# Long cycles in fullerene graphs

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**Abstract**

It is conjectured that every fullerene graph is hamiltonian. Jendrol' and Owens proved [J. Math. Chem. 18 (1995), pp. 83–90] that every fullerene graph on $n$ vertices has a cycle of length at least $4n/5$. In this paper we, improve this bound to $5n/6 - 2/3$.

## 1 Introduction

*Fullerenes* are carbon-cage molecules comprised of carbon atoms that are arranged on a sphere with twelve pentagon-faces and other hexagon-faces. The icosahedral $C_{60}$, well-known as Buckministerfullerene, was found by Kroto et al. [8], and later confirmed through experiments by Krätchmer et al. [7] and Taylor et al. [13]. Since the discovery of the first fullerene molecule, the fullerenes have been objects of interest to scientists in many disciplines.

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Many properties of fullerene molecules can be studied using mathematical tools and results. Thus, *fullerene graphs* were defined as cubic (i.e. 3-regular) planar 3-connected graphs with pentagonal and hexagonal faces. Such graphs are suitable models for fullerene molecules: carbon atoms are represented by vertices of the graph, whereas the edges represent bonds between adjacent atoms. It is known that there exists a fullerene graph on $n$ vertices for every even $n \geq 20$, $n \neq 22$. See the monograph of Fowler and Manolpoulos [2] for more information on fullerenes.

The hamiltonicity of planar 3-connected cubic graph has been attracting much interest of mathematicians since Tait [12] in 1878 gave a short and elegant (but also false) proof of the Four Color Theorem based on the "fact" that planar 3-connected cubic graphs are hamiltonian. The missing detail of the proof was precisely the previously mentioned "act" which became known as Tait's Conjecture. Later, Tutte [15] disproved Tait's Conjecture.

The hamiltonicity of various subclasses of 3-connected planar cubic graphs was additionally investigated. Grünbaum and Zaks [5] asked whether the graphs in the family $\mathcal{G}_3(p,q)$ of 3-connected cubic planar graphs whose faces are of size $p$ and $q$ with $p < q$ are hamiltonian for any $p, q$. Note that $p \in \{3, 4, 5\}$ by Euler's formula. Also note that fullerene graphs correspond to $\mathcal{G}_3(5,6)$. Goodey [3, 4] has proved that all graphs contained in $\mathcal{G}_3(3,6)$ and $\mathcal{G}_3(4,6)$ are hamiltonian. Zaks [17] found non-hamiltonian graphs in the family $\mathcal{G}_3(5,k)$ for $k \geq 7$. Similarly, Walther [16] showed that families $\mathcal{G}_3(3,q)$ for $7 \leq q \leq 10$ and $\mathcal{G}_3(4, 2k+1)$ for $k \geq 3$, contain non-hamiltonian graphs. For more results in this area, also see [9, 10, 11, 14].

Let us restrict our attention to $\mathcal{G}_3(5,6)$. Ewald [1] proved that every fullerene graph contains a cycle which meets every face of $G$. This implies that there is a cycle through at least $n/3$ of the vertices of any fullerene graph on $n$ vertices. It is well known that each planar graph $G$ has a dominating cycle $C$, i.e. a cycle $C$ such that each edge of $G$ has an end-vertex on $C$. If $G$ is a fullerene graph, then its 3-connectivity yields that $G-C$ is comprised of a (possibly empty) set of isolated vertices. This immediately improves the bound from $n/3$ to $3n/4$. Jendrol' and Owens [6] gave a better bound of $4n/5$. In this paper, we improve the bound to $5n/6 - 2/3$.

## 2 Preliminary observations

We follow the terminology of Jendrol' and Owens [6]. We consider a longest cycle $C$ of a fullerene graph; a vertex contained in $C$ is *black* and a vertex

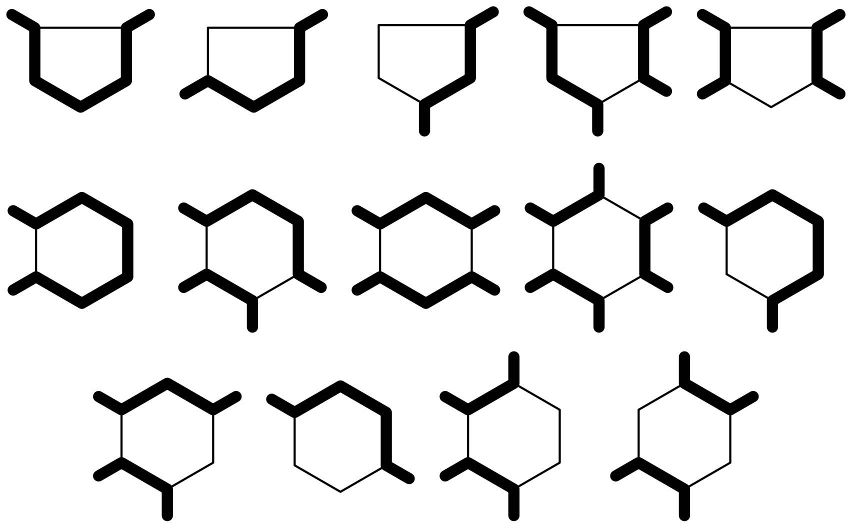

Figure 1: The possible ways for a cycle $C$ to traverse a face of size five or six (up to symmetry) without forming a path of three white vertices. The cycle $C$ is indicated by bold edges.

not contained in $C$ is *white*. Our aim is to show that there are at most $n/6 + 2/3$ white vertices for an $n$-vertex fullerene graph $G$. The following was shown [6].

**Lemma 1.** *Let $G$ be a fullerene graph and $C$ a longest cycle in $G$. The graph $G$ contains no path comprised of three white vertices.*

Lemma 1 implies that no face of $G$ is incident with more than two white vertices (see Figure 1 for all possibilities, up to symmetry, how the cycle $C$ can traverse a face of $G$). The faces incident with two white vertices are called *white* and the faces incident with no white vertices are called *black*. Let us now observe the following simple fact.

**Lemma 2.** *If $C$ is a longest cycle in a fullerene graph $G$, then there are no white faces of size five.*

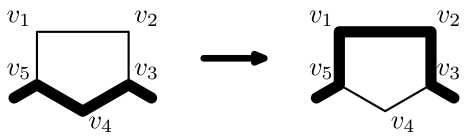


Figure 2: Prolonging the cycle $C$ if the graph $G$ contains a white face of size five.

*Proof.* Assume that there is a white face $v_1v_2v_3v_4v_5$. By symmetry we can assume, that the cycle $C$ contains the path $v_3v_4v_5$. Replacing the path $v_3v_4v_5$ with the path $v_3v_2v_1v_5$ (see Figure 2) yields a cycle of $G$ longer than $C$, a contradiction. □

In the sequel, we use the following notion. Given a face $f$ with vertices $v_1, v_2, \ldots, v_k$ (in cyclic order), we let $f_{i,i+1}$ be the face different from $f$ that contains the edge $v_iv_{i+1}$ (the indices are taken modulo $k$).

# 3 Initial charge and discharging rules

Using a discharging argument, we argue that the number of white vertices with respect to a longest cycle $C$ in an $n$-vertex fullerene graph $G$ is at most $n/6 + 2/3$. Fix such a cycle $C$. Each white vertex initially receives 3 units of charge. Next, each white vertex sends 1 unit of charge to each of the three incident faces. Observe that each white face has 2 units of charge, each black face has no charge and each remaining face has 1 unit of charge each.

The charge is now redistributed based on the following rules (the indices are taken modulo the length of the considered face where appropriate).

**Rule A** A black face $f_0 = v_1 \ldots v_6$ receives 1/2 unit of charge from the face $f_{i,i+1}$ if the path $v_{i-1}v_iv_{i+1}v_{i+2}$ is contained in the cycle $C$ and the face $f$ is white.

**Rule B** A black face $f_0 = v_1 \ldots v_6$ receives 1 unit of charge from the face $f_{i,i+1}$ if the edge $v_iv_{i+1}$ is contained in the cycle $C$, neither the edge $v_{i-1}v_i$ nor the edge $v_{i+1}v_{i+2}$ is contained in $C$ and the face $f$ is white.

The Rules A and B are illustrated in Figure 3.

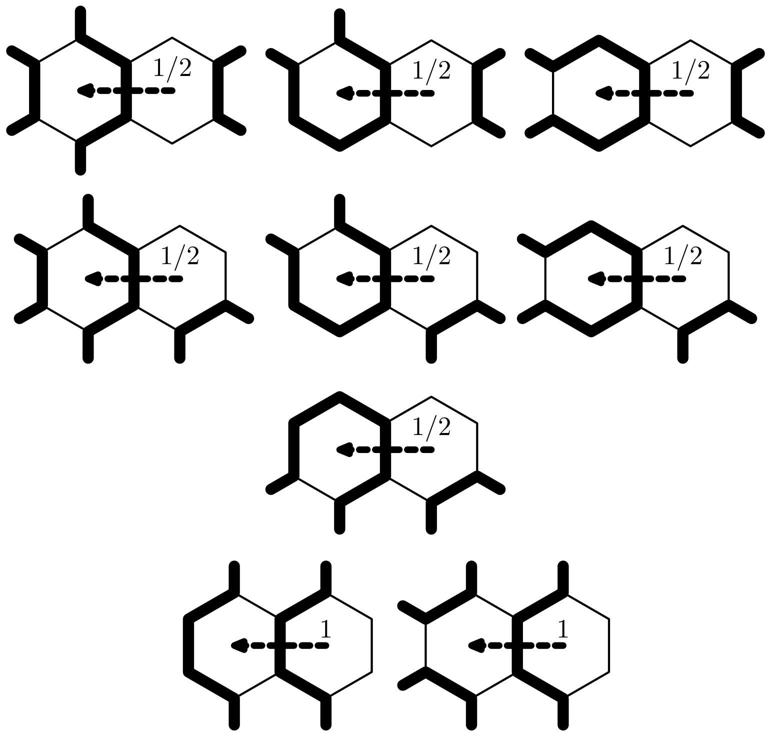


Figure 3: Configurations (up to symmetry) to which Rules A and B are applied.

In Sections 4 and 5, we show that each face has at most 1 unit of charge after applying Rules A and B. Based on this fact, we conclude in Section 6 that the number of white vertices is at most $f/3$ where $f$ is the number of faces of $G$. The bound on the length of the cycle $C$ will then follow.

# 4 Final charge of white faces

In this section, we analyze the final amount of charge of white faces. By Lemma 2, we can restrict our attention to faces of size six.

**Lemma 3.** *Let $C$ be a longest cycle of a fullerene graph $G$. Assume that the discharging rules as described in Section 3 have been applied. If $f = v_1v_2v_3v_4v_5v_6$ is a white face of $G$ such that the edges $v_2v_3$ and $v_5v_6$ are contained in $C$, then the final amount of charge of $f$ is 1 unit.*

*Proof.* The initial amount of charge of the face $f$ is 2 units. If both the face $f_{23}$ and $f_{56}$ are black faces of size six, then the face $f$ sends $1/2$ unit of charge to each of them by Rule A and thus its final amount of charge is 1 unit.

Assume that the face $f_{56}$ is not a black face of size six. Hence, the graph $G$, up to symmetry, contains one of the configurations depicted in the left column of Figure 4. Rerouting the cycle $C$ as indicated in the figure yields a cycle longer than $C$, a contradiction. Since our arguments translate to the case the face $f_{23}$ is not a black face of size six, the proof of the lemma is finished. □

**Lemma 4.** *Let $C$ be a longest cycle of a fullerene graph $G$. Assume that the discharging rules as described in Section 3 have been applied. If $f = v_1v_2v_3v_4v_5v_6$ is a white face of $G$ such that the edges $v_4v_5$, $v_5v_6$ and $v_6v_1$ are contained in $C$, then the final amount of charge of $f$ is 1 unit.*

*Proof.* First, suppose that the face $f_{56}$ is a face of size five. Rerouting the cycle $C$ as indicated in the top line of Figure 5 yields a face of size five incident with two or more white vertices (the vertices $v_5$ and $v_6$ become white). This is excluded by Lemma 2.

We conclude that the face $f_{56}$ has size six. For $i \in \{5, 6\}$, let $v_i'$ be the neighbor of the vertex $v_i$ that is not incident with the face $f$. The vertex $v_5'$ cannot be white: otherwise, rerouting the cycle $C$ as indicated in the

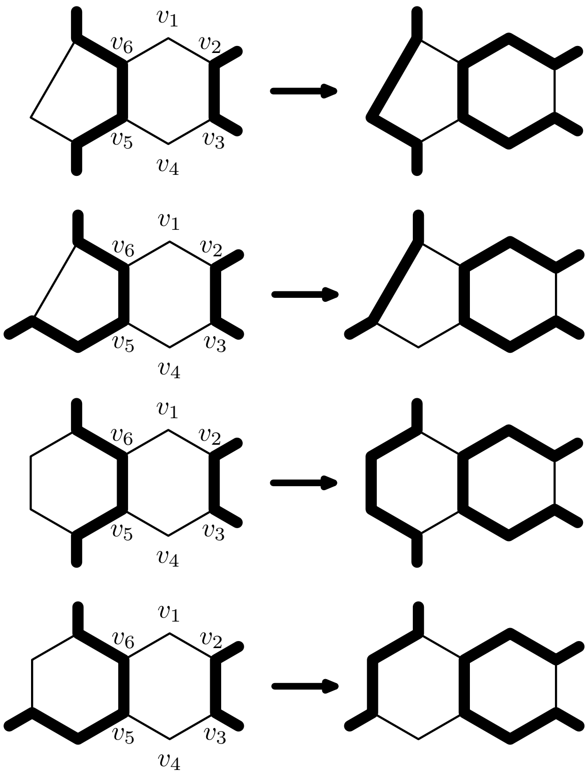


Figure 4: Configurations analyzed in the proof of Lemma 3.

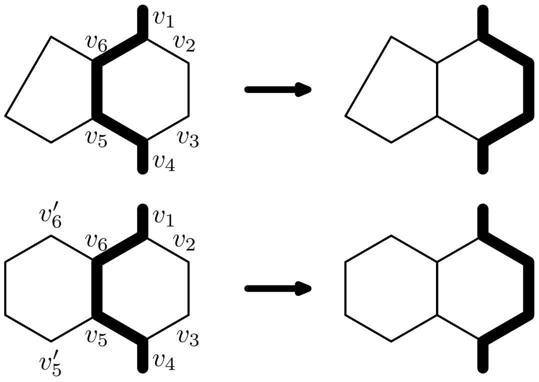


Figure 5: Configurations analyzed in the proof of Lemma 4.

bottom line of Figure 5 yields a path formed by three white vertices. This is impossible by Lemma 1. Thus, the vertex $v_5'$ is black. Similarly, the vertex $v_6'$ is black. Consequently, the face $f_{56}$ is black and by Rule B, the face $f_{56}$ receives 1 unit of charge from the face $f$. Since the face $f$ sends charge to no other face and its initial amount of charge is 2 units, its final amount of charge is 1 unit. □

**Lemma 5.** *Let $C$ be a longest cycle of a fullerene graph $G$. Assume that the discharging rules as described in Section 3 have been applied. If $f = v_1v_2v_3v_4v_5v_6$ is a white face of $G$ such that the edges $v_3v_4$ and $v_5v_6$ are contained in $C$ and the edge $v_4v_5$ is not contained in $C$, then the final amount of charge of $f$ is 1 unit.*

*Proof.* The initial amount of charge of the face $f$ is 2 units. If both the face $f_{34}$ and $f_{56}$ are black faces of size six, then the face $f$ sends 1/2 unit of charge to each of them by Rule A and thus its final amount of charge is 1 unit.

Assume that the face $f_{56}$ is not a black face of size six. Hence, the graph $G$, up to symmetry, contains one of the configurations depicted in the left column of Figure 6. Rerouting the cycle $C$ as indicated in the figure yields a cycle of $G$ longer than $C$, a contradiction. Since our arguments translate to the case where the face $f_{34}$ is not a black face of size six, the proof of the lemma is finished. □

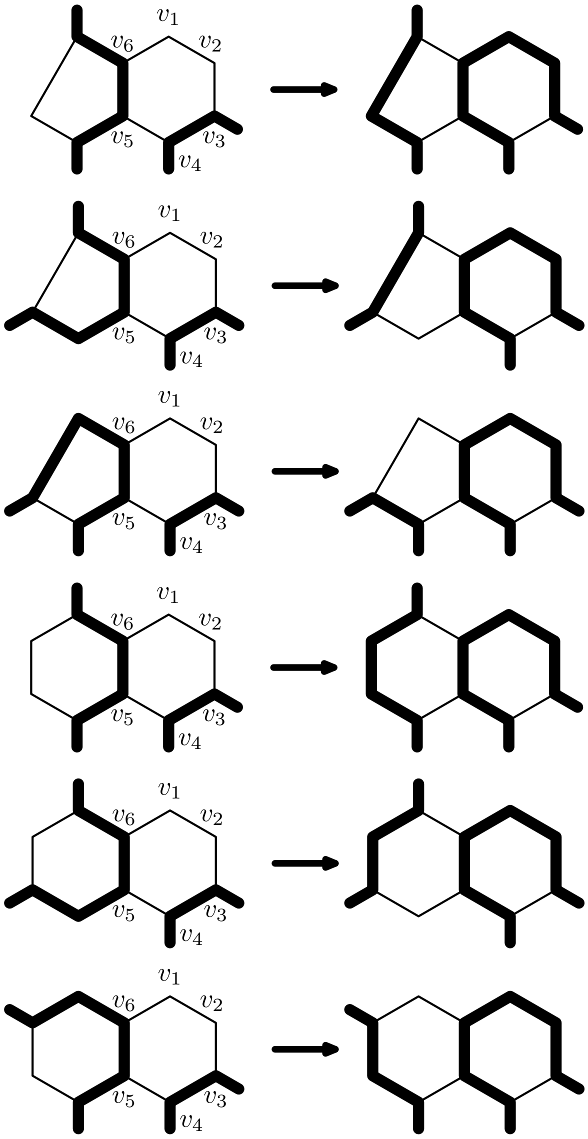


Figure 6: Configurations analyzed in the proof of Lemma 5.

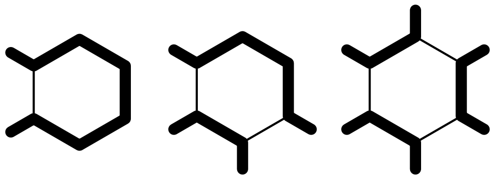

Figure 7: Black faces of size six that could receive more than 1 unit of charge.

Lemmas 2, 3, 4 and 5 yield the following.

**Lemma 6.** *Let $C$ be a longest cycle of a fullerene graph $G$. Assume that the discharging rules as described in Section 3 have been applied. The final amount of charge of any white face of $G$ is* 1 *unit.*

## 5 Final charge of black faces

This section is devoted to the analysis of the final charge of black faces. Since no black face of size five receives any charge, we can restrict our attention to black faces of size six. The final charge of a black face $f$ of size six is at most one unless the face $f$ is isomorphic to one of the faces depicted in Figure 7—note that the amount of charge of $f$ can exceed 1 unit only if Rule A applies three times to $f$, Rule B applies twice to $f$ or both Rules A and B apply to $f$. We analyze each of the configurations separately in a series of three lemmas.

**Lemma 7.** *Let $C$ be a longest cycle of a fullerene graph $G$. Assume that the discharging rules as described in Section 3 have been applied. If $f = v_1v_2v_3v_4v_5v_6$ is a black face of $G$ such that the edges $v_5v_6$, $v_6v_1$, $v_1v_2$, $v_2v_3$ and $v_3v_4$ are contained in $C$ and the edge $v_4v_5$ is not, then the final amount of charge of $f$ is at most* 1 *unit.*

*Proof.* The face $f$ can receive charge only by Rule A from the faces $f_{61}$, $f_{12}$ and $f_{23}$. Assume for the sake of contradiction that $f$ receives charge of 1/2 unit from each of these three faces. In particular, $G$ contains, up to symmetry, one of the configurations depicted in Figure 8 (recall that $G$ cannot contain a path formed by three white vertices by Lemma 1).

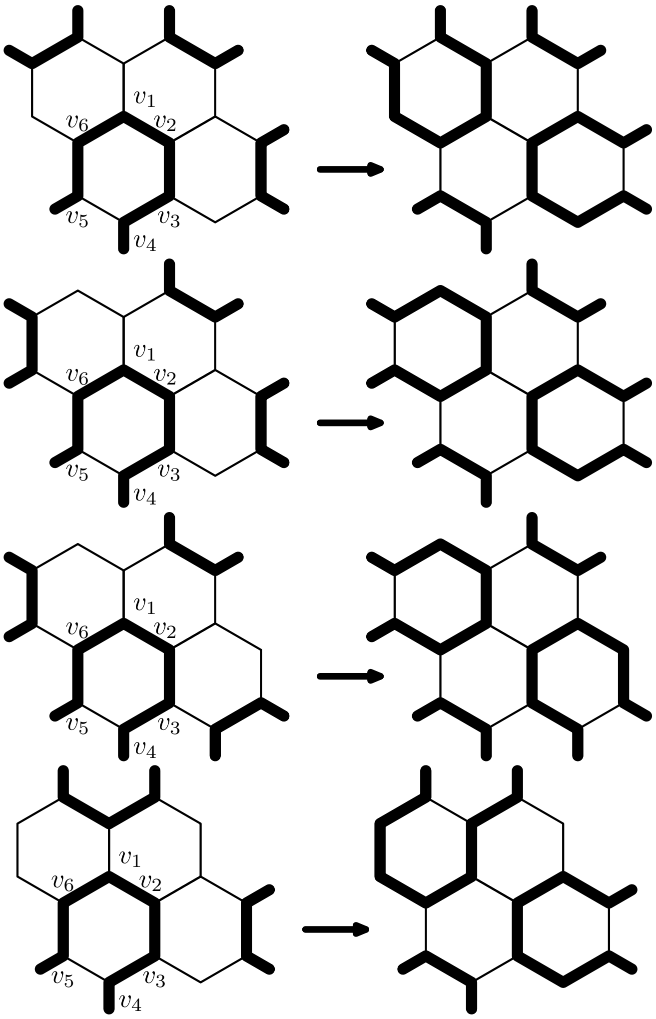


Figure 8: Configurations analyzed in the proof of Lemma 7.

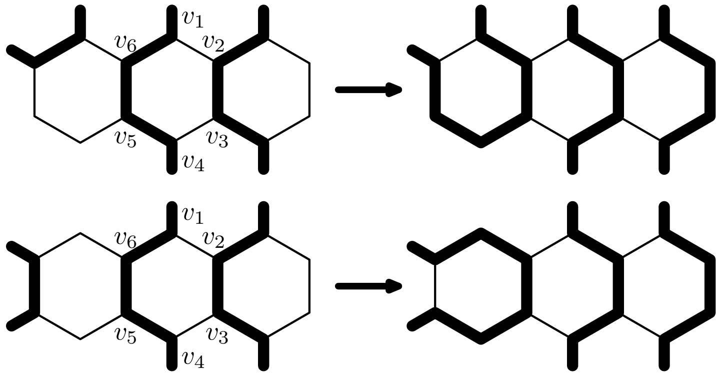


Figure 9: Configurations analyzed in the proof of Lemma 8.

Rerouting the cycle $C$ as indicated in the figure yields a cycle of $G$ longer than the cycle $C$ which contradicts our choice of $C$. We conclude that Rule A can apply at most twice to the face $f$. □

**Lemma 8.** *Let $C$ be a longest cycle of a fullerene graph $G$. Assume that the discharging rules as described in Section 3 have been applied. If $f = v_1v_2v_3v_4v_5v_6$ is a black face of $G$ such that the edges $v_2v_3$, $v_4v_5$, $v_5v_6$ and $v_6v_1$ are contained in $C$ and the edges $v_1v_2$ and $v_3v_4$ are not, then the final amount of charge of $f$ is at most 1 unit.*

*Proof.* If the final amount of charge of $f$ is greater than 1 unit, then $f$ receives 1 unit of charge from the face $f_{23}$ by Rule B and 1/2 unit of charge from the face $f_{56}$ by Rule A. Hence, $G$ contains one of the two configurations depicted in Figure 9. In either of the two cases, it is possible to reroute the cycle $C$ as indicated in Figure 9 to obtain a cycle of $G$ longer than $C$, a contradiction. □

**Lemma 9.** *Let $C$ be a longest cycle of a fullerene graph $G$. Assume that the discharging rules as described in Section 3 have been applied. If $f = v_1v_2v_3v_4v_5v_6$ is a black face of $G$ such that the edges $v_2v_3$, $v_4v_5$ and $v_6v_1$ are contained in $C$ and the edges $v_1v_2$, $v_3v_4$ and $v_5v_6$ are not, then the final amount of charge of $f$ is at most 1 unit.*

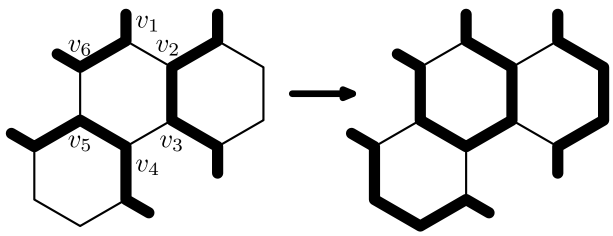


Figure 10: The configuration analyzed in the proof of Lemma 9.

*Proof.* The face $f$ can receive charge only by Rule B. Assume that Rule B applies twice to $f$. By symmetry, we may assume that the charge is given by the faces $f_{23}$ and $f_{45}$. In particular, the graph $G$ contains the configuration depicted in Figure 10. Reroute now the cycle $C$ as indicated in the figure. Since the obtained cycle is longer than the cycle $C$, we conclude that Rule B cannot apply twice to the face $f$. $\square$

Lemmas 7, 8 and 9 yield the following.

**Lemma 10.** *Let $C$ be a longest cycle of a fullerene graph $G$. Assume that the discharging rules as described in Section 3 have been applied. The final amount of charge of any black face of $G$ is at most 1 unit.*

# 6 Main result

**Theorem 11.** *Let $G$ be a fullerene graph with $n$ vertices. The graph $G$ contains a cycle of length at least $5n/6 - 2/3$.*

*Proof.* Consider a longest cycle $C$ contained in the graph $G$ and apply the discharging procedure described in Section 3. By Lemmas 6 and 10, every white and black face has final charge of at most 1 unit. Since the initial amount of charge of other faces is 1 unit and the other faces do not send out or receive any charge, we conclude that the final amount of charge of any face of $G$ is at most 1 unit.

Each white vertex has initially been assigned 3 units of charge. Since the final amount of charge of every face is at most 1 unit, the amount of charge was preserved during the discharging phase and vertices do not have any charge at the end of the process, there are at most $f/3$ white vertices where $f$ is the number of faces of $G$. By Euler's formula, $n = 2f - 4$. Hence, there are at most $n/6 + 2/3$ white vertices. Consequently, there are at least $5n/6 - 2/3$ black vertices and thus the length of the cycle $C$ is at least $5n/6 - 2/3$. $\square$

# References


[1] G. Ewald, *On shortness exponents of families of graphs*, Israel J. Math. **16** (1973) 53–61.

[2] P. W. Fowler, D. E. Manolpoulos, *An Atlas of Fullerenes*, Oxford University Press, Oxford, 1995.

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

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

[5] B. Grünbaum, J. Zaks, *The excistence of certain planar maps*, Discrete Math. **10** (1974) 93-115.

[6] S. Jendrol' and P. J. Owens, *Longest cycles in generalized Buckminsterfullerene graphs*, J. Math. Chem. **18** (1995) 83–90.

[7] W. Krätschmer, L. D. Lamb, K. Fostiropoulos, D. R. Huffman, *Solid $C_{60}$: a new form of carbon*, Nature **347** (1990) 354–358.

[8] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl and R. E. Smalley, *$C_{60}$ Buckminsterfullerene*, Nature **318** (1985) 162–163.

[9] P. J. Owens, *Non-hamiltonian simple 3-polytopes whose faces are all 5-gons or 7-gons*, Discrete Math. **36** (1981) 227–230.

[10] P. J. Owens, *Non-hamiltonian simple 3-polytopes with only one type of face besides triangles*, Ann. Discrete Math. **20** (1984), 241-251.

[11] P. J. Owens, *Regular planar graphs with faces of only two types and shortness parameters*, J. Graph Theory **8** (1984) 253–257.

[12] P. G. Tait, *Remarks on the coloring of maps*, Proc. Royal Soc. Edin. **10** (1878-1880) 501-503.

[13] R. Taylor, J. P. Hare, A. K. Abdul-Sada, H. W. Kroto, *Isolation, separation and characterisation of the fullerenes $C_{60}$ and $C_{70}$: the third form of carbon*, J. Chem. Soc. Chem. Commum. (1990) 1423–1425.

[14] M. Tkáč, *On shortness coefficients of simple* 3*-polytopal graphs with only one type of faces besides triangles*, Discrete Math. **128** (1994) 407–413.

[15] W. T. Tutte, *On hamiltonian cicuits*, J. London Math. Soc. **21** (1946) 98–101.

[16] H. Walther, *Note on two problems of J. Zaks concerning hamiltonian* 3*-polytopes*, Discrete Math. **33** (1981) 107–109.

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