

Fullerenes Which are Cayley Graphs ¹

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Abstract: Inspired by the fact that the buckminster fullerene is a Cayley graph, we are devoted to characterizing fullerenes which are Cayley graphs. Here we prove that the buckminster fullerene is the unique fullerene which is a Cayley graph.

1 Introduction

A fullerene is a cubic planar graph with all faces 5-cycles or 6-cycles. It is the topological structure of a molecule which contains only carbon atoms, and each carbon atom is bonded to exactly three others.

Let f_5 and f_6 denote the numbers of faces of a fullerene F with size 5 and 6 respectively, then we have the following result.

Lemma 1.1 (Lemma 9.8.1 in [1]) $f_5 = 12$, $n = 2f_6 + 20$, where $n = |V(F)|$.

By Lemma 1.1 we see that $n \geq 20$. Thus the dodecahedron is the smallest fullerene.

Not all fullerenes correspond to molecules which exist in nature. One necessary condition believed by many chemists is that no two 5-cycles can share a common vertex. Such fullerenes are called isolated pentagon fullerenes. By Lemma 1.1, any isolated pentagon fullerene has at least 60 vertices. There is an example on 60 vertices known

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as buckminsterfullerene. To introduce this fullerene, we need the definition of Cayley graphs.

Let G be a finite group and S an inverse-closed subset of G not containing the identity 1 of G . The Cayley graph of G related to S , denoted by $C(G, S)$, is the graph with vertex set G and, for any $x, y \in G$, x and y are adjacent in $C(G, S)$ if and only if $x^{-1}y \in S$. Now we can define the buckminsterfullerene. Let A_5 be the alternating group on the set $\{1, 2, 3, 4, 5\}$ and $T = \{(12)(34), (12345), (15432)\}$. Then the buckminsterfullerene is just the Cayley graph $C(A_5, T)$ ([1], page 209). Inspired by this fact, Professor Fuji Zhang posed the following questions: Are there any other fullerenes which are Cayley graphs? or further, can we characterize the fullerenes which are Cayley graphs? In this paper, we show the following result.

Theorem 1.1 *The buckminsterfullerene is the unique fullerene which is a Cayley graph.*

It should be noted that Klein and Liu has proved in [3] that the sole *preferable cage* (the definition of which can be found in [3]) with fewer than 70 vertices is the buckminsterfullerene. On the other hand, we prove in this paper (Lemma 2.2) that if a fullerene of order n is a Cayley graph, then one of three cases occurs, the largest n being 60. Thus Theorem 1.1 follows readily. However, we go further to provide a new proof which has much algebraic taste.

For discussion of the next section, we cite some known results as our next lemma.

Lemma 1.2[5] *Let G be a finite group and S an inverse-closed subset of G with $1 \notin S$. Then*

- (i) $C(G, S)$ is connected if and only if S generates G .
- (ii) $C(G, S)$ is vertex transitive.
- (iii) If $T = \alpha(S)$ for $\alpha \in \text{Aut}(G)$, then $C(G, S) \cong C(G, T)$

Notation and definitions not defined here are referred to [1]. For more results on fullerene, see [2] and [4].

2 Proof of the main result

To prove our main result, we first establish a sequence of lemmas. The first lemma is obvious.

Lemma 2.1 *Every cycle of length 5 or 6 in a fullerene is the boundary of a face.*

Lemma 2.2 *Let F be a fullerene of order n which is a Cayley graph. Then one of the following statements holds:*

- (i) $n = 60$, $f_6 = 20$, every vertex of F is contained in exactly one cycle of length 5 and exactly two cycles of length 6.
- (ii) $n = 30$, $f_6 = 5$, every vertex of F is contained in exactly two cycles of length 5 and exactly one cycle of length 6.
- (iii) $n = 20$, $f_6 = 0$, every vertex of F is contained in exactly three cycles of length 5.

Proof. By Lemma 1.1 we have

$$n = 2f_6 + 20 \quad (1)$$

Since Cayley graph is vertex transitive, the number of cycles of length 5 or 6 containing a vertex is independent of the choice of vertices. Therefore, we may let n_r be such number for $r = 5$ or 6. Then we have

$$n_5 \times n = 60, \quad (2)$$

and

$$n_6 \times n = 6f_6. \quad (3)$$

Since $n \geq 20$, (2) has three solutions: $(n_5, n) = (1, 60), (2, 30), (3, 20)$. For $n = 60, 30, 20$, by (1) we have $f_6 = 20, 5, 0$, respectively. Then by (3) we have $n_6 = 2, 1, 0$, respectively. The result follows. \square

Let $F = C(G, S)$ be a 3-regular connected Cayley graph. Then $|S| = 3$, S is a generating set of G and can be written as one of the following forms:

- (i) $S = \{a, b, c\}$, $a^2 = b^2 = c^2 = 1$.
- (ii) $S = \{a, b, b^{-1}\}$, $a^2 = b^k = 1$, $k \geq 3$.

Lemma 2.3 *Let G be a finite group and $S = \{a, b, c\}$ be a generating set of G with $a^2 = b^2 = c^2 = 1$. Then the Cayley graph $C(G, S)$ is not a fullerene.*

Proof. By contradiction, suppose $C(G, S)$ is a fullerene. Then by Lemma 2.2 we may assume that C is a 5-cycle containing the identity 1 of G . Since the neighbor set $N(1)$

of 1 is S , we have $|V(C) \cap S| = 2$. Without loss of generality, we may assume that $V(C) \cap S = \{a, c\}$. Then there exists $u_1, u_2, u_3 \in S$ such that

$$C = (1, a, au_1, au_1u_2, au_1u_2u_3 = c)$$

Clearly, $u_1 \neq a$, $u_2 \neq u_1$, $u_3 \neq u_2$ and $u_3 \neq c$. Then $u_1 \in \{b, c\}$. We now consider two cases.

Case 1. $u_1 = b$;

Since $u_2 \neq u_1$, $u_2 \neq b$, we have $u_2 \in \{a, c\}$.

If $u_2 = a$, then $u_3 = b$ and $c = (ab)^2$. Thus G can be generated by $\{a, ab\}$ with $a^2 = (ab)^4 = 1$ and $a(ab)a = ba = (ab)^{-1}$. It follows that $|G| = 8$, a contradiction.

If $u_2 = c$, then $u_3 = a$ and $c = abca$. Thus $b = (ac)^2$. Now G can be generated by $\{a, ac\}$ with $a^2 = (ac)^4 = 1$ and $a(ac)a = (ac)^{-1}$. But these imply that $|G| = 8$, a contradiction.

Case 2. $u_1 = c$;

By a similar argument as above we can obtain a contradiction. \square

In what follows, we consider the case where $S = \{a, b, b^{-1}\}$ with $a^2 = b^k = 1$ and $k \geq 3$.

Lemma 2.4 *Let G be a finite group and $S = \{a, b, b^{-1}\}$ be a generating set of G with $a^2 = b^k = 1$ and $k \geq 3$. Suppose that $C(G, S)$ is a fullerene and C is a 5-cycle containing 1 of G . If $a \in V(C)$, then $aba = b^{\pm 2}$, $k = 15$ and $|G| = 30$.*

Proof. Assume, without loss of generality that $V(C) \cap S = \{a, b\}$. Then there exist $u_1, u_2, u_3 \in S$ such that

$$C = (1, a, au_1, au_1u_2, au_1u_2u_3 = b)$$

Clearly, $u_1 \neq a$, $u_2 \neq u_1^{-1}$, $u_3 \neq u_2^{-1}$ and $u_3 \neq b$. It follows that $u_3 \in \{a, b^{-1}\}$, and if $u_1 = b$, then $u_2 \in \{a, b\}$; if $u_1 = b^{-1}$, then $u_2 \in \{a, b^{-1}\}$. We now consider two cases.

Case 1. $u_1 = b$ and $u_2 \in \{a, b\}$;

If $u_2 = a$ then $u_3 = b^{-1}$, and so $aba = b^2$; If $u_2 = b$ then $u_3 = a$, and so $ab^2a = b$, that is, $aba = b^2$.

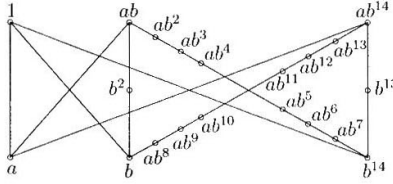


Figure 1: $C(G, S)$ has a subgraph that is a subdivision of $K_{3,3}$

Case 2. $u_1 = b^{-1}$ and $u_2 \in \{a, b^{-1}\}$;

If $u_2 = a$ then $u_3 = b^{-1}$, and so $ab^{-1}ab^{-1} = b$, that is, $aba = b^{-2}$; If $u_2 = b^{-1}$ and $u_3 = a$ then $aba = b^{-2}$; If $u_2 = b^{-1}$ and $u_3 = b^{-1}$ then $a = b^4$.

From the above discussion we know that there are only two situations: $a = b^4$ or $aba = b^{\pm 2}$. In the former case, G contains subgroup $\langle b \rangle$ of order 8. Hence $|G| \neq 20, 30, 60$. In the later case, the order k of b must be odd and so $|G| = 2k$. By Lemma 2.2 we conclude that $k = 15$ and $|G| = 30$. \square

Corollary 2.1 *If the Cayley graph $C(G, S)$ is a fullerene, then $|G| \neq 20$.*

Proof. By Lemma 2.3, we can write $S = \{a, b, b^{-1}\}$, $a^2 = b^k = 1$, $k \geq 3$. If $|G| = 20$, then by Lemma 2.2, every vertex is contained in three 5-cycles. Thus, there exists a 5-cycle C containing 1 such that $V(C) \cap S = \{a, b\}$. But then, by Lemma 2.4, we have $|G| = 30$, a contradiction. \square

Corollary 2.2 *If the Cayley graph $C(G, S)$ is a fullerene, then $|G| \neq 30$.*

Proof. By Lemma 2.3, we can write $S = \{a, b, b^{-1}\}$, $a^2 = b^k = 1$, $k \geq 3$. If $|G| = 30$, then by Lemma 2.2, every vertex is contained in exactly two 5-cycles. Therefore, there exists a 5-cycle C containing a . Without loss of generality we may assume that $V(C) \cap S = \{a, b\}$. Then from the proof of Lemma 2.4 we have $aba = b^{\pm 2}$, $k = 15$ and $|G| = 30$. We only consider the case where $aba = b^2$, the other case can be similarly discussed. Now $abi a = b^{2i}$, $i = 1, 2, \dots, 15$, especially, $ab^8 a = b$, $ab^7 a = b^{14}$ and $ab^{14} a = b^{13}$. From these we can see that $C(G, S)$ contains a subgraph depicted in Figure 1.

This subgraph is a subdivision of $K_{3,3}$, thus $C(G, S)$ is not planar, a contradiction. \square

This subgraph is a subdivision of $K_{3,3}$, thus $C(G, S)$ is not planar, a contradiction. \square

Lemma 2.5 *If the Cayley graph $C(G, S)$ is a fullerene with $S = \{a, b, b^{-1}\}$, then $|G| = 60$, $b^5 = 1$ and the unique 5-cycle C containing 1 must contain b and b^{-1} .*

Proof. By Lemma 2.2, Corollary 2.1 and Corollary 2.2 we have $|G| = 60$. Now we show that $b, b^{-1} \in V(C)$. If, to the contrary, $\{b, b^{-1}\} \not\subseteq V(C)$, then $a \in V(C)$. By Lemma 2.4 we have $|G| = 30$, a contradiction. Thus $V(C) \cap S = \{b, b^{-1}\}$. Then there exist $u_1, u_2, u_3 \in S$ such that

$$C = (1, b, bu_1, bu_1u_2, bu_1u_2u_3 = b^{-1}) \quad (4)$$

Thus $u_1u_2u_3 = b^{-2}$. If only one of u_1, u_2 and u_3 is a , then we have $a = b^m, m \leq 4$. Thus G is a cyclic group of order no more than $2m \leq 8$, a contradiction. If there are two a 's in $\{u_1, u_2, u_3\}$, then, from (4) we have, $u_1 = u_3 = a$. But then $aba = b^{\pm 2}$ and, by the proof of Lemma 2.4, $|G| = 30$, a contradiction. Thus $u_1, u_2, u_3 \in \{b, b^{-1}\}$. Clearly, $u_1 \neq b^{-1}$, we have $u_1 = b$, and therefore $u_2 = u_3 = b$. This gives $b^5 = 1$. \square

Lemma 2.6 *Let G be a group of order 60 and $S = \{a, b, b^{-1}\}$ be a generating set of G with $a^2 = b^5 = 1$. If the Cayley graph $C(G, S)$ is a fullerene, then 6-cycles containing 1 must contain a .*

Proof. Let C be a 6-cycle containing 1. By way of contradiction, if $a \notin V(C)$, then $V(C) \cap S = \{b, b^{-1}\}$. Thus, there exist $u_1, u_2, u_3, u_4 \in S$ such that

$$C = (1, b, bu_1, bu_1u_2, bu_1u_2u_3, bu_1u_2u_3u_4 = b^{-1}) \quad (5)$$

From (5), $u_1u_2u_3u_4 = b^{-2}$. If $u_1 = b$, then $u_2u_3u_4 = b^{-3}$, by a similar argument as in the proof of Lemma 2.5 we can deduce that $|G| \leq 30$, a contradiction. Thus $u_1 \neq b$. If $u_4 = b$, then $u_1u_2u_3 = b^{-3}$. By the similar argument as above we can obtain a contradiction. Thus $u_4 \neq b$. Again from (5), $u_1 \neq b^{-1}$ and $u_4 \neq b^{-1}$. Therefore $u_1 = u_4 = a$ and $u_2u_3 = ab^{-2}a$. Since $u_2u_3 \neq 1$, u_2u_3 is one of ab, ba, b^2 and b^{-2} , and further $ab^{-2}a = b^{\pm 2}$. Since $b^5 = 1$, $aba = b^{\pm 1}$ and so $|G| = 10$, a contradiction. \square

Proof of Theorem 1.1. Let the Cayley graph $C(G, S)$ be a fullerene. Then by Lemma 2.3 we see that $S = \{a, b, b^{-1}\}$ with $a^2 = b^k = 1$. By Lemma 2.5 we have $|G| = 60$ and $k = 5$.

Let C be a 6-cycle containing 1. Then by Lemma 2.6, $a \in V(C)$. Without loss of generality, we may assume that $V(C) \cap S = \{a, b^{-1}\}$. Then there exist $u_1, u_2, u_3, u_4 \in S$ such that

$$b^{-1} = au_1u_2u_3u_4, \quad (6)$$

and the cycle C can be written as

$$C = (1, a, au_1, au_1u_2, au_1u_2u_3, au_1u_2u_3u_4 = b^{-1}) \quad (7)$$

From (7), we know that $u_1 \neq a$, $u_2 \neq u_1^{-1}$, $u_3 \neq u_2^{-1}$ and $u_4 \neq b^{-1}$.

Claim 1. $u_1 = b$; Otherwise, $u_1 = b^{-1}$, and so $u_2 \in \{a, b^{-1}\}$. From (6) we have

$$u_2u_3u_4 = bab^{-1}.$$

First suppose that $u_2 = a$. Then $u_3 \in \{b, b^{-1}\}$. If $u_3 = b$, we have $u_4 = b$ or $u_4 = a$. The former leads to $ab^2 = bab^{-1}$, that is $aba = b^3$, which implies $|G| = 10$, a contradiction; The later leads to $aba = bab^{-1}$, and further $b^2 = 1$, a contradiction. If $u_3 = b^{-1}$, we have $u_4 = b^{-1}$ or $u_4 = a$. If $u_4 = a$ occurs, then $ab^{-1}a = bab^{-1}$, and further $b^2 = 1$, a contradiction.

Next suppose that $u_2 = b^{-1}$. Then $u_3 = b^{-1}$ or a . In the former case we have $u_4 = a$. Therefore $aba = b^{-1}$ and $|G| = 10$. In the later case, we have $u_4 = b$. Therefore $b^{-1}ab = bab^{-1}$, that is $ab^2a = b^2$. Since $b^5 = 1$, this gives $aba = b$ and so $|G| = 10$, a contradiction.

Claim 2. $u_2 = a$; Otherwise, $u_2 = b$ and $u_3 = a$ or b . From (6) and Claim 1, we have

$$u_2u_3u_4 = b^{-1}ab^{-1} \quad (8)$$

If $u_3 = a$, we have $u_4 = b$ and $bab = b^{-1}ab^{-1}$, that is, $ab^2a = b^{-2}$. Since $b^5 = 1$, we have $aba = b^{-1}$. Thus $\langle b \rangle$ is a normal subgroup of G and $|G| = 10$, a contradiction. If $u_3 = b$, then $u_4 \in \{a, b\}$. If $u_4 = a$, then $b^{-1}ab^{-1} = b^2a \implies aba = b^{-3}$. This gives $|G| = 10$, a contradiction. If $u_4 = b$, then $b^3 = b^{-1}ab^{-1} \implies a = b^5 = 1$, again a contradiction.

Claim 3. $u_3 = b$; Otherwise, $u_3 = b^{-1}$ and $u_4 = a$. Then $ab^{-1}a = b^{-1}ab^{-1}$, and so $b^2 = 1$, this is impossible.

Claim 4. $u_4 = a$; Otherwise, $u_4 = b$. Then $ab^2 = b^{-1}ab^{-1}$, that is, $b^{-3} = aba$. But then $|G| = 10$, a contradiction.

From the above four Claims and (6) we deduce the following relations for the elements of S :

$$a^2 = b^5 = 1 \text{ and } (ab)^3 = 1$$

Then it is not difficult to show that any element in G must be one of the following forms:

$$b^i, b^i ab^j, b^i(ab^2a)b^j, b^i(ab^2ab^{-2}a), \text{ where } 0 \leq i, j \leq 4$$

Since $|G| = 60$, the above representation for the elements of G is unique. In the alternating group A_5 of degree 5, if we let $\bar{a} = (12)(34)$ and $\bar{b} = (12345)$, then $\bar{b}^{-1} = (15432)$ and $\bar{a}^2 = \bar{b}^5 = (\bar{a}\bar{b})^3 = 1$. Therefore the elements of A_5 can also be expressed in the following forms:

$$\bar{b}^i, \bar{b}^i \bar{a} \bar{b}^j, \bar{b}^i (\bar{a} \bar{b}^2 \bar{a}) \bar{b}^j, \bar{b}^i (\bar{a} \bar{b}^2 \bar{a} \bar{b}^{-2} \bar{a}), \text{ where } 0 \leq i, j \leq 4$$

Then the following mapping

$$\sigma : \begin{cases} b^i & \longrightarrow \bar{b}^i \\ b^i ab^j & \longrightarrow \bar{b}^i \bar{a} \bar{b}^j \\ b^i ab^2 ab^j & \longrightarrow \bar{b}^i \bar{a} \bar{b}^2 \bar{a} \bar{b}^j \\ b^i ab^2 ab^{-2} ab^j & \longrightarrow \bar{b}^i \bar{a} \bar{b}^2 \bar{a} \bar{b}^{-2} \bar{a} \bar{b}^j \end{cases} \quad \text{where } 0 \leq i, j \leq 4$$

defines a group isomorphism from G to A_5 , and under this mapping, we have $a \longrightarrow \bar{a}$, $b \longrightarrow \bar{b}$ and $b^{-1} \longrightarrow \bar{b}^{-1}$. Thus if we set $T = \{\bar{a}, \bar{b}, \bar{b}^{-1}\}$, then by Lemma 2.2 we have $C(G, S) \cong C(A_5, T)$. The result follows. \square

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