O'Hara, J.
Osaka J. Math.
50 (2013), 477–489

THE CONFIGURATION SPACE OF EQUILATERAL AND EQUIANGULAR HEXAGONS

JUN O'HARA

(Received July 25, 2011, revised September 20, 2011)

Abstract

We study the configuration space of equilateral and equiangular spatial hexagons for any bond angle by giving explicit expressions of all the possible shapes. We show that the chair configuration is isolated, whereas the boat configuration allows one-dimensional deformations which form a circle in the configuration space.

1. Introduction

Let $\mathcal{P}$ be a closed polygon with n vertices in $\mathbb{R}^3$. We express $\mathcal{P}$ by its vertices, $\mathcal{P} = (P_0, P_1, \dots, P_{n-1})$, with suffixes modulo n. A polygon $\mathcal{P}$ is called *equilateral* if the edge length $|P_{i+1} - P_i|$ is constant, and *equiangular* if the angle $\angle P_{i-1}P_iP_{i+1}$ is constant. This angle between two adjacent edges is called the *bond angle* and will be denote by θ in this paper. An equilateral and equiangular polygon can be considered as a mathematical model of a cycloalkane. We are interested in the set of all the possible shapes (which are called conformations in chemistry) of such polygons when the number n of the vertices and the bond angle θ is fixed, i.e. the configuration space of equilateral and equiangular polygons. We remark that we allow intersections of edges and overlapping of vertices in this paper. If the condition for the bond angles is dropped off, the configuration space of equilateral polygons has been intensively studied. See, for example, [3], which is an excellent survey of linkages, [5], [6], [7], and [8]. On the other hand, an equilateral and equiangular polygon is called a *θ-regular stick knot* if the edges meet only at their common vertices. This subject has appeared in [11], and the space of θ-regular stick knots and unknots has been studied in [10] for the ideal tetrahedral bond angle $\cos^{-1}(-1/3) \approx 109.47^\circ$ (Fig. 1) and for general values of θ in [1, 4, 9]. In particular, the space of θ-regular stick hexagonal knots was studied in [9].

Gordon Crippen studied the configuration space of equilateral and equiangular polygons for $n \leq 7$ ([2]). To be precise, what he obtained is not the configuration space itself, but the space of the "*metric matrices*", which are $n \times n$ matrices whose entries are inner products of pairs of edge vectors, and then he gave the corresponding conformations. When $n = 4$ (cyclobutanes) and $n = 5$ (cyclopentanes) he considered all the possible bond angles, but when $n = 6$ (cyclohexanes) and $n = 7$ (cyclopentanes) he fixed the

2000 Mathematics Subject Classification. Primary 65D18; Secondary 51E12, 55R80.

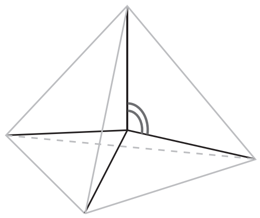

Fig. 1. $\theta = \cos^{-1}(-1/3)$.

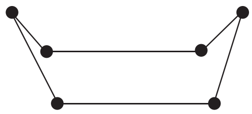

Fig. 2. a *boat*.

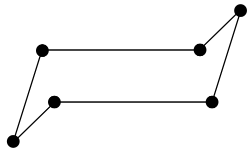

Fig. 3. a *chair*.

bond angle to be the ideal tetrahedral bond angle. He showed that if $n = 6$ the conformation space is a union of a circle which contains a *boat* (Fig. 2) and an isolated point of a *chair* (Fig. 3), and that if $n = 7$ it 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 of the entries of the metric matrix through numerical experiment with 0.05 step size.

In this paper we show that when $n = 6$ a chair cannot be continuously deformed into a boat for any bond angle. As there does not seem to be any geometric invariant which implies that a chair and a boat belong to different components of the configuration space, we will describe the configuration space of hexagons explicitly. Namely, we express all the possible configurations in terms of the parameters illustrated in Fig. 7 by trigonometric computation.

The topological type of the configuration space depends on the bond angle θ. First remark that we distinguish vertices in our study, and hence our configuration space is not equal to the space of shapes. If θ is big ($\pi/3 < \theta < 2\pi/3$) the situation is same as that of cyclohexanes of ideal tetrahedral bond angle studied by Crippen. On the other hand, if θ is small ($0 < \theta < \pi/3$), a new configuration ("*inward crown*" illustrated in Fig. 10) appears, and the one dimensional continuum of deformation of a boat is divided into two pieces, which implies that we cannot deform a boat into its mirror image. In between these two general cases, there is an exceptional case $\theta = \pi/3$, when the inward crown, which degenerates to a doubly covered triangle, can be deformed to boats via newly appeared families of configurations. In any case, a chair is an isolated configuration, whereas a boat allows one-dimensional deformations starting from and ending at it. Moving pictures of deformation of a boat for some values of θ can be found at `http://www.comp.tmu.ac.jp/knotNRG/math/configuration.html`. They illustrate how the configuration spaces when θ is close to $\pi/3$ degenerate as θ approaches $\pi/3$. Of course, as extremal cases, we have a 6 times covered multiple edge and a regular hexagon when $\theta = 0, 2\pi/3$.

This paper is based on the author's talk at "Knots and soft-matter physics, Topology of polymers and related topics in physics, mathematics and biology", YITP, Kyoto, 2008 (A short announcement of the result without proof was reported in *Bussei Kenkyuu* **92**, (2009), 119–122).

Fig. 4. A chair when θ is small and its mirror image.

The author thanks Jorge Alberto Calvo for the information of the study of the α-regular stick knots and the reference [1].

NOTATIONS. Throughout the paper, we agree that $C = \cos(\theta/2)$ and $S = \sin(\theta/2)$. The suffixes are understood modulo n. The angle $\angle P_i$ means $\angle P_{i-1}P_iP_{i+1}$.

2. Preliminaries

DEFINITION 2.1. Put

$$\tilde{\mathcal{M}}_n(\theta) = \left\{ \begin{matrix} \mathcal{P} = (P_0, \dots, P_{n-1}) \\ (P_i \in \mathbb{R}^3) \end{matrix} \;\middle|\; \begin{matrix} |P_i - P_{i+1}| = 1, \\ \angle P_{i-1}P_iP_{i+1} = \theta \end{matrix} \quad (\forall i \pmod n) \right\}.$$

Let G be the group of orientation preserving isometries of $\mathbb{R}^3$. Put $\mathcal{M}_n(\theta) = \tilde{\mathcal{M}}_n(\theta)/G$, and call it the *configuration space of θ-equiangular unit equilateral n-gons* ($0 \le \theta < \pi$). Let us denote the equivalence class of a polygon $\mathcal{P}$ by $[\mathcal{P}]$.

REMARK 2.2. (1) We allow intersections of edges and overlapping of vertices.
(2) We distinguish the vertices when we consider our configuration space. Therefore, two configurations illustrated in Fig. 4 correspond to different points in $\mathcal{M}_6$, although their *shapes* are the same.
(3) When we express an equilateral and equiangular polygon we may fix the first three vertices, P_0, P_1, and P_2. There are $(n-3)$ more vertices, whereas we have $(n-2)$ conditions for the lengths of the edges, and $(n-1)$ conditions for the angles. Therefore, we may expect that the dimension of $\mathcal{M}_n(\theta)$ is equal to $3(n-3)-(n-2)-(n-1) = n-6$ in general if the conditions are independent, which is not the case when $n \le 6$ as we will see.

When $n \le 5$ the configuration space is given as follows. It can be proved by trigonometric computation.

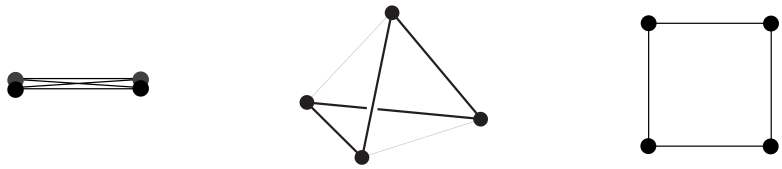

Fig. 5. $n = 4$ case. The middle is a non-planar configuration.

Fig. 6. $n = 5$ case. A regular star shape (left) and a regular pentagon (right).

Proposition 2.3 ([2]). *The configuration spaces $\mathcal{M}_n(\theta)$ of equilateral and θ-equiangular n-gons* ($n = 3, 4, 5$) *and the shapes of polygons which correspond to the elements are given by the following.*

$$\mathcal{M}_3(\theta) \cong \begin{cases} \{1 \text{ point}\} & (\theta = \pi/3) \text{ regular triangle,} \\ \emptyset & \text{otherwise,} \end{cases}$$

$$\mathcal{M}_4(\theta) \cong \begin{cases} \{1 \text{ point}\} & (\theta = 0) \text{ 4-folded edge (Fig. 5 left),} \\ \{2 \text{ points}\} & (0 < \theta < \pi/4) \text{ folded rhombus (Fig. 5 center)} \\ & \text{and its mirror image,} \\ \{1 \text{ point}\} & (\theta = \pi/4) \text{ square (Fig. 5 right),} \\ \emptyset & \text{otherwise,} \end{cases}$$

$$\mathcal{M}_5(\theta) \cong \begin{cases} \{1 \text{ point}\} & (\theta = \pi/5) \text{ regular star shape (Fig. 6 left),} \\ \{1 \text{ point}\} & (\theta = 3\pi/5) \text{ regular pentagon (Fig. 6 right),} \\ \emptyset & \text{otherwise.} \end{cases}$$

3. Equilateral and equiangular hexagons

Put $C = \cos(\theta/2)$ and $S = \sin(\theta/2)$.

First note that P_0, P_2, and P_4 form a regular triangle of edge length $2S$. We may fix

$$P_0 = \begin{pmatrix} -S \\ 0 \\ 0 \end{pmatrix}, \quad P_2 = \begin{pmatrix} S \\ 0 \\ 0 \end{pmatrix}, \quad P_4 = \begin{pmatrix} 0 \\ \sqrt{3}S \\ 0 \end{pmatrix}. \tag{3.1}$$

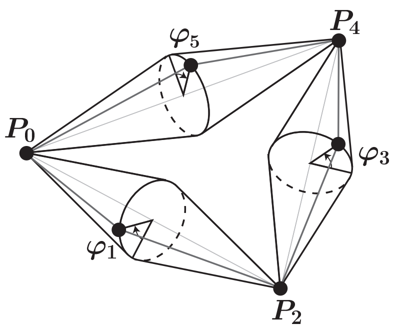

Fig. 7. Double cone or suspension expression.

Any element in $\mathcal{M}_6(\theta)$ has exactly one representative hexagon with P_0, P_2, and P_4 being as above. Let us use a "*double cone*" or suspension expression of a hexagon (Fig. 7), namely, we express P_1, P_3, and P_5 by

$$P_1 = \begin{pmatrix} 0 \\ -C\cos\varphi_1 \\ C\sin\varphi_1 \end{pmatrix}, \quad P_3 = \begin{pmatrix} \frac{1}{2}S + \frac{\sqrt{3}}{2}C\cos\varphi_3 \\ \frac{\sqrt{3}}{2}S + \frac{1}{2}C\cos\varphi_3 \\ C\sin\varphi_3 \end{pmatrix},$$

$$P_5 = \begin{pmatrix} -\frac{1}{2}S - \frac{\sqrt{3}}{2}C\cos\varphi_5 \\ \frac{\sqrt{3}}{2}S + \frac{1}{2}C\cos\varphi_5 \\ C\sin\varphi_5 \end{pmatrix} \tag{3.2}$$

for some φ_1, φ_3, and φ_5. Now the conditions $|P_j - P_{j+1}| = 1$ $(\forall j)$ and $\angle P_1 = \angle P_3 = \angle P_5 = \theta$ are satisfied.

The condition $\angle P_{i+1} = \theta$ $(i = 1, 3, 5)$ is equivalent to

$$\begin{aligned} &C^2(\cos\varphi_i \cos\varphi_{i+2} - 2\sin\varphi_i \sin\varphi_{i+2}) + \sqrt{3}SC(\cos\varphi_i + \cos\varphi_{i+2}) \\ &= 3 - 5C^2, \end{aligned} \tag{3.3}$$

which is equivalent to

$$\begin{aligned} &C(C\cos\varphi_i + \sqrt{3}S)\cos\varphi_{i+2} - 2C^2 \sin\varphi_i \sin\varphi_{i+2} \\ &= 3 - 5C^2 - \sqrt{3}SC\cos\varphi_i. \end{aligned} \tag{3.4}$$

Remark that the equations $ax + by = d$ $(a^2 + b^2 > 0)$ and $x^2 + y^2 = 1$ have solutions

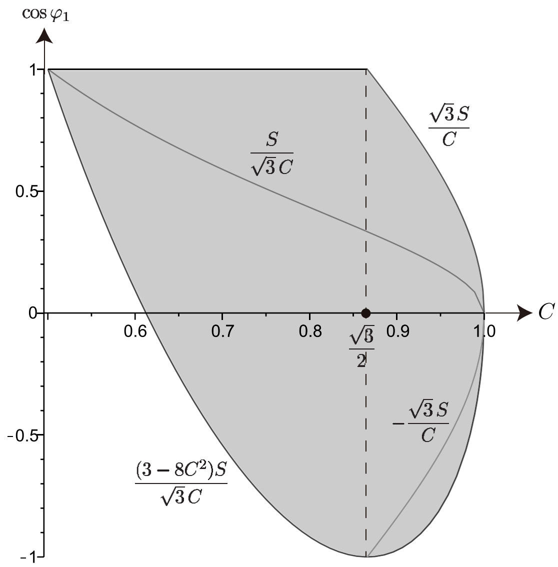

Fig. 8. The region of $\cos\varphi_1$ so that there are φ_3 and φ_5 satisfying $\angle P_0 = \angle P_2 = \theta$.

if and only if $a^2 + b^2 - d^2 \geq 0$, when we have

$$x = \frac{ad \pm b\sqrt{a^2+b^2-d^2}}{a^2+b^2}, \quad y = \frac{bd \mp a\sqrt{a^2+b^2-d^2}}{a^2+b^2}. \tag{3.5}$$

In our case (3.4), by substituting

$$\begin{aligned} a &= C(C\cos\varphi_i + \sqrt{3}S), \quad b = -2C^2\sin\varphi_i, \\ d &= 3 - 5C^2 - \sqrt{3}SC\cos\varphi_i, \end{aligned} \tag{3.6}$$

we have $a^2 + b^2 = 4 - (S - \sqrt{3}C\cos\varphi_i)^2$, which is positive unless $\theta = \pi/3$ and $\varphi_i = \pi$, and

$$a^2 + b^2 - d^2 = -\sqrt{3}(C\cos\varphi_i - \sqrt{3}S)(\sqrt{3}C\cos\varphi_i - (3-8C^2)S). \tag{3.7}$$

It follows that when $(\theta, \varphi_1) \neq (\pi/3, \pi)$ there are φ_3 and φ_5 so that $\angle P_0 = \angle P_2 = \theta$ if and only if $\cos\varphi_1$ satisfies

$$\frac{(3-8C^2)S}{\sqrt{3}C} \leq \cos\varphi_1 \leq \frac{\sqrt{3}S}{C},$$

which can happen if and only if $C = \cos\theta/2 \geq 1/2$, i.e. $0 \leq \theta \leq 2\pi/3$ (Fig. 8).

3.1. The general case when $(\theta, \varphi_1) \neq (\pi/3, \pi)$. Let us first assume that θ and φ_1 satisfy the conditions above mentioned and search for the case when φ_3 and φ_5 that make $\angle P_0 = \angle P_2 = \theta$ also satisfy $\angle P_4 = \theta$. (We will study the case when $(\theta, \varphi_1) = (\pi/3, \pi)$ later.) We have two cases, either $\varphi_3 \neq \varphi_5$ or $\varphi_3 = \varphi_5$.

CASE I. Assume $\varphi_3 \neq \varphi_5$. Remark that this can occur if and only if φ_1 satisfies

$$\frac{(3-8C^2)S}{\sqrt{3}C} < \cos\varphi_1 < \frac{\sqrt{3}S}{C} \quad (0 < \theta < 2\pi/3).$$

Then the conditions $\angle P_0 = \angle P_2 = \theta$ imply that φ_3 and φ_5 are given by

$$\begin{aligned} &\{(\cos\varphi_3, \sin\varphi_3), (\cos\varphi_5, \sin\varphi_5)\} \\ &= \left\{\left(\frac{ad \pm b\sqrt{a^2+b^2-d^2}}{a^2+b^2}, \frac{bd \mp a\sqrt{a^2+b^2-d^2}}{a^2+b^2}\right)\right\}, \end{aligned} \tag{3.8}$$

where a, b, and d are given by (3.6). Computing the left hand side of (3.3), we have

$$\begin{aligned} &C^2\left(\frac{a^2d^2 - b^2(a^2+b^2-d^2)}{(a^2+b^2)^2} - 2\frac{b^2d^2 - a^2(a^2+b^2-d^2)}{(a^2+b^2)^2}\right) + \sqrt{3}SC\frac{2ad}{a^2+b^2} \\ &= 3 - 5C^2, \end{aligned}$$

which implies that the condition $\angle P_4 = \theta$ is always satisfied in this case. Now (3.2) shows that P_3 and P_5 are given by

$$\begin{aligned} P_3 &= \begin{pmatrix} S - \dfrac{\sqrt{3}C\cos\varphi_1 - (3-8C^2)S \pm \sqrt{3}C\sin\varphi_1\sqrt{a^2+b^2-d^2}}{4-(S-\sqrt{3}C\cos\varphi_i)^2} \\ \dfrac{2}{\sqrt{3}}S - \dfrac{C\cos\varphi_1 - (1/\sqrt{3})(3-8C^2)S \pm C\sin\varphi_1\sqrt{a^2+b^2-d^2}}{4-(S-\sqrt{3}C\cos\varphi_i)^2} \\ -\dfrac{2C(3-5C^2-\sqrt{3}SC\cos\varphi_1)\sin\varphi_1 \pm (C\cos\varphi_1+\sqrt{3}S)\sqrt{a^2+b^2-d^2}}{4-(S-\sqrt{3}C\cos\varphi_i)^2} \end{pmatrix}, \\ P_5 &= \begin{pmatrix} -S + \dfrac{\sqrt{3}C\cos\varphi_1 - (3-8C^2)S \mp \sqrt{3}C\sin\varphi_1\sqrt{a^2+b^2-d^2}}{4-(S-\sqrt{3}C\cos\varphi_i)^2} \\ \dfrac{2}{\sqrt{3}}S - \dfrac{C\cos\varphi_1 - (1/\sqrt{3})(3-8C^2)S \mp C\sin\varphi_1\sqrt{a^2+b^2-d^2}}{4-(S-\sqrt{3}C\cos\varphi_i)^2} \\ -\dfrac{2C(3-5C^2-\sqrt{3}SC\cos\varphi_1)\sin\varphi_1 \mp (C\cos\varphi_1+\sqrt{3}S)\sqrt{a^2+b^2-d^2}}{4-(S-\sqrt{3}C\cos\varphi_i)^2} \end{pmatrix}, \end{aligned} \tag{3.9}$$

where $a^2 + b^2 - d^2$ is given by (3.7).

CASE II. Assume $\varphi_3 = \varphi_5$. Let us first study the condition for $\angle P_4 = \theta$ without assuming $\angle P_0 = \angle P_2 = \theta$. If $\varphi_3 = \varphi_5$, which we denote by φ, and $\angle P_4 = \theta$, then (3.3) implies that φ must satisfy

$$\cos\varphi = -\frac{\sqrt{3}S}{C} \quad \text{or} \quad \frac{S}{\sqrt{3}C}.$$

CASE II-1. Assume

$$(\cos\varphi_3, \sin\varphi_3) = (\cos\varphi_5, \sin\varphi_5) = \left(\frac{S}{\sqrt{3}C}, \frac{\sqrt{4C^2-1}}{\sqrt{3}C}\right).$$

Then (3.3) implies that $\angle P_0 = \angle P_2 = \theta$ if and only if

$$(\cos\varphi_1, \sin\varphi_1) = \left(\frac{S}{\sqrt{3}C}, \frac{\sqrt{4C^2-1}}{\sqrt{3}C}\right) \quad \text{or} \quad \left(\frac{(3-8C^2)S}{\sqrt{3}C}, \frac{(4C^2-3)\sqrt{4C^2-1}}{\sqrt{3}C}\right).$$

Note that we have $\overrightarrow{P_0P_5} = \overrightarrow{P_2P_3}$ by (3.2). The points P_1 and P_4 are in the opposite (or same) side of the plane containing P_0, P_2, P_3, and P_5 if $\cos\varphi_1 = S/(\sqrt{3}C)$ (or respectively $\cos\varphi_1 = (3-8C^2)S/(\sqrt{3}C)$). Namely, the hexagon is a chair if $\varphi_1 = \varphi_3 = \varphi_5$ and a boat if $\varphi_1 \neq \varphi_3 = \varphi_5$ in this case. Both coincide if and only if $\theta = 0$ or $2\pi/3$, when $\mathcal{P}$ is a 6-times covered multiple edge or a regular hexagon. The chair is given by

$$P_1 = \begin{pmatrix} 0 \\ -\dfrac{S}{\sqrt{3}} \\ \dfrac{\sqrt{4C^2-1}}{\sqrt{3}} \end{pmatrix}, \quad P_3 = \begin{pmatrix} S \\ \dfrac{2S}{\sqrt{3}} \\ \dfrac{\sqrt{4C^2-1}}{\sqrt{3}} \end{pmatrix}, \quad P_5 = \begin{pmatrix} -S \\ \dfrac{2S}{\sqrt{3}} \\ \dfrac{\sqrt{4C^2-1}}{\sqrt{3}} \end{pmatrix},$$

whereas the boat is given by substituting $(\cos\varphi_1, \sin\varphi_1) = ((3-8C^2)S/(\sqrt{3}C), (4C^2-3)\sqrt{4C^2-1}/(\sqrt{3}C))$ to (3.9),

$$P_1 = \begin{pmatrix} 0 \\ -\dfrac{(3-8C^2)S}{\sqrt{3}} \\ \dfrac{(4C^2-3)\sqrt{4C^2-1}}{\sqrt{3}} \end{pmatrix}, \quad P_3 = \begin{pmatrix} S \\ \dfrac{2S}{\sqrt{3}} \\ \dfrac{\sqrt{4C^2-1}}{\sqrt{3}} \end{pmatrix}, \quad P_5 = \begin{pmatrix} -S \\ \dfrac{2S}{\sqrt{3}} \\ \dfrac{\sqrt{4C^2-1}}{\sqrt{3}} \end{pmatrix}.$$

CASE II-2. Assume

$$(\cos\varphi_3, \sin\varphi_3) = (\cos\varphi_5, \sin\varphi_5) = \left(-\frac{\sqrt{3}S}{C}, \frac{\sqrt{4C^2-3}}{C}\right),$$

which can occur if and only if $\sqrt{3}/2 \le C \le 1$, namely, $0 \le \theta \le \pi/3$. Then (3.3) implies that $\angle P_0 = \angle P_2 = \theta$ if and only if $2C\sqrt{4C^2-3}\sin\varphi_1 = 8C^2 - 6$. Therefore, when $\theta \ne \pi/3$ (we will study the case when $\theta = \pi/3$ and $\varphi_3 = \varphi_5 = \pi$ later) then $\angle P_0 = \angle P_2 = \theta$ if and only if

$$(\cos\varphi_1, \sin\varphi_1) = \left(-\frac{\sqrt{3}S}{C}, \frac{\sqrt{4C^2-3}}{C}\right) \quad \text{or} \quad \left(\frac{\sqrt{3}S}{C}, \frac{\sqrt{4C^2-3}}{C}\right).$$

Note that P_3 and P_5 are above P_0 and P_2 respectively. When $\varphi_1 = \varphi_3 = \varphi_5$ the hexagon is an "inward crown" (Fig. 10) given by

$$P_1 = \begin{pmatrix} 0 \\ \sqrt{3}S \\ \sqrt{4C^2-3} \end{pmatrix}, \quad P_3 = \begin{pmatrix} -S \\ 0 \\ \sqrt{4C^2-3} \end{pmatrix}, \quad P_5 = \begin{pmatrix} S \\ 0 \\ \sqrt{4C^2-3} \end{pmatrix},$$

whereas the other is given by substituting $(\cos\varphi_1, \sin\varphi_1) = (\sqrt{3}S/C, \sqrt{4C^2-3}/C)$ to (3.9),

$$P_1 = \begin{pmatrix} 0 \\ -\sqrt{3}S \\ \sqrt{4C^2-3} \end{pmatrix}, \quad P_3 = \begin{pmatrix} -S \\ 0 \\ \sqrt{4C^2-3} \end{pmatrix}, \quad P_5 = \begin{pmatrix} S \\ 0 \\ \sqrt{4C^2-3} \end{pmatrix}.$$

Let us summarize the argument above when $\theta \ne \pi/3$.

Theorem 3.1. *Suppose a θ-equiangular unit equilateral hexagon ($\theta \ne \pi/3$) is parametrized by the angles φ_1, φ_3, and φ_5 by* (3.1), (3.2). *Let $C = \cos(\theta/2)$ and $S = \sin(\theta/2)$ as before.*

(1) *When $\theta = 2\pi/3$ i.e. $C = 1/2$ we have*

$$\varphi_1 = \varphi_3 = \varphi_5 = 0,$$

which corresponds to a regular hexagon.

(2) *When $\pi/3 < \theta < 2\pi/3$ i.e. $1/2 < C < \sqrt{3}/2$ we have*

$$-\arccos\left(\frac{(3-8C^2)S}{\sqrt{3}C}\right) \le \varphi_1 \le \arccos\left(\frac{(3-8C^2)S}{\sqrt{3}C}\right).$$

(i) *When $\varphi_1 = \pm\arccos((3-8C^2)S/(\sqrt{3}C))$ we have*

$$\varphi_3 = \varphi_5 = \mp\arccos\left(\frac{S}{\sqrt{3}C}\right),$$

which corresponds to a boat (Fig. 2).

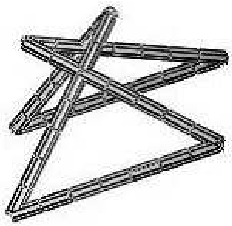

Fig. 9. A boat with a small bond angle.

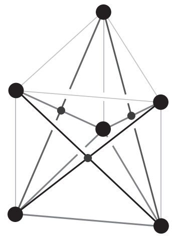

Fig. 10. "*inward crown*" in a prism. Two edges intersect each other in a side face of the prism.

(ii) *When* $-\arccos((3-8C^2)S/(\sqrt{3}C)) < \varphi_1 < \arccos((3-8C^2)S/(\sqrt{3}C))$ *we have either*

- $\varphi_3 \neq \varphi_5$, *which are given by* (3.8),
- $\varphi_1 = \varphi_3 = \varphi_5 = \pm\arccos(S/(\sqrt{3}C))$, *which corresponds to a chair* (Fig. 3).

(3) *When* $0 < \theta < \pi/3$ *i.e.* $\sqrt{3}/2 < C < 1$ *we have*

$$\arccos\left(\frac{\sqrt{3}S}{C}\right) \leq |\varphi_1| \leq \arccos\left(\frac{(3-8C^2)S}{\sqrt{3}C}\right).$$

(i) *When* $\varphi_1 = \pm\arccos((3-8C^2)S/(\sqrt{3}C))$ *we have*

$$\varphi_3 = \varphi_5 = \pm\arccos\left(\frac{S}{\sqrt{3}C}\right),$$

which corresponds to a boat (Fig. 9).

(ii) *When* $\varphi_1 = \pm\arccos(\sqrt{3}S/C)$ *we have*

$$\varphi_3 = \varphi_5 = \pm\arccos\left(-\frac{\sqrt{3}S}{C}\right) = \pm\left(\pi - \arccos\left(\frac{\sqrt{3}S}{C}\right)\right).$$

(iii) *When* $\arccos(\sqrt{3}S/C) < |\varphi_1| < \arccos((3-8C^2)S/(\sqrt{3}C))$ *we have either*

- $\varphi_3 \neq \varphi_5$, *which are given by* (3.8),
- $\varphi_1 = \varphi_3 = \varphi_5 = \pm\arccos(S/(\sqrt{3}C))$, *which corresponds to a chair* (Fig. 4).
- $\varphi_1 = \varphi_3 = \varphi_5 = \pm\arccos(-\sqrt{3}S/C)$, *which corresponds to an "inward crown"* (Fig. 10).

(4) *When* $\theta = 0$ *the hexagon degenerates to a* 6 *times covered multiple edge.*

Corollary 3.2. *The configuration space* $\mathcal{M}_6(\theta)$ *of* θ*-equiangular unit equilateral hexagons* ($\theta \neq \pi/3$) *is homeomorphic to a point if* $\theta = 0, 2\pi/3$, *the union of a circle and a pair of points if* $\pi/3 < \theta < 2\pi/3$, *the union of two circles and four points if* $0 < \theta < \pi/3$, *and the empty set if* $\theta < 0$ *or* $\theta > 2\pi/3$.

Boat configurations are included in circles above mentioned, and chairs are isolated.

We will see that a boat degenerates to a planar configuration when $\theta = \pi/3$.

Corollary 3.3. (1) *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 satisfies* $\pi/3 < \theta < 2\pi/3$.
(2) *A boat and a chair cannot be joined by a path in the configuration space, i.e. they cannot be continuously deformed from one to the other.*

3.2. The exceptional case when $\theta = \pi/3$. Finally we study the exceptional case $\theta = \pi/3$, when the cases when $\varphi_j = \pi$ $(j = 1, 3, 5)$ have not been considered yet.

When $\theta = \pi/3$ the equation (3.3) becomes

$$(\cos\varphi_i + 1)(\cos\varphi_{i+2} + 1) - 2\sin\varphi_i \sin\varphi_{i+2} = 0.$$

If $\angle P_2 = \pi/3$ then φ_3 is determined by φ_1 as follows;

- if $\varphi_1 = \pi$ then φ_3 is arbitrary,
- if $\varphi_1 = 0$ then $\varphi_3 = \pi$,
- if $\varphi_1 \neq 0, \pi$ then $\varphi_3 = \pi$ or $f(\varphi_1)$ $(f(\varphi_1) \neq \pi)$, where $f(\varphi)$ $(\varphi \neq \pm\pi)$ is given by

$$\begin{aligned}&(\cos f(\varphi), \sin f(\varphi)) \\ &= \left(\frac{-(\cos\varphi + 1)^2 + 4\sin^2\varphi}{(\cos\varphi + 1)^2 + 4\sin^2\varphi}, \frac{4\sin\varphi(\cos\varphi + 1)}{(\cos\varphi + 1)^2 + 4\sin^2\varphi}\right).\end{aligned} \tag{3.10}$$

Remark that $f(0) = \pi$ and that $f(\varphi) = \varphi$ if and only if $\varphi = \pm\arccos(1/3)$. Put $f(\pi) = 0$ as $\lim_{\varphi\to\pi} f(\varphi) = 0$.

Theorem 3.4. *Suppose a $\pi/3$-equiangular unit equilateral hexagon is parametrized by the angles φ_1, φ_3, and φ_5 by* (3.1), (3.2). *Then we have*

$$\begin{aligned}&\{\varphi_1, \varphi_3, \varphi_5\} \\ &= \{\pi, \varphi, f(\varphi)\}, \{\pi, \pi, \varphi\}, \quad \textit{or} \quad \left\{\pm\arccos\left(\frac{1}{3}\right), \pm\arccos\left(\frac{1}{3}\right), \pm\arccos\left(\frac{1}{3}\right)\right\},\end{aligned}$$

where φ is arbitrary. The first case contains a boat when $\{\varphi_1,\varphi_3,\varphi_5\} = \{\pi, \pm\arccos(1/3), \pm\arccos(1/3)\}$, *and the last triples correspond to a chair.*

Corollary 3.5. *The configuration space $\mathcal{M}_6(\pi/3)$ of equilateral and $\pi/3$-equiangular hexagons is homeomorphic to the union of a pair of points and the space X illustrated in* Fig. 11 *which is a* 1*-skeleton of a tetrahedron with edges being doubled.*

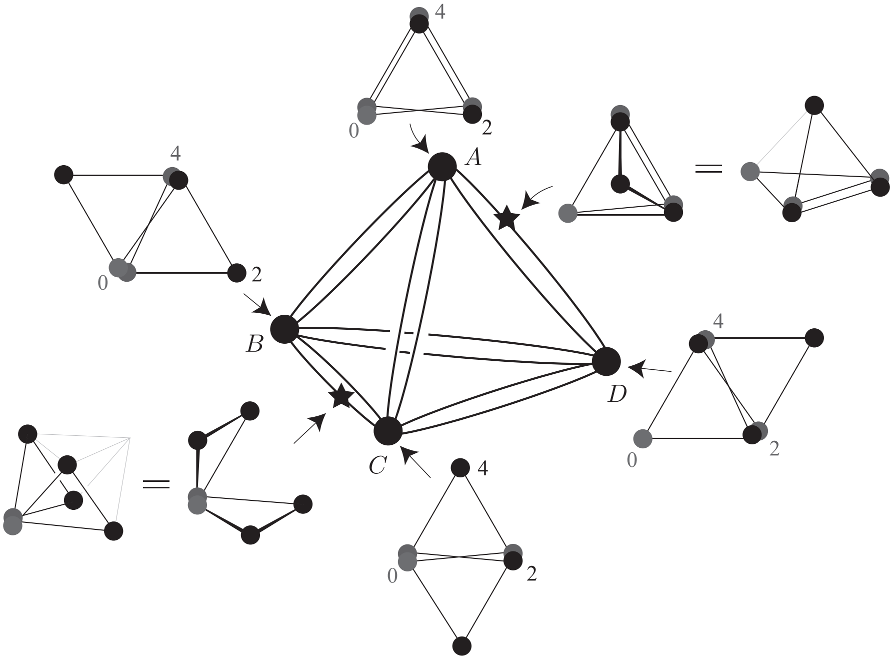

Fig. 11. The configuration space $X = \mathcal{M}_6(\pi/3) \setminus \{\text{chairs}\}$. The numbers $0, 2$, and 4 in the figure indicate the vertices P_0, P_2, and P_4 respectively. The figures of six hexagons around X are seen from above. The non-planar configurations left below is a boat, when P_i occupy five vertices of a regular octahedron. The four vertices A, B, C, and D of X correspond to planar configurations parametrized by $(\varphi_1, \varphi_3, \varphi_5) = (\pi, \pi, \pi)$, $(\pi, \pi, 0)$, $(0, \pi, \pi)$, and $(\pi, 0, \pi)$ respectively. The circle through A and D consists of the configurations parametrized by $(\varphi_1, \varphi_3, \varphi_5) = (\pi, \varphi, \pi)$ $(-\pi \leq \varphi \leq \pi)$. The circle through B and C consists of the configurations parametrized by $(\varphi_1, \varphi_3, \varphi_5) = (\varphi, \pi, f(\varphi))$ $(-\pi \leq \varphi \leq \pi)$.

The author would like to close the article with an open problem: find a new invariant which can show that a boat cannot be deformed continuously into a chair.

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Department of Mathematics and Information Sciences
Tokyo Metropolitan University
1-1 Minami-Ohsawa, Hachiouji-Shi
Tokyo 192-0397
Japan
e-mail: ohara@tmu.ac.jp
Fax: 81-42-677-2481