The configuration space of equilateral and equiangular polygons with up to 6 vertices (等辺等角 n 角形の配置空間 ($n \leq 6$))

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Abstract

We study the configuration space of equilateral and equiangular polygons with n vertices when $n \leq 6$. We illustrate an explicit shape of a polygon which corresponds to a given point in the configuration space.

概要　$\mathbb{R}^3$ の等辺等角 n 角形 ($n \leq 6$) 全体のなす配置空間と、その各点が表す配置を具体的に求めた。

1 Introduction

An equilateral and equiangular polygon is a mathematical model of a cycloalkane. Gordon Crippen studied the space of the shapes of cycloalkanes of n carbons up to the case when $n = 7$ ([C]). He used "*metric matrices*", which are $n \times n$ matrices given by inner products of pairs of edge vectors. He gave the conformaton spaces of cyclobutanes ($n = 4$, the bond angle θ belongs to $[0, \frac{\pi}{4}]$) and of cyclopentanes ($n = 5$, $\theta \in [\frac{\pi}{5}, \frac{3\pi}{5}]$). When the number n of carbons is 6 or 7, for a fixed bond angle $\theta = \cos^{-1}(-\frac{1}{3})$ (Figure 1), he showed that the conformation space of cyclohexanes consists of a circle which includes the conformation of a *boat* (Figure 2) and a point which corresponds to the conformation of a *chair* (Figure 3), and that of cyclopentanes consists of two circles, one for boat/twist-boat and the other for chair/twist-chair. In these two cases, he showed it by searching out all the possible values through numerical experiment with 0.05 step size.

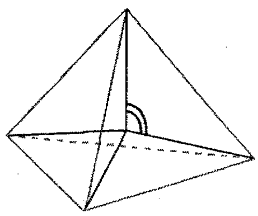

Figure 1: $\theta = \cos^{-1}(-\frac{1}{3})$

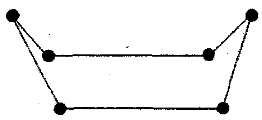

Figure 2: *boat*

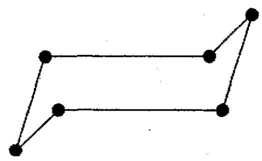

Figure 3: *chair*

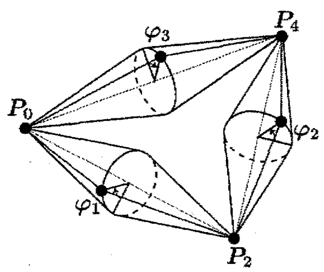

Figure 4: Double cone expression

In this paper we study the configuration space in a different way using a "*double cone*" method (Figure 4). We give the configuration space and an explicit configuration of each element of it in a theoretical way in the case when $n \leq 6$ and for any *mathematically* possible angle θ.

There have been a great number of studies of the configuration spaces of *linkages*. An excellent survey can be found in [D-OR]. Symplectic geometry of polygon spaces was studied in [Kp-M] and [Km-T].

2 The configuration spaces

Definition 2.1 Let n be the number of vertices. Let θ be the "*bond angle*", i.e. the angle between adjacent edges ($0 \leq \theta < \pi$). Put

$$\widetilde{\mathcal{M}}_n(\theta) = \left\{ \mathcal{P} = (P_0, \cdots, P_{n-1}) \,|\, P_i \in \mathbb{R}^3,\ |P_i - P_{i+1}| = 1,\ \angle P_{i-1}P_iP_{i+1} = \theta\ \ (\forall i\ (\mathrm{mod.}\, n)) \right\}.$$

Let G be the group of motions of $\mathbb{R}^3$, i.e. the group of orientation preserving isometries of $\mathbb{R}^3$. Any motion of $\mathbb{R}^3$ can be expressed as a composition of rotations and translations.

Put $\mathcal{M}_n(\theta) = \widetilde{\mathcal{M}}_n(\theta)/G$, and call it the *configuration space of unit equilateral and θ-equiangular n-gons.*

Remark 2.2 (1) We allow intersections of edges and overlapping of vertices.

(2) We distinguish two *configurations* illustrated in Figures 5 and 6 in the configuration space $\mathcal{M}_6$, although their *shapes* are the same.

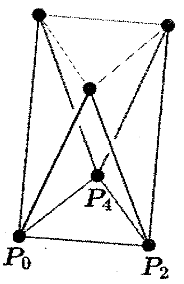

Figure 5: A "*positive crown*"

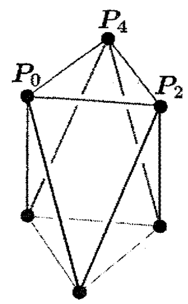

Figure 6: A "*negative crown*"

Cauchy's Arm Lemma (see, for example, [D-OR]) implies

Lemma 2.3 *The configuration space $\mathcal{M}_n(\theta)$ is a non-empty set only if the "bond angle" θ satisfies $0 \leq \theta \leq (1 - \frac{2}{n})\pi$ if n is even or $\frac{\pi}{n} \leq \theta \leq (1 - \frac{2}{n})\pi$ if n is odd. If θ takes one of the extremal values then the configuration space consists of only one point which corresponds to a planar configuration given as follows:*

(1) *If $\theta = (1 - \frac{2}{n})\pi$ then it is a regular n-gon* (Figure 7).

(2) *If n is even and $\theta = 0$ then it is an n times covered single edge* (Figure 8).

(3) *If n is odd and $\theta = \frac{\pi}{n}$ then it is a regular star shape* (Figure 9).

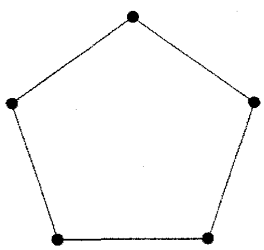

Figure 7: Regular pentagon

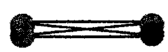

Figure 8: Four times covered edge

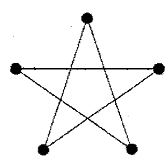

Figure 9: Star pentagon

2.1 $n \leq 5$ cases

Proposition 2.4 (Cf. [C][1]) *The configuration space $\mathcal{M}_n(\theta)$ of equilateral and θ-equiangular n-gons and its elements are given by the following.*

[1]The statement (3) seems different from that of Crippen's.

(1) *When* $n = 3$, $\mathcal{M}_3(\theta) \cong \{1 \text{ point}\}$ *which corresponds to a regular triangle if* $\theta = \frac{\pi}{3}$, *and* $\mathcal{M}_3(\theta) \cong \emptyset$ *otherwise.*

(2) *When* $n = 4$, $\mathcal{M}_4(\theta) \cong \{1 \text{ point}\}$ *which corresponds to a four time covered edge if* $\theta = 0$ *or a square if* $\theta = \frac{\pi}{4}$, *and* $\mathcal{M}_4(\theta) \cong \{2 \text{ points}\}$ *which correspond to a non-planar "folded rhombus in the diagonal" and its mirror image if* $0 < \theta < \frac{\pi}{4}$ (Figure 10).

(3) *When* $n = 5$, $\mathcal{M}_5(\theta) \cong \{1 \text{ point}\}$ *which corresponds to a regular star pentagon if* $\theta = \frac{\pi}{5}$ *or a regular pentagon if* $\frac{3\pi}{5}$, *and* $\mathcal{M}_5(\theta) \cong \emptyset$ *otherwise.*

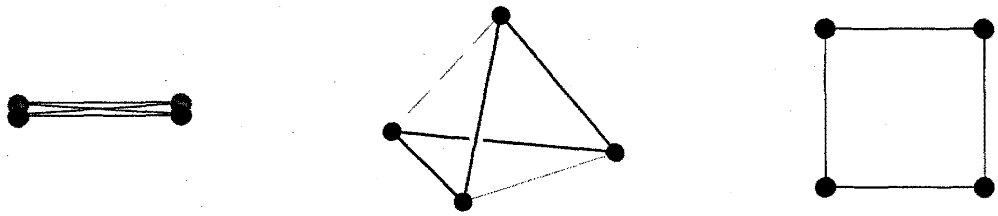

Figure 10: $n = 4$ case. The middle is a non-planar "folded rhombus in the diagonal".

2.2 The space of equilateral and equiangular hexagons

Recall that $\mathcal{M}_6(\theta) \not\cong \emptyset$ only if $0 \leq \theta \leq \frac{2\pi}{3}$. $\mathcal{M}_6(0)$ consists of one point which corresponds to a 6 times covered edge, and $\mathcal{M}_6(\frac{2\pi}{3})$ consists of one point which corresponds to a regular planar hexagon.

Theorem 2.5 *The configuration space* $\mathcal{M}_6(\theta)$ *of equilateral and* θ*-equiangular hexagons* $(0 < \theta < \frac{2\pi}{3})$ *is given as follows.*

(1) *When* $\frac{\pi}{3} < \theta < \frac{2\pi}{3}$ $\mathcal{M}_6(\theta)$ *is a disjoint union of a circle and* 2 *points.*

The circle contains a point which corresponds to the configuration of a boat (Figure 2), *i.e. the circle is the space of reconformatins of a boat, and the* 2 *points correspond to the configuration of a chair* (Figure 3) *and that of its mirror image.*

(2) *When* $0 < \theta < \frac{\pi}{3}$ $\mathcal{M}_6(\theta)$ *is a disjoint union of two circles and* 4 *points.*

One of the circles contains a point which corresponds to the configuration of a boat (Figure 11) *and the other that of its mirror image. Two of the four points correspond to the configurations of a chair and its mirror image, and the remaining two to the configuration illustrated in* Figure 12 *and its mirror image.*

(3) *When* $\theta = \frac{\pi}{3}$ $\mathcal{M}_6(\frac{\pi}{3})$ *is a disjoint union of* 1*-skelton of a tetrahedron with each edge being doubled as illustrated in* Figure 13 *and* 2 *points.*

The two points correspond to the configurations of a chair and its mirror image.

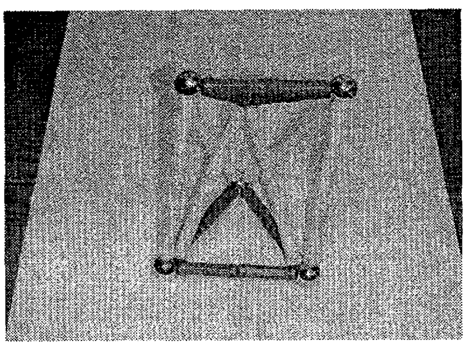

Figure 11: A *boat* with a small bond angle

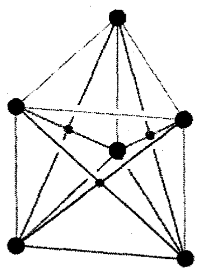

Figure 12: "*inward crown*" in a prism. Two edges intersect each other in a side face of the prism.

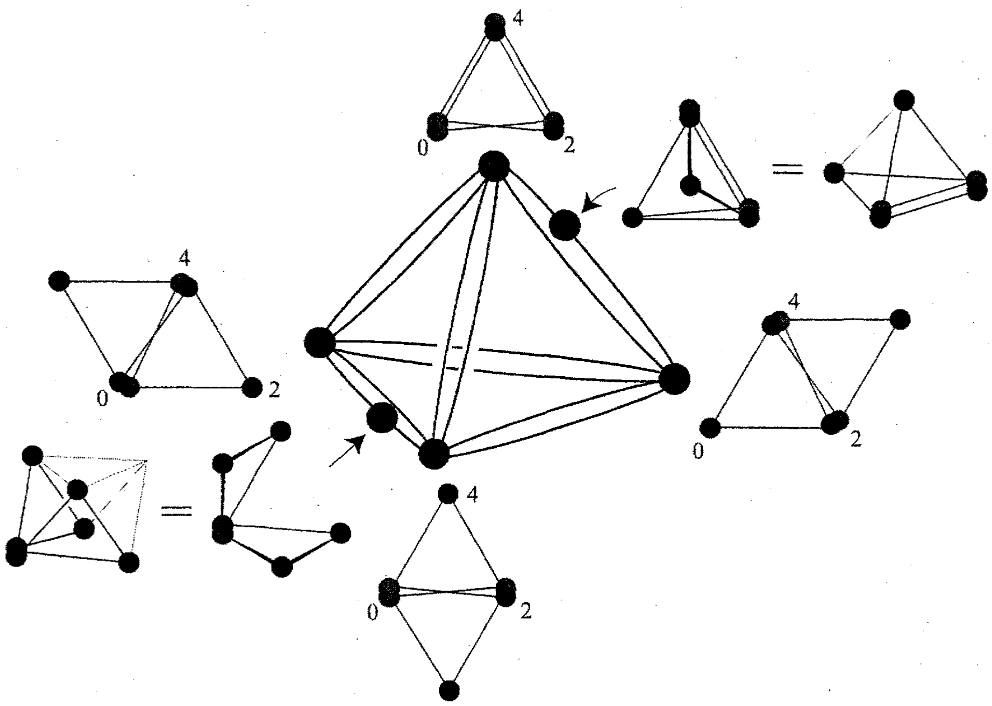

Figure 13: The configuration space $\mathcal{M}_6(\frac{\pi}{3}) \setminus \{\text{chairs}\}$. The numbers $0, 2$, and 4 identify the vertices. One of the vertices (top) corresponds to the configuration of a double-covered regular triangle. The other vertices correspond to the other planar configurations consisting of two regular triangles.
The configurations of the top and the right vertices have the positions of the vertices P_0, P_1, P_2, P_4, and P_5 in common. The circle joining the two vertices in the configuration space consists of the configurations where the vertex P_3 rotates around the axis P_2P_4.
On the other hand, the configurations of the left and bottom veritces have the positions of the vertices P_0, P_2, P_3, and P_4 in common. The circle joining the two vertices in the configuration space consists of the configurations where the vertex P_3 rotates around the axis P_2P_4 and P_5 around P_4P_0. The position of P_5 is determined by that of P_3.

Corollary 2.6 *A boat and its mirror image can be joined by a path in the configuration space, i.e. they can be continuously deformed from one to the other, if and only if the bond angle θ is not smaller than $\frac{\pi}{3}$. (Remark that a boat is planar if $\theta = \frac{\pi}{3}$.)*

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