Parameterization of Fullerenes Via Singularity-Combinations

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Abstract: Fullerene can be embedded in a piecewise linear 2-manifold with singularities corresponding to the non-hexagonal faces. Adjacent two or three singularities can be combined as a whole cut out from a parent cone led by a parent singularity. With proper combinations, fullerene can be simplified to a parent structure easily to be parameterized. In this paper, singularity-combinations of fullerenes were studied, and the symmetries of the combining singularities on the parent cone were revealed. Then, fullerenes with different shapes were studied for parameterization with singularity-combinations, and parameters characterizing its shape were obtained for each type. These parameters are practical for fullerenes, especially those far from icosahedrons.

Keywords: fullerene; parameterization; singularity-combination; manifold; parent structure.

1 Introduction

A fullerene graph (fullerene for short) is a polyhedral graph with only pentagonal and hexagonal faces, modeling an allotrope of carbon. It can be embedded in a piecewise linear manifold, which can be obtained through cut-and-glue from a graphene sheet, with singularities corresponding to the non-hexagonal faces [1-3]. The latticed manifold is called fullerene manifold, or fullerene for short. As easy to measure, the fullerene manifold is the default model of fullerenes for symmetries and parameterization in literature. Researchers have focused on symmetries and parameterization for decades, trying to establish a systematic theory for the structure of fullerene [4, 5].

A fullerene manifold can be treated as the surface of a master polyhedron. With icosahedron (not necessarily regular) as the master polyhedron, the present author has studied the intrinsic symmetries of fullerene and accomplished a general parameterization. However, in some cases, such as carbon nanotubes, the icosahedron model is not perfect as it may be distorted, and the value of some parameters may be negative [1].

In a fullerene manifold, the area around each singularity is a cone. The area around a cluster of singularities is part of a master cone (or cylinder in special). Adjacent two or three singularities can be combined as a cluster cut out from the master cone. If so, the master cone is called the parent cone, and the virtual apex of the master cone is called the parent singularity of the cluster. With a proper combination of singularities, a fullerene may have a simple parent structure. If the parent can be parameterized, the fullerene can also be parameterized.

In 1998, William P. Thurston had proposed that fullerenes can be simplified and parameterized with singularity-combinations [4]. However, the proposal has not attracted enough attention and the related exploration has been delayed for decades.

In this paper, combinations of singularities were studied and parameterizations of different types of fullerenes were explored in light of the combinations. The remainder of the paper is as follows. In section 2 and section 3, the combination of two singularities and the combination of three singularities were studied respectively, and intrinsic symmetries of the combining singularities on their parent cones were revealed. In section 4, in light of the combinations, the caps of tube-like fullerenes are classified and parameterized separately for parameterization of the fullerenes. In Section 5, the octahedral, tetrahedral, and $D_3$ fullerenes were parameterized with the combinations. In section 6, the conclusion and outlook were presented.

This article is a sequel of literature [1]. Readers are recommended to read literature [1] first as many results of [1] are quoted in this paper.
2 Combination of two singularities

2.1 Geometric analysis

Let $S$, $T$ be two adjacent singularities. Cones $S$ and $T$ can be unfolded together as Figure 1a. First, unfold cone $T$ along a generatrix, and then unfold cone $S$ along line segment $ST$. In the figure, $T_1$, and $T_2$ represent the different positions of singularity $T$ after unfolding. As the angular defects of the singularities are all $60^\circ$, the angle between the two positions of the generatrix is $120^\circ$ after twice unfolding. The parent cone can be built up by gluing along the generatrix and filling the opening as the surface extension. Let $P$ be the parent singularity of $S$&$T$ as Figure 1b. Since $T_1$, $T_2$ are coincident after gluing, so, $PT_1 = PT_2$, $\angle T_1PT_2 = 120^\circ$.

As triangle $ST_1T_2$ is equilateral according to unfolding, point $P$ is its center. Then in Figure 1c,

$$\angle SPT_1 = \angle SPT_2 = 120^\circ.$$  

This means that two combining singularities are symmetrically distributed on the parent cone. Their intrinsic field angle from the parent singularity is half of the cone angle, i.e. $120^\circ$.

![Fig.1. combination of two singularities. (a) Together unfolding of two adjacent cones $S$&$T$. (b) Position of the parent singularity $P$. (c) The relationship of $S$, $T$, and $P$. (d) Unconventional singularity.](image)

The singularities $S$ and $T$ can be trimmed out from the parent cone $P$: flatten the surface of the cone $P$ along lines $PS$, $PT$, trim off the apex of the cone along the connecting line segment of $ST$, and seal the remaining part of the cone. Then singularities, each with an angular defect of $60^\circ$, will appear at points $S$ and $T$.

2.2 Coxeter coordinates for the parent singularity

Because of the symmetry, the Coxeter coordinates from point $P$ to $S$ and $T$ are identical. Let the Coxeter coordinates be $(m, n)$, and the Coxeter coordinates between $S$ and $T$ be $(s, t)$ as Figure1c, their relationship can be derived as follows with the Eisenstein plane [2].

The hexagonal lattice is congruent to an Eisenstein plane characterized by a triangular lattice. The Eisenstein plane is a complex plan with unit vectors in the six directions denote with $I$, $\omega$, $\omega^2$. 

\( \omega^3, \omega^4, \omega^5 \), where \( \omega = e^{i2\pi/6} \) is the complex root of equation \( \omega^6 = 1 \). As \( \omega^3 = -1, \omega^2 = \omega - 1 \), each vector in the Eisenstein plane can be express as \( (a+b\omega) \), with \( (a, b) \) known as Eisenstein integers.

In Figure 2c,

\[
\beta_i = \beta + \frac{\beta}{\omega^i}
\]

so

\[
s + t\omega = (n + m\omega^5) + (m + n\omega) \\
= n + m(1 - \omega) + m + n\omega \\
= (n + 2m) + (n - m)\omega
\]

This means

\[
\begin{cases}
s = n + 2m \\
t = n - m
\end{cases}
\]  

(1)

From (1) we can get:

\[
\begin{cases}
m = (s - t)/3 \\
n = (s + 2t)/3
\end{cases}
\]  

(2)

According to formula (2), when \( s \equiv t \mod (3) \), the Coxeter coordinates \( m, n \) are all integers. In this case, the parent singularity corresponds to the center of a square, i.e. a singularity with 4 degrees.

When \( S \) and \( T \) are not congruent with module 3, then \( m \) and \( n \) are not integers. In this case, the parent singularity corresponds to a carbon atom. Such parent singularity is called the first kind of unconventional singularity, to distinguish from another kind in section 3.

3 Combination of three singularities
3.1 Geometric analysis

Let \( A, B, \) and \( C \) be three adjacent singularities. Cones \( A, B, \) and \( C \) can be unfolded together as Figure 2a. First, unfold cone \( C \) along a generatrix, and then unfold cones \( A, B \) along lines segments \( CA, CB \) respectively. As the angular defects of the singularities are all 60°, the angle between two positions of the generatrix is 180° after triple unfolding. The parent cone can be built up by gluing along the generatrix and filling the opening as the surface extension. Let \( P \) be the parent singularity (Figure 2b). As points \( C_1 \) and \( C_2 \) are coincident after gluing, then,

\[ PC_1 = PC_2, \quad \angle C_1PC_2 = 180°. \]

This means point \( P \) (marked with \( \oplus \) in Figure 2) is just at the center point of line segment \( C_1C_2 \), and points \( C_1 \) and \( C_2 \) are symmetrical about point \( P \). The point \( C_1\&C_2 \) after gluing indicates the location of singularity \( C \) on the parent cone. Because of this symmetry, only two of the three locations of \( A, B, \) and \( C \) on the parent cone are independent. As triangles \( BC_1C_3 \) and \( AC_1C_2 \) in Figure 2b are equilateral according to unfolding, with the location of points \( C_1 \) and \( B \), we can obtain the position for points \( C_2, C_3 \), and then for point \( A \).

The quadrilateral \( ABC_1C_2 \) represents the extension area of the parent cone. If \( \angle ACB = 60° \), then \( \angle C_1C_3B + \angle AC_1B + \angle AC_2C_1 = 180° \). In this case, point \( C_3 \) is on line \( C_1C_2 \). Similarly, if \( \angle ACB > 60° \), point \( C_3 \) is inside the quadrilateral; if \( \angle ACB < 60° \), point \( C_3 \) is outside the quadrilateral.

The singularities \( A, B, \) and \( C \) can be truncated out from the parent cone \( P \): take the cone manifold as the surface of triangular pyramid \( PABC \), truncate off the apex through points \( A, B, \) and \( C, \) and extend the lattice to section \( ABC \). Then singularities, each with an angular defect of 60°, will appear at points \( A, B, \) and \( C \). 

3
3.2 Coxeter coordinates for the parent singularity

Let $a$, $b$, $c$, and $A$ be the four parameters for the triangle $ABC$ as literature [1], the Coxeter coordinates from $P$ to $A$, $B$, $C$ be $(m_a, n_a)$, $(m_b, n_b)$, $(m_c, n_c)$, separately. Then the Coxeter coordinates between $C_i$ and $C_2$ in Figure 2c is $(2m_c, 2n_c)$. Just as section 2, with the help of the Eisenstein plane, the following relationship can be obtained:

$$
\begin{align*}
  m_c &= \frac{(c + a)}{2} + \Delta \\
  n_c &= \frac{(c + b)}{2}
\end{align*}
$$

(3)

The expressions of $m_a$, $n_a$, $m_b$, and $n_b$ can also be obtained with the same method. All these expressions can be written in a formula with matrix:

$$
\begin{pmatrix}
  m_a \\
  n_a \\
  m_b \\
  n_b \\
  m_c \\
  n_c
\end{pmatrix} = \begin{pmatrix}
  1/2 & 1/2 & 0 & 1 \\
  0 & 1/2 & 0 & 2 \\
  0 & 1/2 & 1/2 & 0 \\
  1/2 & 0 & 1/2 & 1 \\
  1/2 & 0 & 1/2 & 0
\end{pmatrix} \begin{pmatrix}
  a \\
  b \\
  c \\
  \Delta
\end{pmatrix}
$$

(4)

According to formula (4), if $a$, $b$, and $c$ have the same parity, the Coxeter coordinates of point $A$, $B$, $C$ to point $P$ are all integers. In this case, the parent singularity corresponds to the center of a triangle, i.e. a singularity with three degrees.

If $a$, $b$, and $c$ don't have the same parity, the Coxeter coordinates of point $A$, $B$, $C$ to point $P$ are not all integers. In this case, the parent singularity does not correspond to the center of a triangle, just as Figure 2d. The parent cone can also be obtained by cut-and-glue from a graphene sheet, with vertex corresponding to the center of a carbon bond. Such parent singularity is called the second kind of unconventional singularity.
4 Parameterization of tube-like fullerenes

4.1 Parameterization of caps

Just as carbon nanotubes, most fullerenes have a tube-like structure. The twelve singularities of a tube-like fullerene cluster into two sextuples, each forming a cap of the tube. According to the number of singularities adjacent to the tube, from more to less, the caps can be classified into five types: hexagon, pentagonal pyramid, trimmed square pyramid, truncated triangular pyramid, and trimmed shrunk pyramid. The two caps of one fullerene are not necessarily of the same type.

Cap of pentagonal pyramid

If there are five singularities adjacent to the tube, the cap is a pentagonal pyramid. As shown in Figure 3a, five pairs of Coxeter coordinates \((m_i, n_i)\) for the bottom edges can be selected as the independent parameters for the cap. These parameters determine the relative position of the bottom vertices in the unfolding. As the triangle \(AB_1B_2\) is equilateral according to the unfolding, the position for apex \(A\) is determined, and the detail for the cap can be obtained.

\[
\begin{align*}
5 = 1 = 1 \\
\sum_{i=1}^{5} m_i = \sum_{i=1}^{5} n_i
\end{align*}
\]

Cap of trimmed square pyramid

If there are four singularities adjacent to the tube, the cap can be trimmed out from a square pyramid. Just as figure 4a, four singularities \(A, B, C,\) and \(D\) are adjacent to the tube. They and the parent singularity \(P\) of \(E\&F\) form a square pyramid \(P-ABCD\).

Similar to Figure 3a, four pairs of Coxeter coordinates of the bottom edges can be selected as the independent parameters for the pyramid. According to section 2, \(PE = PF, \angle EPF = 120^\circ\). A pair of Coxeter coordinates are needed to locate the singularities \(E\) and \(F\). These 10 parameters in total are adequate for the cap of trimmed pyramid.

With the locations \(E\) and \(F\), we can draw an equilateral triangle \(EFG\) as Figure 4a. The unfolding of the pyramid falling in the triangle is to be trimmed off. Then we get the detailed unfolding of the cap.

As \(P\) may be the first kind of unconventional singularity, to avoid non-integer values, the Coxeter coordinates for \(E/F\) can refer to the base vertices (point \(A\) for example) of the pyramid instead of the apex \(P\).
If there are three singularities adjacent to the tube, the cap can be truncated out from a triangular pyramid. Just as Figure 4(a), three singularities \(A, B, C\) of the cap are adjacent to the tube. They and the parent singularity \(P\) of \(D, E, \) and \(F\) form a triangular pyramid \(P-ABC\).

Similar to Figure 3(a), the three pairs of Coxeter coordinates of its bottom edges can be selected as its independent parameters. According to section 3, points \(D_1\) and \(D_2\) are symmetrical about point \(P\), triangles \(D_1D_2E\) and \(D_2D_3F\) are equilateral. Two pairs of Coxeter coordinates are needed for two of three locations of singularities \(D, E, \) and \(F\). These 10 parameters in total are adequate for a truncated triangular pyramid.

As \(P\) may be the second kind of unconventional singularity. To avoid non-integer values, the Coxeter coordinates for \(D, E, \) and \(F\) can refer to the base vertices of the pyramid point instead of the apex \(P\) (point \(A\) for \(D, \) point \(B\) for \(E,\) for example).

**Cap of trimmed shrinked pyramid**

If there are only two singularities adjacent to the tube, the cap can be transformed into a shrunk pyramid with combinations. The shrunk pyramid has only two lateral faces. Just as Figure 4c, singularities \(A\) and \(B\) are adjacent to the tube; \(G\) is the parent singularity of \(C\) and \(D; H\) is the parent singularity of \(E\) and \(F.\) The virtual singularities \(G\) and \(H\) can also be combined to get a parent singularity \(P,\) which is the apex of the shrunk pyramid \(P-AB.\) The angular defect of singularity \(P\) is 240° as those of \(G\) and \(H\) are all 120°. Just as the combination of two singularities with angular defects of 60° in section 2, \(G\) and \(H\) are symmetrically distributed on the parent cone \(P,\) and their intrinsic field angle from \(P\) is half of the cone angle. Therefore, in the figure, \(\angle GPH=60°,\) and the triangle \(GHP\) is equilateral.

On the parent cone \(P,\) only three locations of four points \(C, D, E, \) and \(F\) are independent. For
example, if points C and D are known, point G can be obtained according section 2, and then point H can also be obtained according to the symmetry mentioned above. If point E is also known, point F can be obtained. With three pairs of Coxeter coordinates for these locations and two pairs of Coxeter coordinates for the base edges of the shrunk pyramid, the detailed unfolding of the cap can be obtained. These five pairs of Coxeter coordinates can be selected as independent parameters.

Cap of hexagon
If six singularities are all adjacent to the tube, the cap is a hexagon as Figure 4d. As a closed-loop of edges, its shape can be determined by five of the six pairs of Coxeter coordinates for the edges. These five pairs of Coxeter coordinates can be selected as the independent parameters. With the help of the Eisenstein plane, the Coxeter coordinates for the sixth side can be obtained as:

\[
\begin{align*}
m_6 &= m_1 + m_3 - m_5 + n_1 + n_2 - n_4 - n_3 \\
n_6 &= -m_1 - m_2 + m_4 + m_5 - n_1 + n_3 + n_4
\end{align*}
\]

4.2 Independent Parameters for a tube-like fullerene
With an inner point selected as a virtual apex, the hexagon cap can be treated as a hexagonal pyramid. Therefore, each tube-like fullerene has a parent structure as a tube with two caps of pyramids. Just as Figure 3b, to match the tube, the parameters for each pyramid should satisfy two constraint equations similar to formula (5), with different ranges of variable i according to the number of its base edges. For a tube-like fullerene, two pairs of constraint equations can be simplified to two constraint equations without parameters m, n.

Each cap has ten independent parameters. Only 18 of the 20 parameters for the two capes of a tube-like fullerene are independent because of the two constrain equations mentioned above. Together with another two parameters for the relative position of the two caps, as (k, l) in Figure 3, they make up twenty independent parameters for the fullerene.

5 Parameterization of octahedral/tetrahedral/D\textsubscript{3} fullerenes
Except for clustering into two sextuples as a tube-like fullerene, the 12 singularities of a fullerene may also evenly cluster into three quads, four triples, or six pairs. In these cases, they have simple polyhedral parent structures.

Octahedral fullerenes
A fullerene whose singularities cluster into six pairs is called an octahedral fullerene, or O-fullerene for short, as its parent structure has an octahedral master polyhedron.

If the parent singularities of the six pairs are all conventional 4-degree singularities, the octahedral fullerene is a trimmed (4,6)-fullerene. As each pair of singularities have two independent parameters according to section 2, a trimmed (4,6)-fullerene has 12 such parameters in total. Together with the 8 independent parameters for the parent (4,6)-fullerene selected in literature [1], they make up 20 independent parameters for the trimmed (4,6)-fullerene.

Just as Figure 5a, if the lattice is refined with one-third-sized hexagons, the first kind of unconventional singularity will become a conventional 4-degree singularity. Therefore, other octahedral fullerenes can be parameterized with the same method as trimmed (4,6)-fullerenes, and the difference is that the value of the parameters may not be integers.

Tetrahedral fullerenes
A fullerene whose singularities cluster into four triples is called a tetrahedral fullerene [5], or T-fullerene for short [6], as its parent structure has a tetrahedral master polyhedron.

If the parent singularities for each cluster are all conventional 3-degree singularities, the
tetrahedral fullerene is a truncated (3,6)-fullerene. As each triple of singularities has four independent parameters according to section 3, a truncated (3,6)-fullerene has 16 such parameters in total. Together with the 4 independent parameters for the parent (3,6)-fullerene selected in literature [1], they make up 20 independent parameters for the truncated (3,6)-fullerene.

Just as Figure 5b, if the lattice is refined with half-sized hexagons, the second kind of unconventional singularities will become conventional 3-degree singularities. Therefore, other tetrahedral fullerenes can also be parameterized as truncated (3,6)-fullerenes, and the difference is that the value of the parameters may not be integers.

![Fig.5. Transformation of unconventional singularities.](image)

(a) If the lattice is refined with one-third-sized hexagons, the first kind of unconventional singularity will be transformed to a conventional 4-degree singularity. (b) If the lattice is refined with half-sized hexagons, the second kind of unconventional singularity will be transformed to a conventional 3-degree singularity.

The Tetrahedral fullerene mentioned in literature [5] is a truncated (3,6)-fullerene. Its parent fullerene is a Goldberg polyhedron with two independent parameters. The truncations for its four cones are all regular truncations with the same pair of parameters. Therefore, the tetrahedral fullerene has only four independent parameters.

**D₃-fullerenes**

A fullerene whose singularities cluster into three quads is called D₃-fullerene [6], as its parent has a master polyhedron as dihedron D₃. Just as singularities C, D, E, and F in Figure 4c, each quad has six independent parameters. Therefore, a D₃-fullerene has 18 such parameters in total. Its parent structure, the triangular dihedron, has only two independent parameters [4]. Together, they make up 20 independent parameters for the D₃-fullerene.

6 Conclusion and outlook

Fullerenes come in different shapes depending on the distribution of their singularities. Their parent structures which represent their major shape as frameworks can be obtained by singularity-combinations. Fullerenes can be parameterized with the parameters of their parent structures.
together with those of the location of the combining singularities. Characterizing the shapes of the fullerenes, these parameters may vary from type to type, but they are practical, especially for those fullerenes far from icosahedrons.

A pair of Coxeter coordinates from a four-degree singularity has two possible trimming results. Two pairs of Coxeter coordinates from a three-degree singularity can correspond to up to six possible truncations. Therefore, it is essential to specify the Coxeter coordinates for parameters (illustrate in the unfolding graph for example) or eliminate ambiguity with further classification.

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