Chapter

The Topology of the Configuration Space of a Mathematical Model for Cycloalkenes

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Abstract

As a mathematical model for cycloalkenes, we consider equilateral polygons whose interior angles are the same except for those of the both ends of the specified edge. We study the configuration space of such polygons. It is known that for some case, the space is homeomorphic to a sphere. The purpose of this chapter is threefold: First, using the h-cobordism theorem, we prove that the above homeomorphism is in fact a diffeomorphism. Second, we study the best possible condition for the space to be a sphere. At present, only a sphere appears as a topological type of the space. Then our third purpose is to show the case when a closed surface of positive genus appears as a topological type.

Keywords: cycloalkene, polygon, configuration space, h-cobordism theorem, closed surface

1. Introduction

The configuration space of mechanical linkages in the Euclidean space of dimension three, also known as polygon space, is the central objective in topological robotics. The linkage consists of n bars of length $l_1, \cdots, l_n$ connected by revolving joints forming a closed spatial polygonal chain.

The polygon space is quite important in various engineering applications: In molecular biology they describe varieties of molecular shapes, in robotics they appear as spaces of all possible configurations of some mechanisms, and they play a central role in statistical shape theory.

Mathematically, these spaces are also very interesting: The symplectic structure on the polygon space was studied in the seminal paper [1]. The integral cohomology ring was determined in [2] applying methods of toric topology. We refer to [3] for an excellent exposition with emphasis on Morse theory.

Recently, mathematicians are interested in a mathematical model for monocyclic hydrocarbons. The model is defined by imposing conditions on the interior angles of a polygon. The configuration space of such polygons corresponds in chemistry to the conformations of all possible shapes of a monocyclic hydrocarbon. Hence the configuration space is interesting both in mathematics and chemistry.

In order to give more detailed account, recall that monocyclic hydrocarbons are classified into two types: One is saturated type, and the other is unsaturated type. Mathematicians constructed a mathematical model for each type. We summarize the correspondence between chemical and mathematical terminologies in the following **Table 1**.

Below we explain **Table 1**.

i. Monocyclic saturated hydrocarbons are monocyclic hydrocarbons that contain only single bonds between carbon atoms. Monocyclic saturated hydrocarbons are called *cycloalkanes*. (See **Figure 1** for the 6-membered cycloalkane.)

- The mathematical model for cycloalkanes is the equilateral and equiangular polygons. Let $\mathcal{M}_n(\theta)$ be the configurations of such n-gons with interior angle θ. The study of the topological type of $\mathcal{M}_n(\theta)$ originated in [4]. See the next item for more details.

- The topological type of $\mathcal{M}_4(\theta)$ and $\mathcal{M}_5(\theta)$ was determined in [4] for arbitrary θ, and that of $\mathcal{M}_6(\theta)$ was determined in [5] for arbitrary θ. The paper [4] also determined the topological type of $\mathcal{M}_7(\theta)$ for the case that θ is the ideal tetrahedral bond angle, i.e. $\theta = \arccos\left(-\frac{1}{3}\right) \approx 109.47°$. The result was generalized in [6] for generic θ.

ii. Monocyclic unsaturated hydrocarbons are monocyclic hydrocarbons with at least one double or triple bond between carbon atoms.

- Hereafter, for simplicity, we consider only the monocyclic unsaturated hydrocarbons that contain exactly one multiple bond.

- It is not mathematically important whether the multiple bond is a double or triple bond. Hence we assume that the multiple bond is a double bond.

Chemistry	Mathematics
Monocyclic hydrocarbon	Equilateral polygon in $\mathbb{R}^3$
Bond of a monocyclic hydrocarbon	Edge of a polygon
Bond angle of a monocyclic hydrocarbon	Interior angle of an equilateral polygon
Conformations	Configuration space
Cycloalkanes	Equilateral and equiangular polygons. Their configuration space is denoted by $\mathcal{M}_n(\theta)$.
Cycloalkenes	Equilateral polygons whose interior angles are the same except for those of the both ends of the specified edge. Their configuration space is denoted by $C_n(\theta)$.

Table 1.
The correspondence between chemical and mathematical terminologies.

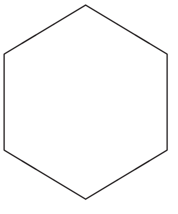

Figure 1.
Cyclohexane (6-membered cycloalkane).

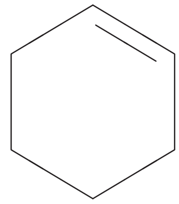

Figure 2.
Cyclohexene (6-membered cycloalkene).

- Such monocyclic unsaturated hydrocarbons are called *cycloalkenes*. (See **Figure 2** for the 6-membered cycloalkene.)

- The mathematical model for cycloalkenes is the equilateral polygons whose interior angles are the same except for those of the both sides of the specified edge. Here the specified edge corresponds to the double bond. Let $C_n(\theta)$ be the configurations of such n-gons with interior angle θ. (See (1) for more precise definition of $C_n(\theta)$.) The study of the topological type of $C_n(\theta)$ originated in [7] and the result was generalized in [8]. See the next item for more details.

- The following result was proved in [8] (see Theorem 6): There exists θ_0 such that for all $\theta \in \left(\theta_0, \frac{n-2}{n}\pi\right)$, $C_n(\theta)$ is *homeomorphic* to S^{n-4}.

- Except for the above result in [8], we do not know strong results about the topology of $C_n(\theta)$.

On the other hand, as a combinatorial result, the necessary and sufficient condition for $\mathcal{M}_n(\theta)$ and $C_n(\theta)$ to be non-empty was proved in [9]. (See Theorem 3 about the result for $C_n(\theta)$.)

As stated in the last item of the above ii, we do not have enough information about the topology of $C_n(\theta)$. The purpose of this chapter is to obtain systematic information about $C_n(\theta)$. More precisely, we study the following:

Problem 1. (i) We prove that the above homeomorphism in [8] is in fact a diffeomorphism.

(ii) We study the best possible value about the above θ_0 in [8].

(iii) At present, only a sphere appears as a topological type of $C_n(\theta)$. We determine the topological type of $C_6(\theta)$ for all θ. The result shows that for some θ, $C_6(\theta)$ is a closed surface of positive genus.

This chapter is organized as follows. In §2, we state our main results. In §3-§5, we prove them. In §6, we state the conclusions.

2. Main results

We give the definition of the configuration space. Let θ be a real number satisfying $0 \le \theta \le \pi$. We set

$$C_n(\theta) := \left\{P = (u_1, \cdots, u_n) \in \left(S^2\right)^n \mid \text{the following i, ii and iii hold}\right\}. \tag{1}$$

i. $u_1 = (1, 0, 0)$ and $u_n = (-\cos\theta, -\sin\theta, 0)$.

ii. $\sum_{i=1}^{n} u_i = 0$.

iii. $\langle u_i, u_{i+1}\rangle = -\cos\theta$ for $1 \le i \le n-3$, where $\langle\ ,\rangle$ denotes the standard inner product on $\mathbb{R}^3$.

About the conditions in (1), the following explanations are in order.
(See **Table 1** for chemical terminologies.)

- The element u_i denotes the unit vector in the direction of the edge of a polygon. Then the condition ii requires the fact that $(u_1, \cdots, u_n)$ is in fact a polygon.

- We specify u_{n-1} to be the special edge, which corresponds to the double bond of a cycloalkene. Then the condition iii requires the fact that the interior angles of an n-gon are θ except for those of the both ends of u_{n-1}.

Remark 2. In some papers, $C_n(\theta)$ is defined as

$$A_n(\theta)/SO(3), \tag{2}$$

where we set

$$A_n(\theta) := \left\{(u_1, \cdots, u_n) \in \left(S^2\right)^n \mid (1)\ \text{ ii, iii and the condition } \langle u_n, u_1\rangle = -\cos\theta \text{ hold}\right\}.$$

Let $SO(3)$ act on $A_n(\theta)$ diagonally. Then for an element $(u_1, \cdots, u_n) \in A_n(\theta)$, we may normalize u_1 and u_n to be as in (1) i. Hence (2) in fact coincides with (1).

The following result is known.

Theorem 3 ([9], Theorems A and B). *(i) For $n \ge 4$, we have $C_n(\theta) \ne \emptyset$ if and only if θ belongs to the following interval:*

$$\begin{cases} \left[2\arcsin\dfrac{1}{n-1}, \dfrac{n-2}{n}\pi\right], & \textit{if } n \textit{ is odd},\\ \left[0, \dfrac{n-2}{n}\pi\right], & \textit{if } n \textit{ is even}. \end{cases} \tag{3}$$

(ii). Let a be an endpoint of the intervals in (3). *Then we have $C_n(a) = \{\text{one point}\}$.*

Example 4. For $n = 4$ or 5, the following results hold, where we omit the cases which can be read from Theorem 3.

i. For $0 < \theta < \frac{\pi}{2}$, we have $C_4(\theta) = \{\text{two points}\}$.

ii. The topological type of $C_5(\theta)$ is given by the following **Table 2**.

Here we define η_1 and η_2 to be the following **Figures 3** and **4**, respectively.

The proof of the example will be given at the end of §5.

In [8], the following proposition is proved using the implicit function theorem.

Proposition 5 ([8], Proposition 1). *There exists θ_0 such that for all $\theta \in \left(\theta_0, \frac{n-2}{n}\pi\right)$, the system of equations defined by* (1) i, ii *and* iii *intersect transversely. Hence for such θ, $C_n(\theta)$ carries a natural differential structure.*

Range of θ	$2\arcsin\frac{1}{4} < \theta < \frac{\pi}{5}$	$\frac{\pi}{5}$	$\frac{\pi}{5} < \theta < \frac{\pi}{3}$	$\frac{\pi}{3}$	$\frac{\pi}{3} < \theta < \frac{3}{5}\pi$
Topological type of $C_5(\theta)$	S^1	η_1	$S^1 \coprod S^1$	η_2	S^1

Table 2.
The topological type of $C_5(\theta)$.

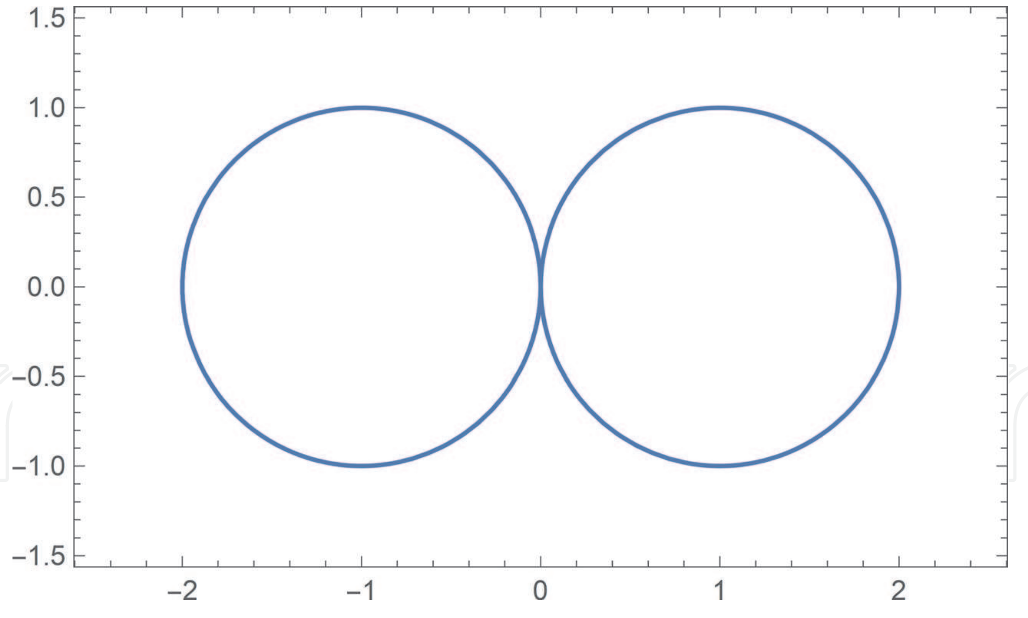

Figure 3.
The space η_1.

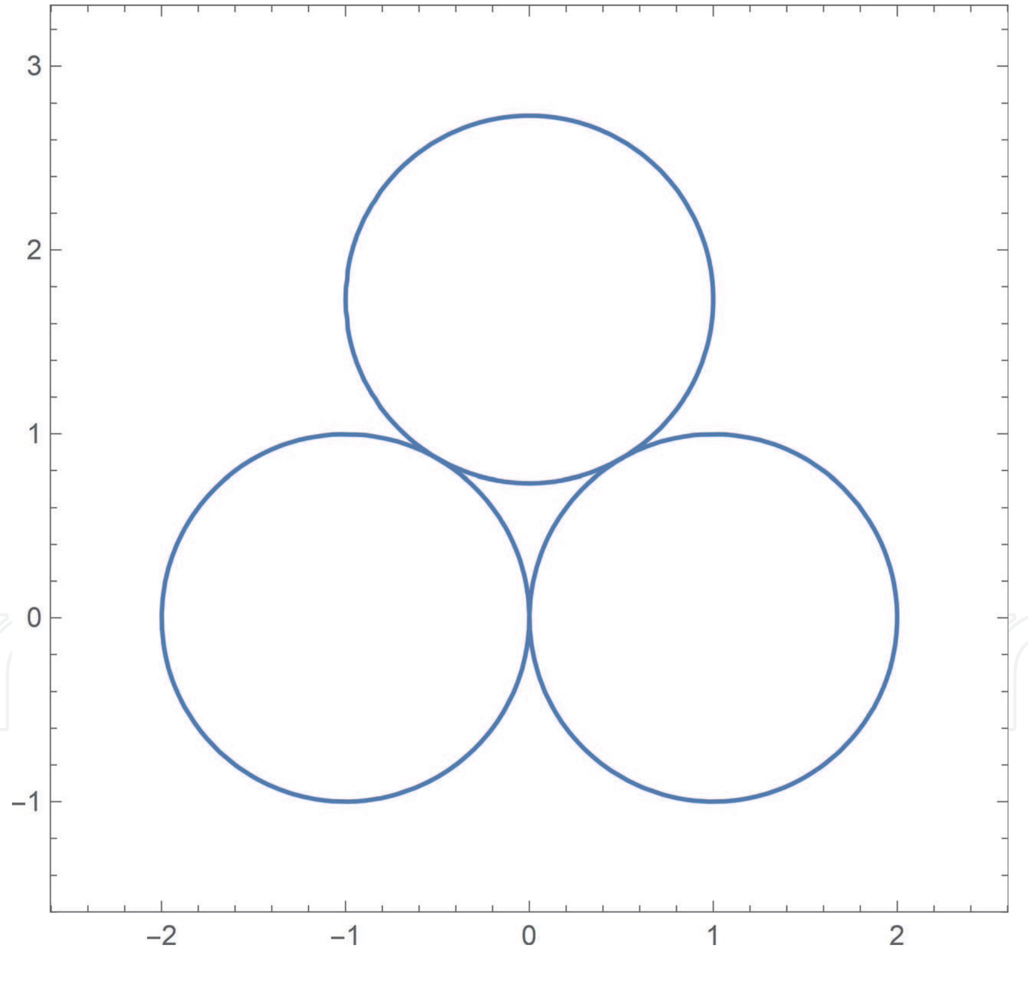

Figure 4.
The space η_2.

The main result in [8] is the following:

Theorem 6 ([8], Theorem 1)**.** *Let θ_0 be as in Proposition 5. Then for all $\theta \in \left(\theta_0, \frac{n-2}{n}\pi\right)$, $C_n(\theta)$ is homeomorphic to S^{n-4}.*

Remark 7. In [8], Theorem 6 is proved by the following method: We construct a function $f : C_n(\theta) \to \mathbb{R}$ and show that f has exactly two critical points. Then Reeb's theorem implies Theorem 6. Note that with this method, we cannot improve the assertion from homeomorphism to diffeomorphism. (See ([10], p. 25) for Reeb's theorem and remarks about it.)

The following theorem is the answer to Problem 1 (i).

Theorem A. *We equip S^{n-4} with the standard differential structure. Let θ_0 be as in Proposition 5. Then for all $\theta \in \left(\theta_0, \frac{n-2}{n}\pi\right)$, $C_n(\theta)$ is diffeomorphic to S^{n-4}.*

Next we consider Problem 1 (ii). We set

$$\alpha_n := \inf \left\{\theta_0 \in (0,\pi)\ \mathrm{C_n}(\theta) \cong \mathrm{S}^{\mathrm{n}-4}\,\text{holds for all}\,\theta \in \left(\theta_0, \frac{\mathrm{n}-2}{\mathrm{n}}\pi)\right\}.$$

Here in what follows, the notation $X \cong Y$ means that X is homeomorphic to Y. Note that among the values of θ_0 in Theorem 6, α_n is the best possible one.

The following result is known.

Theorem 8 ([11]). *(i) We have $\alpha_n = \frac{n-4}{n-2}\pi$ for $4 \le n \le 7$.*

(ii). We have $\alpha_8 < \frac{5}{7}\pi$.

Remark 9. About Theorem 8 (i), we can read α_4 and α_5 from the above Example 4, and α_6 from **Table 4** in Theorem D below.

From Theorem 8, we naturally encounter the following:

Question 10. (i) Is it true that $\alpha_n = \frac{n-4}{n-2}\pi$ holds for $n \ge 4$?

(ii) Is it true that $\alpha_n < \frac{n-3}{n-1}\pi$ holds for $n \ge 4$? Note that if (i) is true then (ii) holds automatically.

The following theorem is the answer to Problem 1 (ii).

Theorem B. *For $4 \le n \le 14$, the following* **Table 3** *holds.*

The following theorem is the answer to Question 10.

Theorem C. *(i) The statement in Question 10* (i) *is false for $n \ge 8$. In fact, we have $\frac{n-4}{n-2}\pi < \alpha_n$ for $n \ge 8$.*

(ii) The statement in Question 10 (ii) *is false for $n \ge 13$. In fact, we have $\frac{n-3}{n-1}\pi < \alpha_n$ for $n \ge 13$.*

The following theorem is the answer to Problem 1 (iii).

Theorem D. *The topological type of $C_6(\theta)$ is given by the following* **Table 4***, where we omit the cases which can be read from Theorem 3.*

n	α_n	$\frac{n-4}{n-2}\pi$	$\frac{n-3}{n-1}\pi$	$\frac{n-2}{n}\pi$
4	0	0	0.333π	0.500π
5	0.333π	0.333π	0.500π	0.600π
6	0.500π	0.500π	0.600π	0.667π
7	0.600π	0.600π	0.667π	0.714π
8	0.676π	0.667π	0.714π	0.750π
9	0.729π	0.714π	0.750π	0.778π
10	0.767π	0.750π	0.778π	0.800π
11	0.795π	0.778π	0.800π	0.818π
12	0.817π	0.800π	0.818π	0.833π
13	0.834π	0.818π	0.833π	0.846π
14	0.848π	0.833π	0.846π	0.857π

Table 3.
The value of α_n for $4 \le n \le 14$.

Range of θ	$0 < \theta < \frac{\pi}{3}$	$\frac{\pi}{3} < \theta < \frac{\pi}{2}$	$\frac{\pi}{2} < \theta < \frac{2}{3}\pi$
Topological type of $C_6(\theta)$	$\#_3(S^1 \times S^1)$	$\#_3(S^1 \times S^1)$	S^2

Table 4.
The topological type of $C_6(\theta)$.

Remark 11. (i) As indicated in Problem 1 (iii), not only S^2 but also $\#_3(S^1 \times S^1)$ appears in **Table 4** as a topological type of $C_6(\theta)$

(ii) We can also determine the topological type of $C_6\left(\frac{\pi}{2}\right)$ and $C_6\left(\frac{\pi}{3}\right)$. (See Remark 18 in §5.) In particular, they have singular points.

3. Proof of Theorem A

Following the method of [12], we set

$$X_n := \left\{ (P, \theta) \in \left(S^2\right)^n \times \left(0, \frac{n-2}{n}\pi\right] \mid P \in C_n(\theta) \right\}. \tag{4}$$

We define the function $\mu : X_n \to \mathbb{R}$ by

$$\mu(P, \theta) = \theta. \tag{5}$$

Note that for all $\theta \in (0, \pi]$, we have

$$\mu^{-1}(\theta) = C_n(\theta). \tag{6}$$

The following proposition holds:

Proposition 12. (i) *Let θ_0 be as in Proposition 5. Then the space $\mu^{-1}\left(\theta_0, \frac{n-2}{n}\pi\right]$ is a manifold, where $\mu^{-1}\left(\theta_0, \frac{n-2}{n}\pi\right]$ denotes the inverse image of the interval.*

(ii) *Any element of $\mu^{-1}\left(\theta_0, \frac{n-2}{n}\pi\right)$ is a regular point of μ.*

(iii) *Consider the case $n = 8$. Then $C_8\left(\frac{6}{8}\pi\right)$ is a non-degenerate critical point of μ.*

In order to prove the proposition, we need a lemma. We set

$$D_n := \left\{ (u_1, \cdots, u_{n-2}, \theta) \in \left(S^2\right)^{n-2} \times (0, \pi) \mid \text{the following i and ii hold} \right\}.$$

i. $u_1 = (1, 0, 0)$.

ii. $\langle u_i, u_{i+1} \rangle = -\cos\theta$ for $1 \le i \le n-3$.

Lemma 13. *(i) There is a diffeomorphism*

$$f : \left(S^1\right)^{n-3} \times (0, \pi) \underset{\cong}{\to} D_n.$$

(ii) We define the map $L : D_n \to \mathbb{R}$ by

$$L(u_1, \cdots, u_{n-2}, \theta) = \|(-\cos\theta, -\sin\theta, 0) + \sum_{i=1}^{n-2} u_i\|^2.$$

Then we have the following commutative diagram:

$$\begin{tikzcd} X_n \arrow[rr, "g", "\cong"'] \arrow[dr, "\mu"'] & & (L\circ f)^{-1}(1) \arrow[dl, "p"] \\ & \mathbb{R} & \end{tikzcd} \tag{7}$$

Here the maps p and g are defined as follows.

- *Let*

$$Pr : \left(S^1\right)^{n-3} \times (0, \pi) \to \mathbb{R} \tag{8}$$

be the projection to the $(0, \pi)$*-component and we denote by p the restriction of Pr to* $(L \circ f)^{-1}(1)$:

$$p := Pr|_{(L\circ f)^{-1}(1)}.$$

- *The map g is a homeomorphism which will be defined in* (13).

(iii) For all $\theta \in (0, \pi)$, *the restriction of the map g in* (7) *naturally induces a homeomorphism*

$$g|_{C_n(\theta)} : C_n(\theta) \underset{\cong}{\to} p^{-1}(\theta). \tag{9}$$

Proof of Lemma 13*:* (i) From an element

$$\left(e^{i\phi_1}, \cdots, e^{i\phi_{n-3}}, \theta\right) \in \left(S^1\right)^{n-3} \times (0, \pi),$$

we construct the element $(u_1, \cdots, u_{n-2}, \theta) \in D_n$ as follows: In the process of constructing u_i, we also construct the elements $v_i \in S^2$ such that $\langle u_i, v_i \rangle = 0$. We set

$$u_{i+1} := -(\cos\theta)u_i + (\sin\theta\cos\phi_i)v_i + (\sin\theta\sin\phi_i)u_i \times v_i \tag{10}$$

and

$$v_{i+1} := -(\sin\theta)u_i - (\cos\theta\cos\phi_i)v_i - (\cos\theta\sin\phi_i)u_i \times v_i, \tag{11}$$

where $u_i \times v_i$ denotes the cross product.

In (10) and (11) for $i = 1$, we set $u_1 := (1, 0, 0)$ and $v_1 := (0, 1, 0)$. Then we obtain u_2 and v_2. Next using (10) and (11) for $i = 2$, we obtain u_3 and v_3. Repeating this process, we obtain u_i and v_i for $1 \le i \le n-2$. Now we define f by

$$f\left(e^{i\phi_1}, \cdots, e^{i\phi_{n-3}}, \theta\right) := (u_1, \cdots, u_{n-2}, \theta).$$

From the construction, f is a diffeomorphism.

(ii) We define the map $h : X_n \to L^{-1}(1)$ by

$$h(u_1, \cdots, u_n, \theta) := (u_1, \cdots, u_{n-2}, \theta). \tag{12}$$

Since $(u_1, \cdots, u_n)$ is an element of $C_n(\theta)$, the right-hand side of (12) is certainly an element of $L^{-1}(1)$. It is clear that h is a homeomorphism. Hence if we define the map g by

$$g := f^{-1} \circ h, \tag{13}$$

then g is also a homeomorphism. From the construction, it is clear that the diagram (7) is commutative.

(iii) The item is clear from (6) and the diagram (7).

Proof of Proposition 12: Recall that $(L \circ f)^{-1}(1)$ in (7) is a subspace of $(S^1)^{n-3} \times (0, \pi)$. In order to prove Proposition 12, we calculate in the universal covering space. Let

$$q : \mathbb{R}^{n-3} \times (0, \pi) \to (S^1)^{n-3} \times (0, \pi)$$

be the universal covering space and we define the map

$$\widetilde{Pr} : \mathbb{R}^{n-3} \times (0, \pi) \to \mathbb{R}$$

by $\widetilde{Pr} := Pr \circ q$, where the map Pr is defined in (8). Then in addition to (7), we have the following commutative diagram:

$$\begin{tikzcd}
\mathbb{R}^{n-3} \times (0,\pi) \arrow[rr, "q"] \arrow[dr, "\widetilde{Pr}"'] & & (S^1)^{n-3} \times (0,\pi) \arrow[r, "f", "\cong"'] \arrow[dl, "Pr"] & D_n \arrow[r, "L"] & \mathbb{R} \\
& \mathbb{R} & & &
\end{tikzcd} \tag{14}$$

(i) Let $x \in \mathbb{R}^{n-3} \times (0, \pi)$ be any element which satisfies the condition

$$q(x) \in p^{-1}\left(\theta_0, \frac{n-2}{n}\pi\right]. \tag{15}$$

Note that if we use the diagram (14), then (15) is equivalent to saying that

$$\widetilde{Pr}(x) \in \left(\theta_0, \frac{n-2}{n}\pi\right] \quad \text{and} \quad (L \circ f \circ q)(x) = 1.$$

We set

$$\operatorname{grad}_x(L \circ f \circ q) := \left(\frac{\partial(L \circ f \circ q)}{\partial \phi_1}(x), \cdots, \frac{\partial(L \circ f \circ q)}{\partial \phi_{n-3}}(x), \frac{\partial(L \circ f \circ q)}{\partial \theta}(x)\right). \tag{16}$$

In order to prove Proposition 12 (i), it will suffice to prove that

$$\operatorname{grad}_x(L \circ f \circ q) \neq (0, \cdots, 0) \tag{17}$$

(a) *The case when* $\widetilde{Pr}(x) = \frac{n-2}{n}\pi$.

We claim that x has the form

$$x = \left(0, \cdots, 0, \frac{n-2}{n}\pi\right). \tag{18}$$

To prove this, recall the homeomorphism $g|_{C_n(\theta)}$ was defined in (9). Since $\left(g|_{C_n(\theta)}\right)^{-1}(q(x))$ is the regular n-gon, (18) follows.

We shall prove that

$$\mathrm{grad}_x(L\circ f\circ q) = (0,\cdots,0,r) \tag{19}$$

for some positive real number r.

First, note that the real-valued function $(L\circ f\circ q)\left(\phi_1,\cdots,\phi_{n-3},\frac{n-2}{n}\pi\right)$ takes the minimum value 0 at $(\phi_1,\cdots,\phi_{n-3}) = (0,\cdots,0)$. Hence the first $(n-3)$-terms of the both sides of (19) coincide.

Second, direct computations show that

$$(L\circ f\circ q)(0,\cdots,0,\theta) = \begin{cases} 4\left(\displaystyle\sum_{i=1}^{m}(-1)^i\sin\frac{2i-1}{2}\theta\right)^2, & \text{if } n = 2m+1, \\ \left(1+2\displaystyle\sum_{i=1}^{m-1}(-1)^i\cos i\theta\right)^2, & \text{if } n = 2m. \end{cases} \tag{20}$$

The number r in (19) equals to the derivative of (20) at $\theta = \frac{n-2}{n}\pi$. It is easy to see that

$$\begin{cases} (-1)^i\cos\dfrac{(2i-1)(2m-1)}{4m+2}\pi < 0, & \text{for } 1\le i\le m, \\ (-1)^{i+1}\sin\dfrac{i(2m-2)}{2m}\pi > 0, & \text{for } 1\le i\le m-1 \end{cases} \tag{21}$$

and

$$\begin{cases} \displaystyle\sum_{i=1}^{m}(-1)^i\sin\frac{(2i-1)(2m-1)}{4m+2}\pi = -\frac{1}{2}, \\ 1+2\displaystyle\sum_{i=1}^{m-1}(-1)^i\cos\frac{i(2m-2)}{2m}\pi = 1. \end{cases} \tag{22}$$

Using (21) and (22), we can check that the derivative of (20) at $\theta = \frac{n-2}{n}\pi$ is positive, i.e., r is positive. Thus we have obtained (19). This completes the proof of (17) for the case (a).

(b) *The case when* $\widetilde{Pr}(x)\in\left(\theta_0,\frac{n-2}{n}\pi\right)$.

By Proposition 5, we have

$$\left(\frac{\partial(L\circ f\circ q)}{\partial\phi_1}(x),\cdots,\frac{\partial(L\circ f\circ q)}{\partial\phi_{n-3}}(x)\right)\neq(0,\cdots,0). \tag{23}$$

Then using (16), we obtain (17). This completes the proof of (17) for the case (b), and hence also that of (i).

(ii) In order to prove by contradiction, assume that $\mu^{-1}\left(\theta_0,\frac{n-2}{n}\pi\right)$ contains a critical point of μ. Then using (7), $p^{-1}\left(\theta_0,\frac{n-2}{n}\pi\right)$ contains a critical point of p. Lifting to the universal covering space using (14), there exists an element $x\in\mathbb{R}^{n-3}\times(0,\pi)$ which satisfies the following two items:

- We have $\widetilde{Pr}(x)\in\left(\theta_0,\frac{n-2}{n}\pi\right)$.

- The point x is a critical point of the function $\widetilde{Pr}$ under the constraint

$$(L \circ f \circ q)(\phi_1, \cdots, \phi_{n-3}, \theta) = 1. \tag{24}$$

We apply the Lagrange multiplier method to (24). Since $\widetilde{Pr}(\phi_1, \cdots, \phi_{n-3}, \theta) = \theta$, there exists $\lambda \in \mathbb{R}$ such that

$$(0, \cdots, 0, 1) = \lambda \, \mathrm{grad}_x (L \circ f \circ q). \tag{25}$$

We compare the first $(n-3)$-components of the both sides of (25). Then by (23), we have $\lambda = 0$. But this contradicts the last component of (25). Hence (25) cannot occur. This completes the proof of (ii).

(iii) Consider the Eq. (24). Using the implicit function theorem, we may assume that θ is a function with variables $\phi_i \ \ (1 \le i \le n-3)$: $\theta = \theta(\phi_1, \cdots, \phi_{n-3})$. Note that

$$\widetilde{Pr}(\phi_1, \cdots, \phi_{n-3}, \theta(\phi_1, \cdots, \phi_{n-3})) = \theta(\phi_1, \cdots, \phi_{n-3}).$$

Hence it will suffice to prove the following result for $n = 8$:

$$\left| \left(\frac{\partial^2 \theta(\phi_1, \cdots, \phi_{n-3})}{\partial \phi_i \partial \phi_j} (0, \cdots, 0) \right)_{1 \le i,j \le n-3} \right| \ne 0, \tag{26}$$

where || denotes the determinant. Computing by the method of second implicit derivative, we see that the value of the left-hand side of (26) for $n = 8$ is $\frac{1-\sqrt{2}}{16384}$. Hence (26) holds for $n = 8$. This completes the proof of (iii), and hence also that of Proposition 12.

In order to prove Theorem A, we recall the following:

Theorem 14 ([13], Corollary B). *For $d \ge 2$, let M be a d-dimensional smooth manifold without boundary and $F : M \to \mathbb{R}$ a smooth function. We set* $\max F(M) = m$ *and assume that m is attained by unique point $z \in M$. Let $a \in \mathbb{R}$ satisfy the following four conditions:*

i. $a < m$.

ii. $F^{-1}[a, m]$ is compact.

iii. *There are no critical points in $F^{-1}[a, m)$.*

iv. $d \ne 5$.

Then there is a diffeomorphism $F^{-1}(a) \cong S^{d-1}$.

Remark 15. For the proof of Theorem 14, the h-cobordism theorem (see [14], p. 108, Proposition A) is crucial. Hence we cannot drop the condition $d \ne 5$.

Proof of Theorem A: First, we consider the case $n \ne 8$.

- For F in Theorem 14, we consider

$$\mu : \mu^{-1}\left(\theta_0, \frac{n-2}{n}\pi\right] \to \mathbb{R}.$$

More precisely, we denote the restriction of μ in (5) to $\mu^{-1}\left(\theta_0, \frac{n-2}{n}\pi\right]$ by the same symbol μ. Note that from the definition of F, z in Theorem 14 is $C_n\left(\frac{n-2}{n}\pi\right)$.

- By Proposition 12 (i), $\mu^{-1}\left(\theta_0, \frac{n-2}{n}\pi\right]$ is in fact a manifold.

- For a in Theorem 14, we consider any element θ in $\left(\theta_0, \frac{n-2}{n}\pi\right)$.

Below we check that the conditions i, ii, iii and iv in Theorem 14 are satisfied. The items i and ii are clear. The item iii follows from Proposition 12 ii. The item iv follows from the following argument: Since dim $X_n = n - 3$, we have dim $\mu^{-1}\left(\theta_0, \frac{n-2}{n}\pi\right] \neq 5$ if and only if $n \neq 8$.

Now we can apply Theorem 14 and obtain that $\mu^{-1}(\theta)$ is diffeomorphic to S^{n-4} if θ satisfies that $\theta_0 < \theta < \frac{n-2}{n}\pi$. By (6), this is equivalent to saying that $C_n(\theta)$ is also diffeomorphic to S^{n-4}. This completes the proof of Theorem A for $n \neq 8$.

Second, we consider the case $n = 8$. If we apply the Morse lemma to Proposition 12 (iii), then we obtain that $\mu^{-1}(\theta)$ is diffeomorphic to S^4 if θ satisfies that $\theta_0 < \theta < \frac{6}{8}\pi$. Hence $C_8(\theta)$ is also diffeomorphic to S^4. This completes the proof of Theorem A for $n = 8$.

4. Proofs of Theorems B and C

Proof of Theorem B: In ([8], Lemma 1), certain conditions on an element $(u_1, \cdots, u_n)$ of $C_n(\theta)$ are listed. For example, a condition is given by

$$u_2 = u_n. \tag{27}$$

Let Λ be the set of the conditions. For $\lambda \in \Lambda$, we set

$$\Theta_\lambda := \inf \ \left\{\theta_0 \in \left(0, \frac{n-2}{n}\pi\right) \ \middle| \ \text{for all } \theta \in \left(\theta_0, \frac{n-2}{n}\pi\right), C_n(\theta) \text{ does not contain an element which satisfies the condition } \lambda\right\}. \tag{28}$$

Using this, we set

$$\beta_n := \max \ \{\Theta_\lambda \ | \ \lambda \in \Lambda\}. \tag{29}$$

Then it is proved in ([8], Proposition 1) that

$$\alpha_n = \beta_n. \tag{30}$$

We explain how to compute Θ_λ. As an example of λ, we consider the condition (27). We construct the continuous function

$$R_\lambda : (0, \pi) \to \mathbb{R} \tag{31}$$

which satisfies the following two properties:

a. We have $R_\lambda(\theta) \geq 0$ for all θ.

b. An element $\theta \in (0, \pi)$ satisfies $R_\lambda(\theta) = 0$ if and only if $C_n(\theta)$ contains an element which satisfies the condition (27).

In order to construct R_λ in (31), we first fix θ and define the space $Y_n(\theta)$ as follows:

$$Y_n(\theta) := \left\{(u_1, \cdots, u_n) \in \left(S^2\right)^n \ \mid \ \text{the following i and ii hold}\right\}.$$

i. $u_1 = (1, 0, 0)$ and $u_2 = u_n = (-\cos\theta, -\sin\theta, 0)$.

ii. $\langle u_i, u_{i+1}\rangle = -\cos\theta$ for $2 \le i \le n-3$.

Second, we define the function $r_\lambda : Y_n(\theta) \to \mathbb{R}$ as follows: For $(u_1, \cdots, u_n) \in Y_n(\theta)$, we set

$$r_\lambda(u_1, \cdots, u_n) := \left\| \sum_{i=1}^{n} u_i \right\|. \tag{32}$$

Third, we define R_λ in (31) by

$$R_\lambda(\theta) := \min r_\lambda(Y_n(\theta)).$$

Below we check the above properties a and b of R_λ.

The item a is clear.

In order to prove the item b, we claim the following identification holds:

$$r_\lambda^{-1}(0) = \{(u_1, \cdots, u_n) \in C_n(\theta) \ \mid \ u_2 = u_n\}. \tag{33}$$

In fact, an element $(u_1, \cdots, u_n) \in Y_n(\theta)$ belongs to $r_\lambda^{-1}(0)$ if and only if (1) ii holds. Hence (33) follows.

Now the item b is clear from (33). Thus we have checked the above properties a and b.

Next using the properties a and b, we can describe Θ_λ in (28) as

$$\Theta_\lambda = \max\{\theta \in (0, \pi) \ \mid \ R_\lambda(\theta) = 0\}. \tag{34}$$

From the constructions in (10) and (11), we have

$$Y_n(\theta) \cong \left(S^1\right)^{n-4} \times S^2.$$

Using this fact, we can compute the right-hand side of (34) for $n \le 14$.

By a similar method, we compute Θ_λ for each $\lambda \in \Lambda$. Then from the definition of β_n in (29), we can determine β_n. Finally, using (30), we obtain α_n. This completes the proof of Theorem B.

Remark 16. In the above proof of Theorem B, the identification (33) is crucial. Although $r_\lambda^{-1}(0)$ is a critical submanifold of the function r_λ in (32), this fact allows us to compute the right-hand side of (34) for $n \le 14$. See §6 (ii) for further remarks.

Proof of Theorem C: The theorem is clear from **Table 3**.

5. Proof of Theorem D

The following proposition is a refinement of Proposition 12 for $n = 6$.

Proposition 17. *(i) The space X_6 is a manifold, where X_n is defined in* (4).

(ii) The interior angle θ is a critical point of μ if and only if θ equals to $\frac{\pi}{3}$, $\frac{\pi}{2}$ or $\frac{2}{3}\pi$.

Proof: We can prove the proposition is the same way as in Proposition 12. Since the dimension is low, we can perform direct computations.

We apply the first fundamental theorem of Morse theory to Proposition 17. Then we obtain the following assertion: If θ_1 and θ_2 belong to the same interval from the three intervals $\left(0, \frac{\pi}{3}\right)$, $\left(\frac{\pi}{3}, \frac{\pi}{2}\right)$ and $\left(\frac{\pi}{2}, \frac{2}{3}\pi\right)$, then we have $C_6(\theta_1) \cong C_6(\theta_2)$.

The homeomorphism (9) tells us that in order to determine the topological type of $C_6(\theta)$, it will suffice to determine the topological type of $p^{-1}(\theta)$ for $n = 6$. For a fixed $\psi \in [0, 2\pi]$, we set

$$M_\theta(\psi) := \left\{ \left(e^{i\phi_1}, e^{i\phi_2}, e^{i\phi_3}, \theta\right) \in p^{-1}(\theta) \;\middle|\; \phi_1 = \psi \right\}.$$

Since $M_\theta(\psi)$ is a one dimensional object, it is not to difficult to draw its figure. The results are given as follows.

(i) *The case when* $\frac{\pi}{2} < \theta < \frac{2}{3}\pi$.

There exists ω in $(0, \pi)$ such that the following homeomorphism holds:

$$M_\theta(\psi) \cong \begin{cases} \{\text{one point}\}, & \text{if } \psi = \omega \text{ or } 2\pi - \omega, \\ \varnothing, & \text{if } \omega < \psi < 2\pi - \omega, \\ S^1, & \text{otherwise.} \end{cases}$$

From this, we have $p^{-1}(\theta) \cong S^2$. The figure of $C_6(\theta)$ is given by the following **Figure 6**.

(ii) *The case when* $\frac{\pi}{3} < \theta < \frac{\pi}{2}$.

There exists ω in $(0, \pi)$ such that the following homeomorphism holds:

$$M_\theta(\psi) \cong \begin{cases} \sigma, & \text{if } \psi = \omega \text{ or } 2\pi - \omega. \\ S^1, & \text{otherwise,} \end{cases} \tag{35}$$

Here we set

$$\sigma := \bigcup_{i=1}^{2} \left\{ (x, y) \in \mathbb{R}^2 \;\middle|\; x^2 + i^2 y^2 = 1 \right\}.$$

(The figure of σ is given by the following **Figure 5(b)**.)

We claim that the four intersection points in $M_\theta(\omega) \cup M_\theta(2\pi - \omega)$ are saddle points of $p^{-1}(\theta)$. In fact, for a sufficiently small positive real number ε, the following **Figure 5 (a)–(c)** give the shape of $M_\theta(\omega - \varepsilon)$, $M_\theta(\omega)$ and $M_\theta(\omega + \varepsilon)$, respectively. (The deformation of the shape of $M_\theta(\psi)$ when ψ is near $2\pi - \omega$ is also given by **Figure 5**.) Now from **Figure 5**, we see that the four intersection points are in fact saddle points.

Since we identify $M_\theta(0)$ with $M_\theta(2\pi)$, (35) and **Figure 5** give the homeomorphism $p^{-1}(\theta) \cong \underset{3}{\#}(S^1 \times S^1)$. The figure of $C_6(\theta)$ is given by the following **Figure 7**.

(iii) *The case when* $0 < \theta < \frac{\pi}{3}$.

The topological type of $M_\theta(\psi)$ is the same as (35). Hence the argument in (ii) remains valid.

Remark 18. We determine the topological type of $C_6\left(\frac{\pi}{2}\right)$ and $C_6\left(\frac{\pi}{3}\right)$.

(i) The figure of $C_6\left(\frac{\pi}{2}\right)$ is given by the following **Figure 8**.

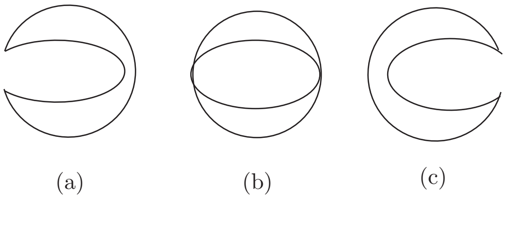

Figure 5.
(a) $M_\theta(\omega - \varepsilon)$; (b) $M_\theta(\omega)$; (c) $M_\theta(\omega + \varepsilon)$.

Thus $C_6\left(\frac{\pi}{2}\right)$ is homeomorphic to the orbit space $S^2/\sim$, where the equivalence relation is generated by

$$(-1,0,0)\sim(1,0,0),\quad (0,-1,0)\sim(0,1,0)\quad \text{and}\quad (0,0,-1)\sim(0,0,1).$$

In particular, $C_6\left(\frac{\pi}{2}\right)$ has three singular pints.

As θ approaches $\frac{\pi}{2}$ from below, each center of the three handles in **Figure 7** shrinks. And when $\theta=\frac{\pi}{2}$, each center pinches to a point and we obtain **Figure 8**. If θ increases further from $\frac{\pi}{2}$, then the pinched point separates and we obtain **Figure 6**.

(ii) The figure of $C_6\left(\frac{\pi}{3}\right)$ is given by the following **Figure 9**.

The space $C_6\left(\frac{\pi}{3}\right)$ contains subspaces

$$N_1,\ \ N_2\ \text{ and }\ N_3 \tag{36}$$

which satisfy the following three properties:

- $N_1\cong S^1\times S^1, .N_2\cong S^1\times S^1$ and $N_3\cong \underset{2}{\#}\left(S^1\times S^1\right)$
- $\bigcup_{i=1}^{3} N_i = C_6\left(\frac{\pi}{3}\right)$.
- $\bigcup_{i<j}\left(N_i\cap N_j\right)\cong \bigcup_{i=1}^{3}\left\{(x,y)\in\mathbb{R}^2\ \mid\ x^2+i^2y^2=1\right\}$.

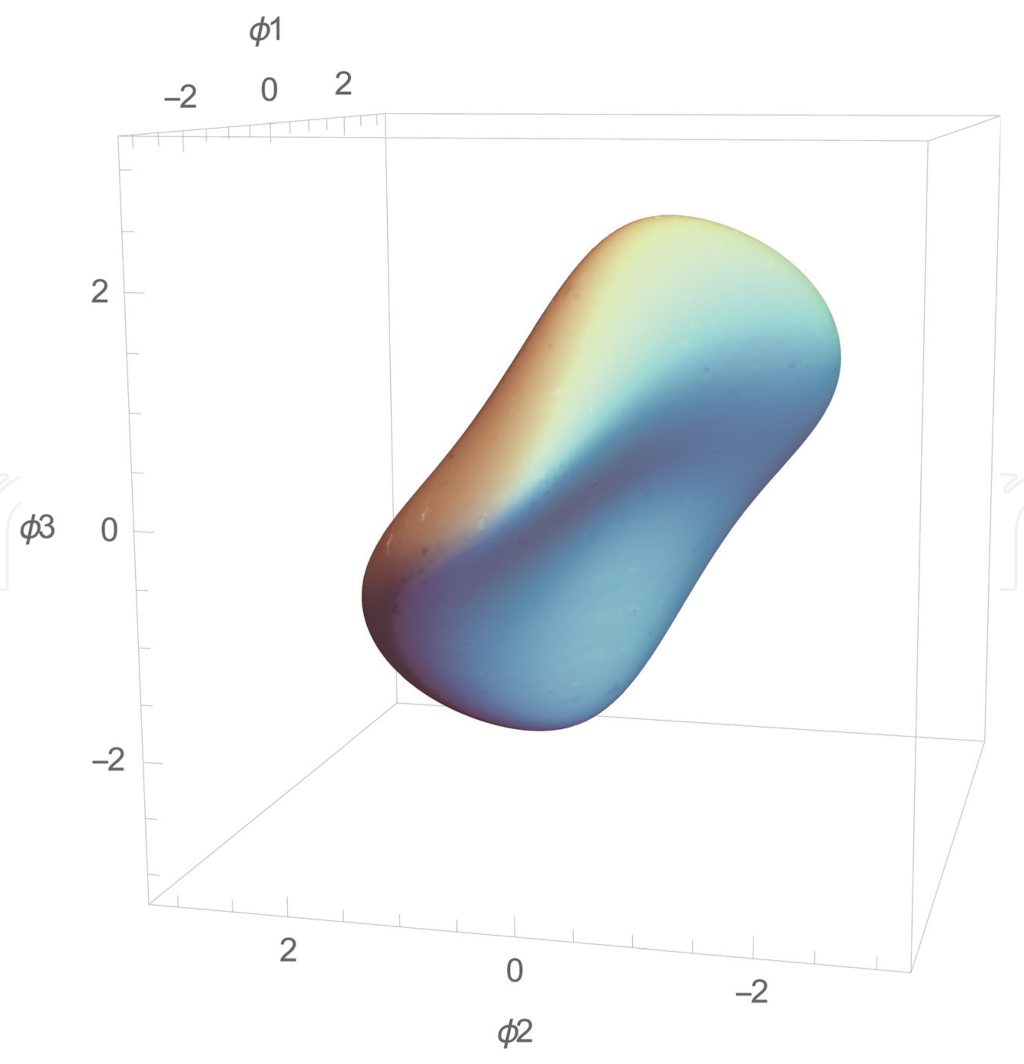

Figure 6.
The space $C_6(\theta)$ for $\frac{\pi}{2}<\theta<\frac{2}{3}\pi$.

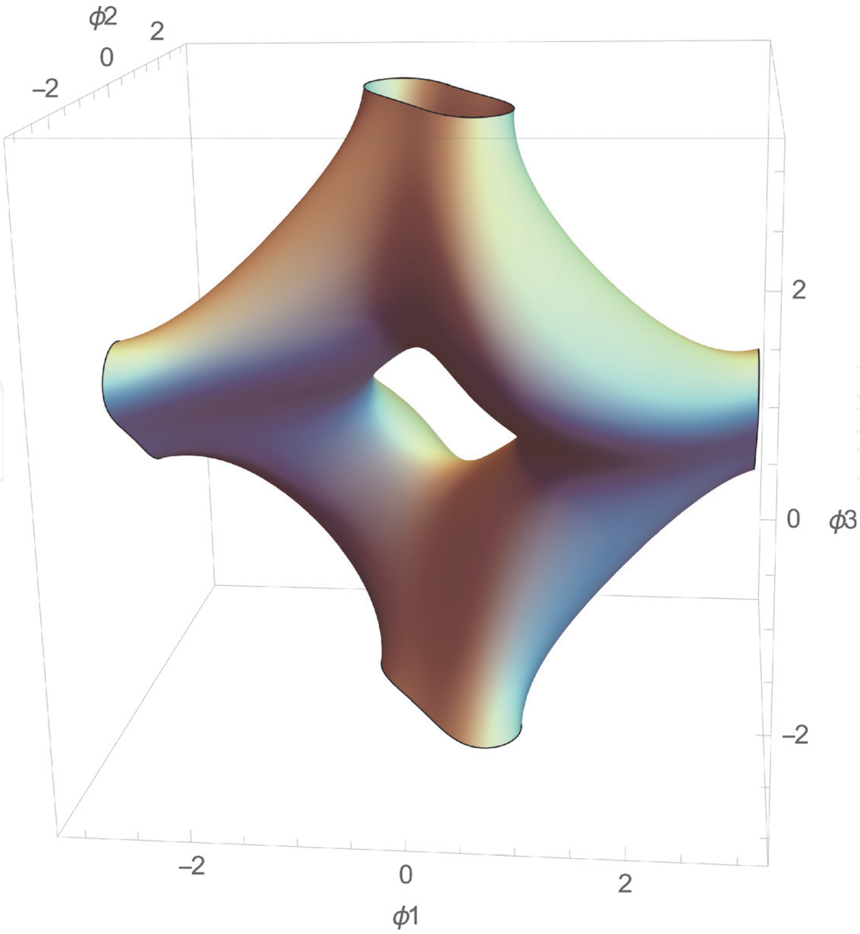

Figure 7.
The space $C_6(\theta)$ for $\frac{\pi}{3} < \theta < \frac{\pi}{2}$, where we identify the opposite boundaries.

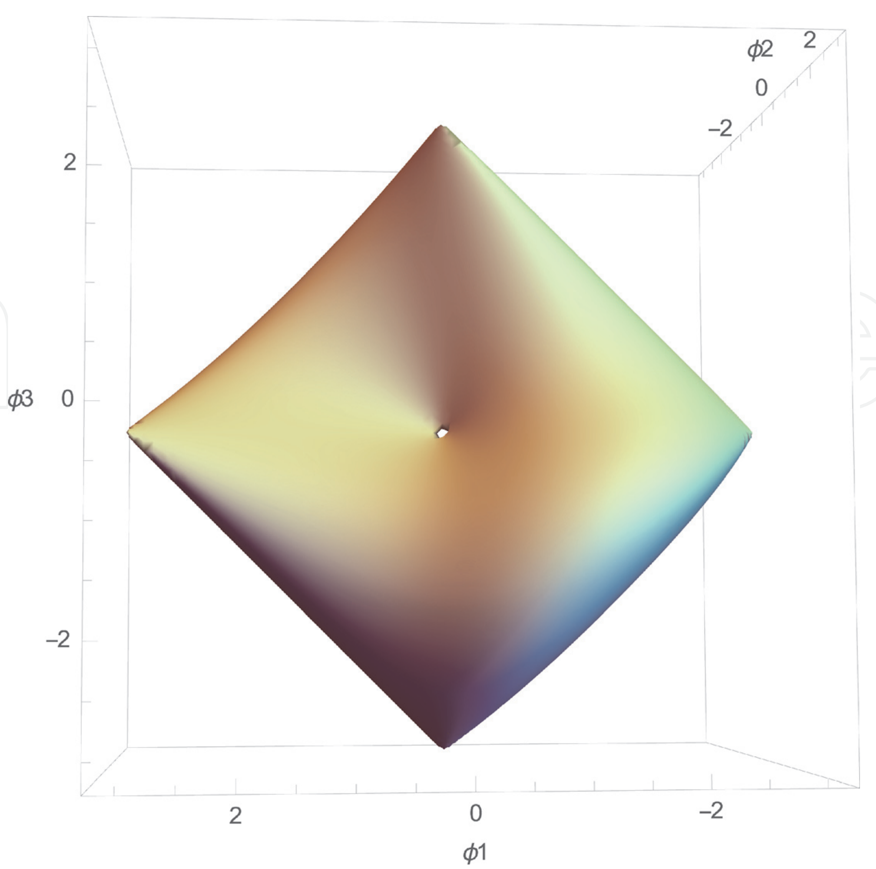

Figure 8.
The space $C_6\left(\frac{\pi}{2}\right)$, where we identify the opposite vertices.

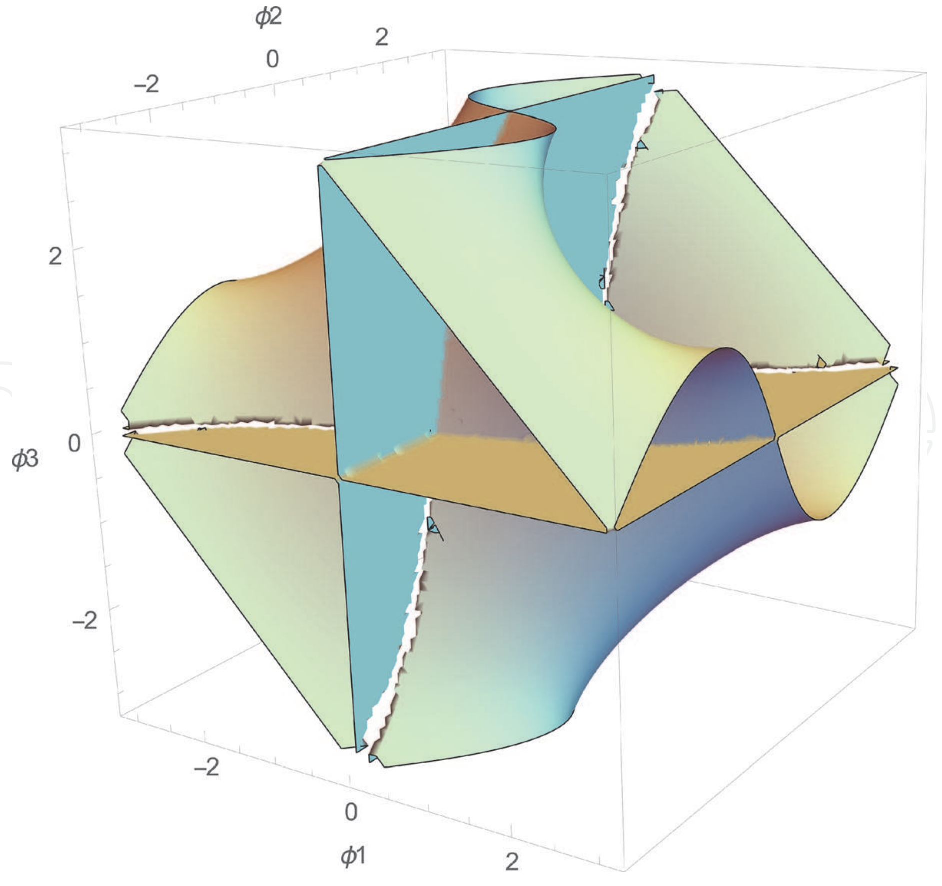

Figure 9.
The space $C_6\left(\frac{\pi}{3}\right)$.

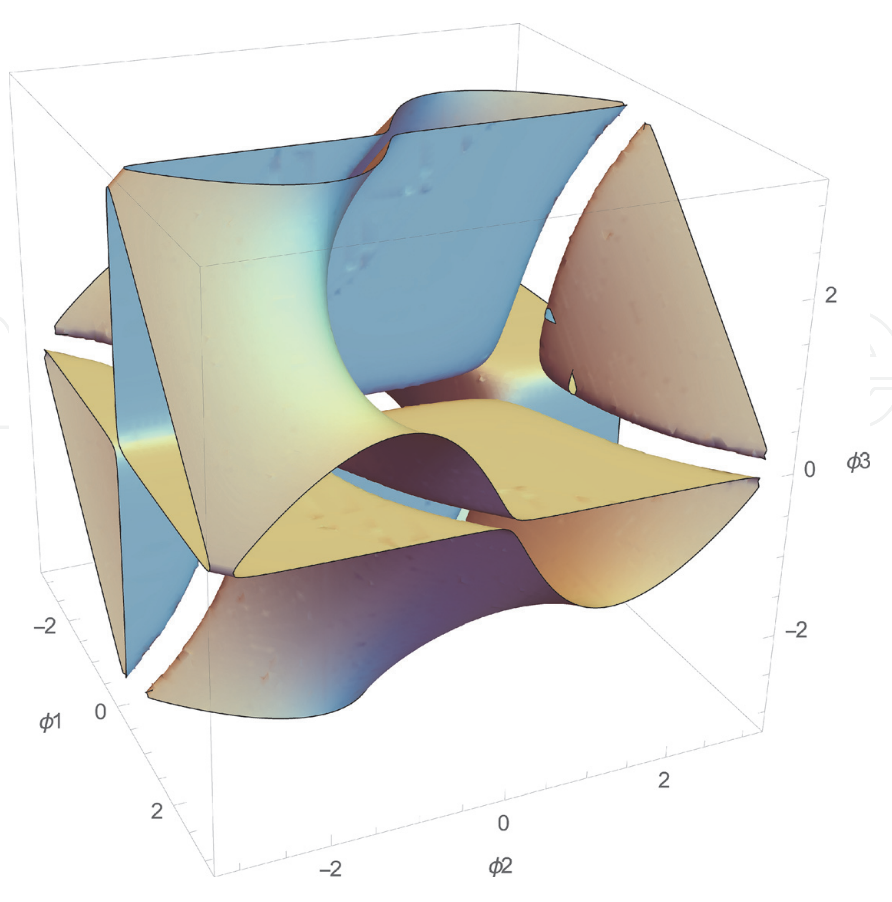

Figure 10.
The space $C_6\left(\frac{\pi}{3} \pm \varepsilon\right)$.

The figure of $C_6\left(\frac{\pi}{3} \pm \varepsilon\right)$ is given by **Figure 10** above.

As θ approaches $\frac{\pi}{3}$, a cross-section of the four tubes in **Figure 7** becomes a union of two circles: In the notation of (36), one circle becomes a handle of N_3. And the other circle is a subspace of $N_1 \cup N_2$.

On the other hand, the hole of the center of **Figure 7** becomes a subspace of $N_1 \cup N_2$.

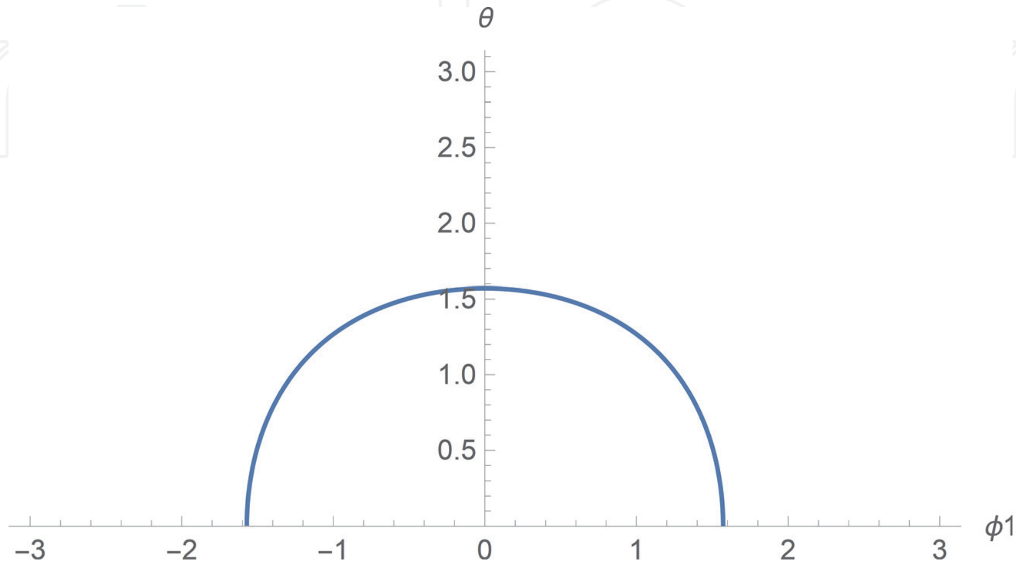

Figure 11.
The space X_4.

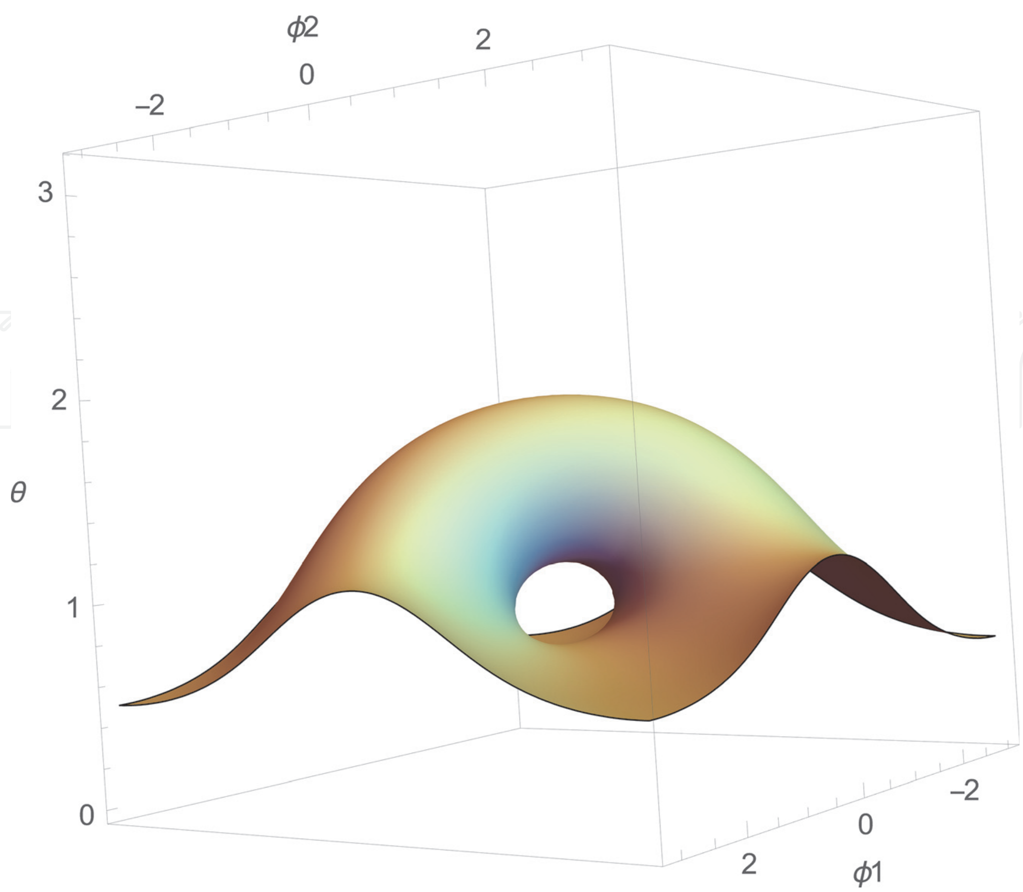

Figure 12.
The space X_5.

Proof of Example 4: We can prove the example in the same way as in Theorem D. We can also prove by the following method. Recall that the space X_n was defined in (4). The figures of X_4 and X_5 are given by **Figures 11** and **12** above, respectively.

The identification (6) tells us that each level set of **Figure 11** gives $C_4(\theta)$, and that of **Figure 12** gives $C_5(\theta)$. Thus we obtain Example 4.

6. Conclusions

i. We have the following comments about the proof of Theorem A. Recall that for the proof of Theorem A given in §3, we used Proposition 5 but we did not use Theorem 6. In other words, we did not use Reeb's theorem. Instead, we used Theorem 14, for which the h-cobordism theorem is crucial. From the computations for small n, it seems that (26) holds for all n. If we could prove this, then we obtain a proof which uses only the Morse lemma. We pose the following question: Is it possible to prove (26) for all n?

ii. We have the following comments about the proof of Theorem B. Recalling (23) and (24), we consider the following system of equations:

$$\left(\frac{\partial(L\circ f\circ q)}{\partial\phi_1}(x), \cdots, \frac{\partial(L\circ f\circ q)}{\partial\phi_{n-3}}(x)\right) = (0, \cdots, 0) \tag{37}$$

and

$$(L\circ f\circ q)(\phi_1, \cdots, \phi_{n-3}, \theta) = 1. \tag{38}$$

If we could solve the system of Eqs. (37) and (38) with respect to the variables $\phi_1, \cdots, \phi_{n-3}$ and θ, then we could determine for which θ, $C_n(\theta)$ has a singular point and the set of singular points of $C_n(\theta)$. In particular, we obtain Proposition 5. But it is not easy to solve a system of equations even if we can use a computer. Hence, as we remarked in Remark 16, we have given the proof of Theorem B such as in §4. We pose the following question: Is it possible to solve the system of Eqs. (37) and (38) with respect to the variables $\phi_1, \cdots, \phi_{n-3}$ and θ?

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References

[1] Kapovich M, Millson J. The symplectic geometry of polygons in the Euclidean space. Journal of Differential Geometry 1996; 44: 479–513. DOI: 10.4310/jdg/1214459218 https://projecteuclid.org/journals/journal-of-differential-geometry/volume-44/issue-3/The-symplectic-geometry-of-polygons-in-Euclidean-space/10.4310/jdg/1214459218.full [Accessed: 30 September 2021]

[2] Hausmann J.-C, Knutson A. The cohomology ring of polygon spaces. Annales de l'Institut Fourier 1998; 48; 281–321. DOI: 10.5802/aif.1619 https://aif.centre-mersenne.org/item/AIF_1998__48_1_281_0 [Accessed: 30 September 2021]

[3] Farber M. Invitation to Topological Robotics. Zurich Lectures in Advanced Mathematics: European Mathematical Society; 2008. 143p. DOI: 10.4171/054

[4] Crippen G. Exploring the conformation space of cycloalkanes by linearized embedding. Journal of Computational Chemistry 1992; 13: 351–361. DOI:10.1002/jcc.540130308 https://www.researchgate.net/publication/30839993_Exploring_the_conformation_space_of_cycloalkanes_by_ linearized_embedding [Accessed: 30 September 2021]

[5] O'Hara J. The configuration space of equilateral and equiangular hexagons. Osaka Journal of Mathematics 2013; 50: 477–489. DOI:10.18910/25093 https://projecteuclid.org/journals/osaka-journal-of-mathematics/ volume-50/issue-2/The-configuration-space-of-equilateral-and-equiangular- hexagons/ojm/1371833496.full [Accessed: 30 September 2021]

[6] Kamiyama Y. The configuration space of equilateral and equiangular heptagons. JP Journal of Geometry and Topology 2020, 25: 25–33 DOI:http://dx.doi.org/10.17654/GT025120025 https://www.researchgate.net/publication/347482448_THE_CONFIGURATION_SPACE_OF_EQUILATERAL_AND_EQUIANGULAR_HEPTAGONS [Accessed: 30 September 2021]

[7] Goto S, Komatsu K. The configuration space of a mathematical model for ringed hydrocarbon molecules. Hiroshima Mathematical Journal 2012; 42: 115–126. DOI: 10.32917/hmj/1333113009 https://projecteuclid.org/journals/hiroshima-mathematical-journal/volume-42/issue-1/The-configuration-space-of-a-model-for-ringed-hydrocarbon-molecules/10.32917/hmj/1333113009.full [Accessed: 30 September 2021]

[8] Goto S, Komatsu K, Yagi J. The configuration space of almost regular polygons. Hiroshima Mathematical Journal 2020; 50: 185–197. DOI: 10.32917/hmj/1595901626 https://projecteuclid.org/journals/hiroshima-mathematical-journal/ volume-50/issue-2/The-configuration-space-of-almost-regular-polygons/ 10.32917/hmj/1595901626.full [Accessed: 30 September 2021]

[9] Kamiyama Y. A filtration of the configuration space of spatial polygons. Advances and Applications in Discrete Mathematics 2019; 22: 67–74. DOI:http://dx.doi.org/10.17654/DM022010067 https://www.researchgate.net/publication/ 336117647_A_FILTRATION_OF_THE_CONFIGURATION_SPACE_OF_SPATIAL_POLYGONS [Accessed: 30 September 2021]

[10] Milnor J. Morse Theory. Annals of Mathematics Studies Volume 51: Princeton University Press; 1963. 153p. DOI: 10.1515/9781400881802

[11] Goto S, Hemmi Y, Komatsu K, Yagi J. The closed chains with spherical configuration spaces. Hiroshima Mathematical Journal 2012, 42: 253–266.

DOI: 10.32917/hmj/1345467073 https://projecteuclid.org/journals/hiroshima-mathematical-journal/ volume-42/issue-2/The-closed-chains-with-spherical-configuration-spaces/ 10.32917/hmj/1345467073.full [Accessed: 30 September 2021]

[12] Kamiyama Y. The Euler characteristic of the regular spherical polygon spaces. Homology Homotopy and Applications 2020, 22: 1–10. DOI: https://dx.doi.org/10.4310/HHA.2020.v22.n1.a1 https://www.intlpress.com/site/pub/pages/journals/items/hha/content/vols/0022/0001/a001 [Accessed: 30 September 2021]

[13] Kamiyama Y. On the level set of a function with degenerate minimum point. International Journal of Mathematics and Mathematical Sciences 2015, Article ID 493217: 6pages. DOI:10.1155/2015/493217 https://downloads.hindawi.com/journals/ijmms/2015/493217.pdf [Accessed: 30 September 2021]

[14] Milnor J. Lectures on the h-cobordism Theorem. Princeton University Press: Princeton; 1965. 122p. DOI: 10.1515/9781400878055