Note that, when a_3, b_3, c_3 are all removed, Case 2 disappears entirely. □

We need a similar result for a white vertex with a white neighbour. Here, we shall be satisfied with a slightly weaker result.

LEMMA 7

Let x be a white vertex with a white neighbour. Then $q(x) \geqslant 4$.

Proof

Let y be the white neighbour of x. At first we assume that all relevant faces (see fig. 5) are 6-gons. Suffixes indicate distances from the nearer of the two vertices

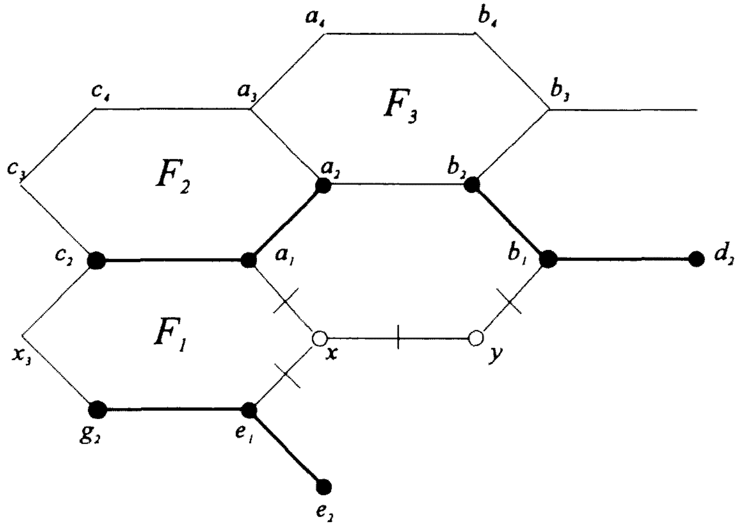

Fig. 5.

x, y. It will be sufficient to consider the contribution to $q(x)$ from vertices that lie above the line xy in the diagram and are at distance 1 or 2 from x. Afterwards, the proof can be completed by adding the contribution from vertices below xy.

As shown, $a_2a_1c_2$ and $b_2b_1d_2$ are black paths so $q(x, a_1) = 1$. We shall show that $q(x, a_2) + q(x, c_2) \geqslant 1$. There are two cases.

Case 1 (a_2b_2 black). The operation $a_1a_2b_2b_1 \rightarrow a_1xyb_1$ leaves $|C|$ unaltered but makes a_2, b_2 white. Hence, by lemma 4, a_3, a_4, b_4, b_3 are black. As a_2b_2 is black, a_2a_3 and b_2b_3 are white and so $c_4a_3a_4b_4b_3$ is a black path. Hence a_2 has no white neighbours and no white 2-neighbours except x. Thus $q(x, a_2) + q(x, c_2) \geqslant q(x, a_2) = 1$.

Case 2 (a_2b_2 white). The edges a_2a_3, b_2b_3 are black, so a_3 and b_3 are black. Hence a_2 has no white neighbours and $q(x, a_2) \geqslant 1/2$. We shall show that either a_2 has no white 2-neighbours except x or c_2 has no white neighbours.

The vertices c_3, c_4 are both black since otherwise one of the operations $a_3a_2a_1c_2 \rightarrow a_3c_4c_3c_2$, $a_3a_2a_1c_2c_3 \rightarrow a_3c_4c_3$, $c_4a_3a_2a_1c_2 \rightarrow c_4c_3c_2$, followed by $b_2b_1 \rightarrow b_2a_2a_1xyb_1$, would lengthen C.

Next, x_3 and a_4 are not both white since otherwise c_2c_3 and a_3c_4 would be black and $c_4a_3a_2a_1c_2c_3 \rightarrow c_4c_3$ followed by $e_1g_2 \rightarrow e_1xa_1c_2x_3g_2$ would leave $|C|$ unaltered but produce a white path $a_4a_3a_2$, contrary to lemma 3. Hence either x_3 is black and $q(x, c_2) \geqslant 1/2$, or a_4 is black and $q(x, a_2) = 1$. Since $q(x, a_2) \geqslant 1/2$ we have $q(x, a_2) + q(x, c_2) \geqslant 1$ in any case.

By similar reasoning $q(x, e_1) = 1$, $q(x, e_2) + q(x, g_2) \geqslant 1$. Hence $q(x) \geqslant 4$, as required.

It remains to consider how to the proof must be modified when some of the relevant faces become 5-gons. By lemma 4, the faces incident with xy cannot be

5-gons. Any one of the faces F_1, F_2, F_3 becomes a 5-gon if we remove (as in lemma 6) one of the vertices x_3, c_4, b_4.

When we remove x_3, g_2 becomes a neighbour of c_2, so c_2 has no white neighbours and $q(x, c_2) \geqslant 1/2$. When we remove c_4, Case 1 remains unaltered (except that c_4 is changed to c_3) and, in Case 2, x_3 and a_4 are not both white for the simpler reason that, otherwise, there would be a black 5-cycle $a_3a_2a_1c_2c_3$. When we remove b_4, Case 1 becomes impossible because $a_1a_2b_2b_1 \rightarrow a_1xyb_1$ leaves two white vertices on the 5-gon F_3, contrary to lemma 4, while the proof in Case 2 is unaltered.

The removal of two or all three of the vertices x_3, c_4, b_4 is dealt with by combining the above changes. □

Since $q(x) \geqslant 4$ for every white vertex, $|C| \geqslant 4n/5$ and the proof of the theorem is complete.

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