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The closed chains with spherical configuration spaces

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Abstract. As a mathematical model of n-membered ringed hydrocarbon molecules, we consider closed chains in $\mathbf{R}^3$. Assume that the bond angle θ satisfies $\frac{n-4}{n-2}\pi < \theta < \frac{n-2}{n}\pi$ when $n = 5, 6, 7$, and that $\frac{5}{7}\pi \leq \theta < \frac{3}{4}\pi$ when $n = 8$. Then the configuration space C_n of the model is homeomorphic to $(n-4)$-dimensional sphere S^{n-4}. By this result, it is possible for approximating larger macrocyclic molecules by smaller ones to be more widely applied.

1. Introduction

In Mathematics, the study of configurations of closed chains has been considered from a topological, an algorithmic or a kinematic viewpoint. See, for example ([2], [6], [8], [10], [11], [12], [15], [17]). As a mathematical model of n-membered ringed hydrocarbon molecules, we consider closed chains in $\mathbf{R}^3$ with rigidity ([3], [5], [9], [14]).

A closed chain is defined to be a graph in $\mathbf{R}^3$ having vertices $\{v_0, v_1, \dots, v_{n-1}\}$ and bonds $\{\beta_1, \beta_2, \dots, \beta_{n-1}, \beta_0\}$, where β_i connects v_{i-1} with v_i $(i = 1, 2, \dots, n-1)$ and β_0 connects v_{n-1} with v_0. For the sake of simplicity, let bond vectors $v_i - v_{i-1}$ be denoted by $\boldsymbol{\beta}_i$ $(i = 1, 2, \dots, n-1)$ and $v_0 - v_{n-1}$ be denoted by $\boldsymbol{\beta}_0$.

We fix θ, and put 3 vertices $v_0 = (0, 0, 0)$, $v_{n-1} = (-1, 0, 0)$, $v_{n-2} = (\cos\theta - 1, \sin\theta, 0)$. We define a configuration space of closed chains by the following:

Definition 1. We define $f_k : (\mathbf{R}^3)^{n-3} \to \mathbf{R}$ by $f_k(v_1, \dots, v_{n-3}) = \frac{1}{2}(\|\boldsymbol{\beta}_k\| - 1)$ for $k = 1, \dots, n-2$, and $g_k : (\mathbf{R}^3)^{n-3} \to \mathbf{R}$ by $g_1(v_1, \dots, v_{n-3}) = \langle -\boldsymbol{\beta}_0, \boldsymbol{\beta}_1 \rangle - \cos\theta$, $g_k(v_1, \dots, v_{n-3}) = \langle -\boldsymbol{\beta}_{k+1}, \boldsymbol{\beta}_{k+2} \rangle - \cos\theta$ for $k = 2, \dots, n-3$, where $\langle\, , \rangle$ denotes the standard inner product in $\mathbf{R}^3$ and $\|\cdot\|$ the standard norm $\|\boldsymbol{x}\| = \sqrt{\langle \boldsymbol{x}, \boldsymbol{x} \rangle}$. We call θ a *bond angle*.

Then the configuration space C_n is defined by the following;

$$C_n = \{p \in (\mathbf{R}^3)^{n-3} \mid f_1(p) = \cdots = f_{n-2}(p) = g_1(p) = \cdots = g_{n-3}(p) = 0\}.$$

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We call f_k, g_k *rigidity maps*. Rigidity maps determine bond lengths and angles of a closed chain in C_n. The closed chains in C_n are equilateral polygons in $\mathbf{R}^3$ with n vertices such that the bond angles are all equal to a given angle θ except for two successive ones.

The standard bond angle of 5,6,7-membered ringed hydrocarbon molecules is equal to $\frac{7}{12}\pi$, $\cos^{-1}\left(-\frac{1}{3}\right)$, $\cos^{-1}\left(-\frac{1}{3}\right)$, respectively. Then the configuration space C_n is homeomorphic to $(n-4)$-dimensional sphere S^{n-4} for $n = 5, 6, 7$ ([4]).

We need to study the condition of the bond angle to satisfy that a configuration space C_n of the model is homeomorphic to $(n-4)$-dimensional sphere S^{n-4} in order to approximate larger macrocyclic molecules by smaller ones as in [3], [5] and [14].

We obtain the following theorem:

Theorem 1. *Assume that the bond angle satisfies* $\frac{n-4}{n-2}\pi < \theta < \frac{n-2}{n}\pi$ *when* $n = 5, 6, 7$ *and that* $\frac{5}{7}\pi \le \theta < \frac{3}{4}\pi$ *when* $n = 8$. *Then the configuration space* C_n *is homeomorphic to* $(n-4)$*-dimensional sphere* S^{n-4} *when* $n = 5, 6, 7, 8$.

This note is arranged as follows. In Section 2 we prove preliminary results for the proof of Theorem 1. In Section 3 we prove Theorem 1.

In the following sections, we assume that $\frac{n-4}{n-2}\pi < \theta < \frac{n-2}{n}\pi$ when $n = 5, 6, 7$ and that $\frac{5}{7}\pi \le \theta < \frac{3}{4}\pi$ when $n = 8$.

2. Preliminaries

We need the following lemmas in the proof of Theorem 1.

Lemma 1.

(1) *When* $n = 5, 6, 7$, *any closed chain in* C_n *does not have the local configurations of successive three bonds* β_k, β_{k+1} *and* β_2 $(k = 0, 3)$ *that the bond vectors satisfy* $\boldsymbol{\beta_k} + \boldsymbol{\beta_{k+1}} = \lambda\boldsymbol{\beta_2}$ *for any nonzero* λ *as in Figs.* 1, 2, 3 *and* 4.

(2) *When* $n = 5, 6, 7, 8$, *any closed chain in* C_n *does not have the local configurations of successive three bonds* β_k, β_{k+1} *and* β_{k+2} *with bond angles* θ *that the bond vectors satisfy* $\boldsymbol{\beta_k} = \boldsymbol{\beta_{k+2}}$ *as in Fig.* 5, *where all indices are modulo n.*

(3) *When* $n = 5, 6, 7, 8$, *all vertices cannot be in one plane for each closed chain in* C_n.

(4) *When* $n = 5, 6, 7, 8$, *the configuration space* C_n *is not the empty set.*

We call such local configurations as (1) *and* (2) *the forbidden local configurations.*

PROOF. (1) First, we give the proof in the case that $k = 0$ and $\lambda > 0$. By using the similar argument, we can prove the case that $k = 3$ and $\lambda > 0$. We consider a non-closed chain $\Gamma_{\beta_{n-1,0,1,2}}$ which consists of four bonds β_{n-1}, β_0, β_1 and β_2, and assume that $\Gamma_{\beta_{n-1,0,1,2}}$ has the configuration as in Fig. 1. Then, the minimal value of the distance between v_{n-2} and v_2 is given by the following function of θ:

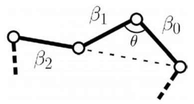

Fig. 1. (1) The forbidden local configuration for $k = 0$ and $\lambda > 0$

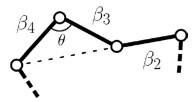

Fig. 2. (1) The forbidden local configuration for $k = 3$ and $\lambda > 0$

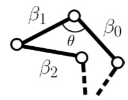

Fig. 3. (1) The forbidden local configuration for $k = 0$ and $\lambda < 0$

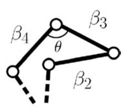

Fig. 4. (1) The forbidden local configuration for $k = 3$ and $\lambda < 0$

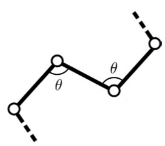

Fig. 5. (2) The forbidden local configuration $\beta_k = \beta_{k+2}$

$$f(\theta) = \sqrt{1 + (1 - 2\cos\theta)^2 + (1 - 2\cos\theta)\sqrt{2 - 2\cos\theta}}.$$

When $n = 5$, we have $f(\theta) > 1$ $(\theta \in (\frac{1}{3}\pi, \frac{3}{5}\pi))$ since $f(\theta)$ is a monotonic increasing function of θ. Thus, we cannot get any closed chains in C_5 from non-closed chain $\Gamma_{\beta_{4,0,1,2}}$ by adding a bond β_3 even if we forget the restriction of the bond angle at v_3.

When $n = 6$, we have $f(\theta) > \sqrt{2 + \sqrt{2}} > \sqrt{3}$ $(\theta \in (\frac{1}{2}\pi, \frac{2}{3}\pi))$ since $f(\theta)$ is a monotonic increasing function of θ. Since the maximal value of the distance between v_2 and v_4 on two bonds β_3, β_4 is $\sqrt{3}$ we cannot get any closed chains in C_6 from non-closed chain $\Gamma_{\beta_{5,0,1,2}}$ by adding two bonds β_3, β_4.

When $n = 7$, we consider a non-closed chain $\Gamma_{\beta_{5,6,0,1,2}}$ which consists of five bonds β_5, β_6, β_0, β_1, β_2, and assume that $\Gamma_{\beta_{5,6,0,1,2}}$ has the configuration as in Fig. 1.

We assume that β_6 is on x-axis and v_6 is the origin. Then, the coordinate of v_4 is given by $(\cos\theta - 1, x_1 \sin\theta, y_1 \sin\theta)$ $(x_1^2 + y_1^2 = 1)$. Note that the coordinate of v_4 is changed into $(x_1 \sin^2\theta + \cos\theta - \cos^2\theta,$ $\sin\theta(1 - \cos\theta - x_1 \cos\theta), y_1 \sin\theta)$ after rotational transformation by clockwise angle $\pi - \theta$ at v_6. On the other hand, the coordinate of v_2 is given by $\left(t(\theta)\cos\left(\frac{3(\pi-\theta)}{4}\right)+1, x_2 t(\theta)\sin\left(\frac{3(\pi-\theta)}{4}\right), y_2 t(\theta)\sin\left(\frac{3(\pi-\theta)}{4}\right)\right)$, where $t(\theta) = \sqrt{2-2\cos\left(\frac{\pi+\theta}{2}\right)}$ and $x_2^2+y_2^2=1$. Thus, we have the following inequality:

$$d(v_4, v_2) \geq |\cos\theta - \cos^2\theta + x_1 \sin^2\theta - (1-\cos\theta\sqrt{2-2\cos\theta})|.$$

Let m be the minimal value of the distance between v_4 and v_2 on $\Gamma_{\beta_{5,6,0,1,2}}$, and $g(\theta)$ a continuous function with respect to θ defined by

$$g(\theta) = |\cos\theta - 2\cos^2\theta + \cos\theta\sqrt{2-2\cos\theta}|.$$

Then, since when $x_1 = 1$ the value of this function of x_1 is the minimal value, we have $m \geq g(\theta)$. Moreover, we have $g(\theta) - \sqrt{2-2\cos\theta} > 0.13 > 0$ by calculating.

Thus, we cannot get closed chains in C_7 from non-closed chain $\Gamma_{\beta_{n-2,n-1,0,1,2}}$ by adding two bonds β_3, β_4 by the restriction of the bond angle at v_3.

Next, we give the proof in the case that $k=0$ and $\lambda < 0$. By the similar argument we can prove the case that $k=3$ and $\lambda < 0$. We consider a non-closed chain $\Gamma_{\beta_{0,1,2}}$ which consists of three bonds β_0, β_1 and β_2, and assume that this chain forms the local configuration as in Fig. 3. We remark that the distance between v_{n-1} and v_2 is equal to $\sqrt{2-2\cos\theta} - 1$.

When $n=5$, we cannot get any closed chains in C_5 from $\Gamma_{\beta_{0,1,2}}$ by adding two bonds β_3, β_4 since the distance between v_2 and v_4 on two bonds β_3, β_4 is equal to $\sqrt{2-2\cos\theta}$ by the restriction of the bond angle at v_3.

When $n=6$, we cannot get any closed chains in C_6 from the non-closed chain $\Gamma_{\beta_{0,1,2}}$ by adding three bonds β_3, β_4, β_5 since the minimal value of the distance between v_2 and v_5 on three bonds β_3, β_4, β_5 is $1-2\cos\theta$.

When $n=7$, we consider a non-closed chain which consists of four bonds $\Gamma_{\beta_{6,0,1,2}}$ constructed by adding β_6 to $\Gamma_{\beta_{0,1,2}}$. By calculating we have the inequality $\sqrt{2-2\cos\theta} > d(v_2, v_5)$.

On the other hand, the minimal value of the distance between v_2 and v_5 on a non-closed chain consisting of β_3, β_4, β_5 is given $1-2\cos\theta$.

Thus, since we have $1-2\cos\theta > \sqrt{2-2\cos\theta}$ we cannot get any closed chains by adding three bonds β_3, β_4, β_5.

(2) When $n=5$, we consider a non-closed chain $\Gamma_{\beta_{k-1,k,k+1}}$ which consists of three bonds β_{k-1}, β_k and β_{k+1}, and assume that this chain forms the local configuration as in Fig. 5. The distance between v_{k-2} and v_{k+1} is given by the function $h(\theta) = \sqrt{5-4\cos\theta}$ of θ.

On the other hand, we have $h(\theta) > \sqrt{3}$ since $h(\theta)$ is a monotonic increasing function. Thus, we cannot get any closed chains in C_5 from $\Gamma_{\beta_{k-1,k,k+1}}$ by adding successive two bonds since the distance between the end-points is at most $\sqrt{\frac{(3+\sqrt{5})}{2}}$ (< 1.62).

For $n = 6$, we consider a non-closed chain $\Gamma_{\beta_{k-1,k,k+1,k+2}}$ which consists of four bonds β_{k-1}, β_k, β_{k+1} and β_{k+2}, and assume that this chain has a local configuration as Fig. 5 constructed by β_k, β_{k+1} and β_{k+2}. We may assume that the bond angles of β_{k-1}, β_k, β_{k+1} and β_{k+2} are θ. When $n = 6$, for the distance $d(v_{k-1}, v_{k+3})$ between v_{k-2} and v_{k+2} on $\Gamma_{\beta_{k-1,k,k+1,k+2}}$, we have $d(v_{k-1}, v_{k+3}) \geq 2 - 2\cos\theta > 2$. Thus, we cannot get any closed chain in C_6 by adding successive two bonds.

For $n = 7, 8$, we consider a non-closed chain $\Gamma_{\beta_{k-2,k-1,k,k+1,k+2}}$ which consists of five bonds β_{k-2}, β_{k-1}, β_k, β_{k+1} and β_{k+2}.

When $n = 7$, we assume that the local configuration as Fig. 5 is constructed by β_{k-1}, β_k and β_{k+1}. Then we have two cases: $k = 0$ (resp. $k = 2$) or $k \neq 0$ (resp. $k \neq 2$). If $k = 0$ or $k = 2$, then the minimal value of the distance between v_{k-2} and v_{k+3} on five bonds β_{k-2}, β_{k-1}, β_k, β_{k+1}, β_{k+2} is $1 - 2\cos\theta$. On the other hand, the maximal value of the distance between v_{k-2} and v_{k+3} on the other bonds is $\sqrt{2 - 2\cos\theta}$. Then, we have $1 - 2\cos\theta - \sqrt{2 - 2\cos\theta} = 1 - 2\cos\theta - \sqrt{2 - 2\cos\theta} > 0$. If $k \neq 0$ and $k \neq 2$, then for the distance $d(v_{k-2}, v_{k+3})$ between v_{k-2} and v_{k+3} on $\Gamma_{\beta_{k-2,k-1,k,k+1,k+2}}$ we have $d(v_{k-2}, v_{k+3}) \geq 2 - \cos\theta > 2$. Thus, we cannot get any closed chain in C_7 by adding successive three bonds by the restriction of the bond angles at v_k, v_{k+1}, v_{k+2}.

When $n = 8$, we assume that the local configuration as Fig. 5 is constructed by β_k, β_{k+1} and β_{k+2}. In the following, we may assume that the bond angles of β_{k-2}, β_{k-1}, β_k, β_{k+1} and β_{k+2} are θ, since the bond angles of five bonds β_{k-3}, β_{k-2}, β_{k-1}, β_k, β_{k+1} or β_{k-1}, β_k, β_{k+1}, β_{k+2}, β_{k+3} are θ if the local configuration as Fig. 5 is constructed by β_{k-1}, β_k and β_{k+1}.

Then, the coordinates of v_{k-3} and v_{k+2} are given by $(\cos\theta - \cos^2\theta + x_1\sin^2\theta, \sin\theta(1 - \cos\theta - x_1\cos\theta), y_1\sin\theta)$ $(x_1^2 + x_2^2 = 1)$ and $(2 - \cos\theta, x_2\sin\theta, y_2\sin\theta)$ $(x_1^2 + x_2^2 = 1)$ respectively, when the origin is v_{k-1} and β_k is on x-axis. By calculating we have $d(v_{k-2}, v_{k+3}) - 3 > 0$. Thus, we cannot get any closed chains in C_6 (resp. C_7, C_8) by adding one bond (resp. successive two bonds, successive three bonds) to $\Gamma_{\beta_{k-2,k-1,k,k+1,k+2}}$.

(3) We assume that all vertices are in one plane for any closed chain. By forgetting the bond β_2 from the closed chain, we have the non-closed chain with the end points v_1, v_2. By Lemma 1 (2) we see that the successive three bonds in the non-closed chain from the planar local configuration as in Fig. 6.

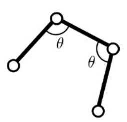

Fig. 6. The planar local configuration of the succcessive three bonds

When $n=5$, the distance between v_1 and v_2 is equal to $|2\cos\theta\sqrt{(2-2\cos\theta)}|$. Then, we have $|2\cos\theta\sqrt{(2-2\cos\theta)}|<1$. When $n=6$, the distance between v_1 and v_2 is less than 1. When $n=7$, the distance between v_1 and v_2 is less than 1. When $n=8$, the distance between v_1 and v_2 is less than 1.

Since the distance between v_1 and v_2 is not equal to 1, all vertices cannot be in one plane for each closed chain in C_n.

(4) We fix the point v_1, and consider the non-closed chains with the end points v_1, v_2. The distance function between v_1 and v_2 is continuous with respect to $v_2,\dots,v_{n-3}$. The distance function between v_1 and v_2 takes a value less than 1 from the above argument. When vertices are not in one plane, it is easy to see that the distance function between v_1 and v_2 can take a value greater than 1. Hence, the configuration space C_n is not the empty set. $\square$

Lemma 2.

(1) *When $n=6,7,8$, any closed chain does not locally contain a planar configuration with $\boldsymbol{\beta_2}=\boldsymbol{\beta_4}$ as in Fig. 7.*

(2) *When $n=8$, any closed chain does not locally contain a planar configuration with $\lambda=-2\cos\theta$, $a\boldsymbol{\beta_2}=b(\boldsymbol{\beta_3}-(\lambda+1)\boldsymbol{\beta_4})$ for some nonzero a, b and the angle $\alpha\in\left(\frac{1}{2}\pi,\theta\right)$ at v_2 as in Figs. 8, 9.*

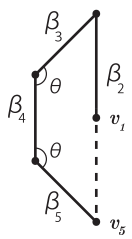

Fig. 7. (1) The forbidden local configuration $\beta_2=\beta_4$

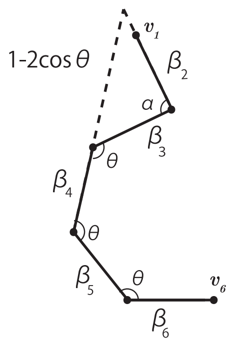

Fig. 8. (2) The forbidden local configuration $ab>0$

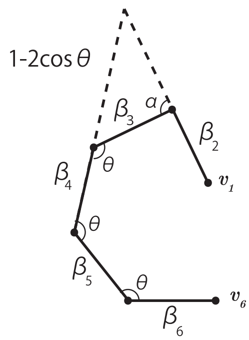

Fig. 9. (2) The forbidden local configuration $ab<0$

Proof. (1) First, we remark that the distance between v_1 and v_5 is given by $-2\cos\theta$. For $n=6,7,8$ we consider a non-closed chain $\Gamma_{\beta_{2,3,4,5}}$ which consists of β_2, β_3, β_4 and β_5, and assume that $\Gamma_{\beta_{2,3,4,5}}$ forms the configuration as in Fig. 7.

When $n=6$, from $\frac{1}{2}\pi<\theta<\frac{2}{3}\pi$ we have $\sqrt{2-2\cos\theta}>1>-2\cos\theta$. Thus, we cannot get any closed chains from $\Gamma_{\beta_{2,3,4,5}}$ adding two bonds by the restriction of the bond angle.

When $n = 7$, the minimal value of the distance between v_1 and v_5 on β_1, β_0, β_6 is equal to $1 - 2\cos\theta$. Thus, we cannot get any closed chains from $\Gamma_{\beta_{2,3,4,5}}$ adding three bonds β_1, β_0, β_6 to $\Gamma_{\beta_{2,3,4,5}}$.

When $n = 8$, the coordinates of v_1 and v_5 on four bonds β_6, β_7, β_0, β_1 can be represented by $(\cos\theta - \cos^2\theta + x_1 \sin^2\theta, \sin\theta(1 - \cos\theta - x_1\cos\theta), y_1 \sin\theta)$ and $(1 - \cos\theta, x_2 \sin\theta, y_2 \sin\theta)$ when the origin is v_7 and β_0 is on x-axis, where $x_1^2 + y_1^2 = 1$ and $x_2^2 + y_2^2 = 1$ respectively. For the distance $d(v_1, v_5)$ between v_1 and v_5 on β_6, β_7, β_0, β_1, we have the inequality $d(v_1, v_5) + 2\cos\theta > 0$ for $\theta \in \left[\frac{5}{7}\pi, \frac{3}{4}\pi\right)$).

This implies that we cannot get any closed chains from $\Gamma_{\beta_{2,3,4,5}}$ adding four bonds β_1, β_0, β_7, β_6 to $\Gamma_{\beta_{2,3,4,5}}$.

(2) First, we consider a non-closed chain $\Gamma_{\beta_{2,3,4,5,6,7}}$ which consists of six bonds β_2, β_3, β_4, β_5, β_6, β_7, and assume that $\Gamma_{\beta_{2,3,4,5,6,7}}$ has the local configuration as in Fig. 8. When the origin is v_5 and β_5 is on x-axis, we have the inequality $d(v_1, v_7) > d(v_2, v_7) \geq \sqrt{2 - 2\cos\theta}$.

Thus, we cannot get any closed chains from $\Gamma_{\beta_{2,3,4,5,6,7}}$ adding two bonds β_1, β_0 to $\Gamma_{\beta_{2,3,4,5,6,7}}$ since the distance between v_1 and v_7 on β_1, β_0 is no less than $\sqrt{2 - 2\cos\theta}$.

Finally, we consider a non-closed chain $\Gamma_{\beta_{2,3,4,5,6}}$ which consists of five bonds β_2, β_3, β_4, β_5, β_6, and assume that $\Gamma_{\beta_{2,3,4,5,6}}$ forms the local configuration as in Fig. 9. We assume that β_3 is on x-axis of which origin is v_2. Then, the coordinate of v_6 is given by $(4\cos^3\theta - 2\cos^2\theta - 2\cos\theta, \sin\theta(4\cos^2\theta - 2\cos\theta), 0)$. Since the coordinate of v_1 is $(\cos(\pi - \alpha), \sin(\pi - \alpha), 0)$, we have the inequality $(1 - 2\cos\theta)^2 - (d(v_2, v_7))^2 > (1 - 2\cos\theta)^2 - ((4\cos^3\theta - 2\cos^2\theta - \cos\theta)^2 + (\sin\theta(4\cos^2\theta - 2\cos\theta - 1))^2) > 0$.

Since the minimal value of distance between v_1 and v_6 on β_1, β_0, β_7 is equal to $1 - 2\cos\theta$, we cannot get any closed chains from $\Gamma_{\beta_{2,3,4,5,6}}$ adding three bonds β_1, β_0, β_7 to $\Gamma_{\beta_{2,3,4,5,6}}$. □

By Lemmas 1 and 2, we obtain the following proposition:

Proposition 1. *The configuration space C_n is an orientable closed $(n-4)$-dimensional submanifold of $\mathbf{R}^{3n-9}$ when $n = 5, 6, 7, 8$.*

Proof. We define $F : (\mathbf{R}^3)^{n-3} \to \mathbf{R}^{2n-5}$ by $F = (f_1, \ldots, f_{n-2}, g_1, \ldots, g_{n-3})$. Then $C_n = F^{-1}(\{\boldsymbol{O}\})$ for $\boldsymbol{O} = (0, \ldots, 0) \in \mathbf{R}^{2n-5}$.

We show that $\boldsymbol{O} \in \mathbf{R}^{2n-5}$ is a regular value of F. So, it suffices to prove that the gradient vectors $(\operatorname{grad} f_1)_p, \ldots, (\operatorname{grad} f_{n-2})_p$, $(\operatorname{grad} g_1)_p, \ldots, (\operatorname{grad} g_{n-3})_p$ are linearly independent for any $p \in F^{-1}(\{\boldsymbol{O}\}) = C_n$, where $(\operatorname{grad} f)_p = \left(\frac{\partial f}{\partial x_j}(p)\right)_j$. It is convenient to decompose the gradient vectors of f_k and g_k into 1×3 blocks. We have the following forms:

$$
\begin{aligned}
(\mathrm{grad}\ f_1)_p &= (\boldsymbol{\beta}_1, \mathbf{0}, \ldots\ldots, \mathbf{0}),\\
&\ \vdots\\
(\mathrm{grad}\ f_k)_p &= (\mathbf{0}, \ldots, \mathbf{0}, -\boldsymbol{\beta}_k, \boldsymbol{\beta}_k, \mathbf{0}, \ldots, \mathbf{0}),\\
&\ \vdots\\
(\mathrm{grad}\ f_{n-2})_p &= (\mathbf{0}, \ldots\ldots, \mathbf{0}, -\boldsymbol{\beta}_{n-2}),\\
(\mathrm{grad}\ g_1)_p &= (-\boldsymbol{\beta}_0, \mathbf{0}, \ldots\ldots, \mathbf{0}),\\
&\ \vdots\\
(\mathrm{grad}\ g_k)_p &= (\mathbf{0}, \ldots, \mathbf{0}, \boldsymbol{\beta}_{k+2}, \boldsymbol{\beta}_{k+1} - \boldsymbol{\beta}_{k+2}, -\boldsymbol{\beta}_{k+1}, \mathbf{0}, \ldots, \mathbf{0}),\\
&\ \vdots\\
(\mathrm{grad}\ g_{n-4})_p &= (\mathbf{0}, \ldots, \mathbf{0}, \boldsymbol{\beta}_{n-2}, \boldsymbol{\beta}_{n-3} - \boldsymbol{\beta}_{n-2}),\\
(\mathrm{grad}\ g_{n-3})_p &= (\mathbf{0}, \ldots\ldots, \mathbf{0}, \boldsymbol{\beta}_{n-1}),
\end{aligned}
$$

where $\boldsymbol{\beta}_k$ denotes the bond vectors of the closed chain corresponding to $p \in C_n$, $\mathbf{0} = (0,0,0)$.

For instance, when $n = 8$, the form is given by the following:

$$
\begin{aligned}
(\mathrm{grad}\ f_1)_p &= (\ \boldsymbol{\beta}_1, && \mathbf{0}, && \mathbf{0}, && \mathbf{0}, && \mathbf{0}),\\
(\mathrm{grad}\ f_2)_p &= (-\boldsymbol{\beta}_2, && \boldsymbol{\beta}_2, && \mathbf{0}, && \mathbf{0}, && \mathbf{0}),\\
(\mathrm{grad}\ f_3)_p &= (\ \mathbf{0}, && -\boldsymbol{\beta}_3, && \boldsymbol{\beta}_3, && \mathbf{0}, && \mathbf{0}),\\
(\mathrm{grad}\ f_4)_p &= (\ \mathbf{0}, && \mathbf{0}, && -\boldsymbol{\beta}_4, && \boldsymbol{\beta}_4, && \mathbf{0}),\\
(\mathrm{grad}\ f_5)_p &= (\ \mathbf{0}, && \mathbf{0}, && \mathbf{0}, && -\boldsymbol{\beta}_5, && \boldsymbol{\beta}_5),\\
(\mathrm{grad}\ f_6)_p &= (\ \mathbf{0}, && \mathbf{0}, && \mathbf{0}, && \mathbf{0}, && -\boldsymbol{\beta}_6),\\
(\mathrm{grad}\ g_1)_p &= (-\boldsymbol{\beta}_0, && \mathbf{0}, && \mathbf{0}, && \mathbf{0}, && \mathbf{0}),\\
(\mathrm{grad}\ g_2)_p &= (\ \mathbf{0}, && \boldsymbol{\beta}_4, && \boldsymbol{\beta}_3 - \boldsymbol{\beta}_4, && -\boldsymbol{\beta}_3, && \mathbf{0}),\\
(\mathrm{grad}\ g_3)_p &= (\ \mathbf{0}, && \mathbf{0}, && \boldsymbol{\beta}_5, && \boldsymbol{\beta}_4 - \boldsymbol{\beta}_5, && -\boldsymbol{\beta}_4),\\
(\mathrm{grad}\ g_4)_p &= (\ \mathbf{0}, && \mathbf{0}, && \mathbf{0}, && \boldsymbol{\beta}_6, && \boldsymbol{\beta}_5 - \boldsymbol{\beta}_6),\\
(\mathrm{grad}\ g_5)_p &= (\ \mathbf{0}, && \mathbf{0}, && \mathbf{0}, && \mathbf{0}, && \boldsymbol{\beta}_7).
\end{aligned}
$$

Assume that the gradient vectors $(\text{grad } f_1)_p, \dots, (\text{grad } f_{n-2})_p$, $(\text{grad } g_1)_p, \dots,$ $(\text{grad } g_{n-3})_p$ are linearly dependent. Then $c_k \neq 0$ and $\sum_{i=1}^{n-2} c_i (\text{grad } f_i)_p + \sum_{i=1}^{n-3} c_{i+n-2} (\text{grad } g_i)_p = (\mathbf{0}, \dots, \mathbf{0})$ for some k.

Now we will show that all vertices of the closed chain corresponding to p are in one plane by using Lemma 1 (1), (2) in what follows. Let $v_0, v_1, \dots, v_{n-1}$ denote the vertices of the closed chain corresponding to p. Since two successive bond vectors $\boldsymbol{\beta}_k$, $\boldsymbol{\beta}_{k+1}$ are linearly independent for $k \neq 1, 2$, we get that $c_2 \neq 0$. Then the first 1×3 blocks of gradient vectors implies that the vertices v_0, v_1, v_2 and v_{n-1} are in one plane and the second 1×3 blocks of gradient vectors implies that the vertices v_1, v_2, v_3 and v_4 are in one plane. When $n = 5$, all vertices are in one plane since β_0, β_1, β_2 and β_2, β_3, β_4 are in one plane respectively.

When $n = 6$, we consider two cases: $c_7 \neq 0$ or $c_7 = 0$.

If $c_7 \neq 0$, all vertices are in one plane. If $c_7 = 0$, we have $c_3 = -c_6$, and β_2, β_3, β_4 has a local configuration as in Fig. 2. This case contradicts Lemma 1 (1).

When $n = 7$, we consider two cases: $c_8 = 0$ or $c_8 \neq 0$.

If $c_8 = 0$, β_2, β_3, β_4 has a configuration as in Fig. 2 from $c_3 = -c_7$. This case contradicts Lemma 1 (1).

If $c_8 \neq 0$, we divide into two cases: $c_9 \neq 0$ or $c_9 = 0$. We remark that β_3, β_4, β_5 are in one plane in this case.

If $c_9 \neq 0$, β_4, β_5, β_6 are in one plane. This implies that all vertices are in one plane.

If $c_9 = 0$, from Lemma 1 (2) we have $\boldsymbol{\beta_3} + 2\cos\theta \boldsymbol{\beta_4} + \boldsymbol{\beta_5} = 0$.

If $-2\cos\theta = 1$, we have $\theta = \frac{2}{3}\pi$. Then, we obtain configurations as in Fig. 1 or 2 since we have $\boldsymbol{\beta_3} - \boldsymbol{\beta_4} + \boldsymbol{\beta_5} = 0$. However, this is impossible to realize from the restriction of the bond angle $\theta = \frac{2}{3}\pi$.

If $-2\cos\theta \neq 1$, we have $c_3 = 0$ by using the above relation. Then any closed chain has a configuration as in Fig. 7. However, this case contradicts Lemma 2 (1).

When $n = 8$, we consider two cases: $c_9 = 0$ or $c_9 \neq 0$.

First, we consider the case $c_9 = 0$. Then, we have two subcases: $c_{10} = 0$ or $c_{10} \neq 0$. If $c_{10} = 0$, from Lemma 1 (2) we have $\boldsymbol{\beta_3} + 2\cos\theta \boldsymbol{\beta_4} + \boldsymbol{\beta_5} = 0$ $(-2\cos\theta \neq 1)$. However, this implies $c_9 \neq 0$.

If $c_{10} \neq 0$, we have two subcases $c_{11} \neq 0$ or $c_{11} = 0$. When $c_{11} \neq 0$, all vertices are in one plane. When $c_{11} = 0$, any closed chain obtains the configuration with the relation $a(\boldsymbol{\beta_3} + \boldsymbol{\beta_4}) = b(\boldsymbol{\beta_5} + \boldsymbol{\beta_6})$ for some nonzero a, b as in Fig. 10. However, this contradicts Lemma 1 (2).

Finally, we consider the case $c_9 \neq 0$. Then, we have two subcases: $c_{10} = 0$ or $c_{10} \neq 0$. If $c_{10} = 0$, from Lemma 1 (2) we have $\boldsymbol{\beta_3} + 2\cos\theta \boldsymbol{\beta_4} + \boldsymbol{\beta_5} = 0$ $(-2\cos\theta \neq 1)$. By using this relation, we have $c_3 = 0$. Since this

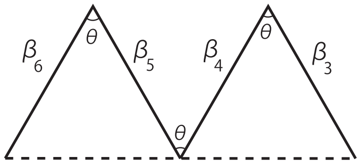

Fig. 10. The forbidden local configuration $a(\boldsymbol{\beta}_3+\boldsymbol{\beta}_4)=b(\boldsymbol{\beta}_5+\boldsymbol{\beta}_6)$

implies that we obtain the configuration as in Fig. 7, this case contradicts Lemma 2 (1). If $c_{10}\neq 0$, we have two cases: $c_{11}\neq 0$ or $c_{11}=0$. When $c_{11}\neq 0$, all vertices are in one plane. When $c_{11}=0$, from Lemma 1 (2) we have $\boldsymbol{\beta}_4+2\cos\theta\boldsymbol{\beta}_5+\boldsymbol{\beta}_6=0$ $(-2\cos\theta\neq 1)$. By using this relation, we have $c_8=(1-2\cos\theta)c_3$. This implies that we obtain the configuration as in Fig. 8 or 9. However, from $2\cos\left(\frac{3}{4}\pi\right)<2\cos\theta\leq 2\cos\left(\frac{5}{7}\pi\right)$ this contradicts Lemma 2 (2).

Hence we see that all vertices $v_0,v_1,\dots,v_{n-1}$ are in the plane through v_1, v_2 and v_{n-1} for $n=5,6,7,8$.

This contradicts Lemma 1 (3). Therefore $\boldsymbol{O}\in\mathbf{R}^{2n-5}$ is a regular value of F and we obtain that C_n is an orientable closed $(n-4)$-dimensional submanifold of $\mathbf{R}^{3n-9}$ by the regular value theorem. The proof of Proposition 1 is completed. □

3. The proof of Theorem 1

We define $h:(\mathbf{R}^3)^{n-3}\to\mathbf{R}$ by $h(v_1,\dots,v_{n-3})=\frac{x_2}{\sqrt{x_2^2+x_3^2}}$, where $v_1=(x_1,x_2,x_3)$. Due to [13, p.25, REMARK1], [16, p.380, Lemma1] we have the extension of Reeb's theorem that M is homeomorphic to a sphere if M is a compact manifold and f is a differentiable function on M with only two critical points.

We show that $h|C_n$ is a differentiable function on C_n with only two critical points. Due to [7] for a function on a manifold embedded in Euclidean space, $p\in C_n$ is a critical point of $h|C_n$ for $h:(\mathbf{R}^3)^{n-3}\to\mathbf{R}$ if and only if there exist $a_i\in\mathbf{R}$ such that $(\mathrm{grad}\,h)_p=\sum_{i=1}^{n-2}a_i(\mathrm{grad}\,f_i)_p+\sum_{i=1}^{n-3}a_{i+n-2}(\mathrm{grad}\,g_i)_p$. We can easily check that $(\mathrm{grad}\,h)_p=\left(0,\frac{x_3^2}{\sin^3\theta},-\frac{x_2x_3}{\sin^3\theta},0,\dots,0\right)$. Note that the first 1×3 block $\left(0,\frac{x_3^2}{\sin^3\theta},-\frac{x_2x_3}{\sin^3\theta}\right)$ is orthogonal to $\boldsymbol{\beta}_0$ and $\boldsymbol{\beta}_1$. So, we see that $a_2\neq 0$ if $(\mathrm{grad}\,h)_p=\sum_{i=1}^{n-2}a_i(\mathrm{grad}\,f_i)_p+\sum_{i=1}^{n-3}a_{i+n-2}(\mathrm{grad}\,g_i)_p$. By the same argument as the proof of Proposition 1 in §2, we obtain that the configuration of the closed chain corresponding to a critical point p satisfies that the vertices v_i $(i=1,\dots,n-1)$ are in one plane $\mathrm{Span}\langle\beta_2,\beta_3\rangle=\mathrm{Span}\langle\beta_2,\dots,\beta_{n-1}\rangle$.

We transform the closed chains by the congruent transformation that maps v_{n-1}, v_{n-2} and v_{n-3} to $(0,0,0)$, $(-1,0,0)$ and $(\cos\theta-1, \sin\theta, 0)$ in this order, and we denote the image of v_k as w_k. This congruent transformation can be expressed by the composition of a translation and a rotation around z-axis and a rotation around x-axis. Because the vertices w_i $(i = 1, \dots, n-1)$ are in the xy-plane, it becomes easy to find the coordinates of the vertices w_i concretely. We only show the case $n = 8$, since other cases can be proved in the same way. When $n = 8$, since $w_1, \dots, w_7$ are in xy-plane, we can calculate the coordinate of w_2 concretely by the restriction of the bond angle at w_3. We have the coordinates of w_2, w_3, w_4, w_5, v_6, v_7.

$$\begin{aligned}
w_2 &= (-8\cos^4\theta + 4\cos^3\theta + 6\cos^2\theta - 2\cos\theta - 1,\\
&\qquad\qquad 2\cos\theta\sin\theta(-4\cos^2\theta + 2\cos\theta + 1), 0),\\
w_3 &= (2\cos\theta(2\cos^2\theta - \cos\theta - 1), 2\sin\theta\cos\theta(2\cos\theta - 1), 0),\\
w_4 &= (\cos\theta(1 - 2\cos\theta), \sin\theta(1 - 2\cos\theta), 0),\\
w_5 &= (\cos\theta - 1, \sin\theta, 0),\\
w_6 &= (-1, 0, 0),\\
w_7 &= (0, 0, 0),
\end{aligned}$$

where $\frac{5}{7}\pi \le \theta < \frac{3}{4}\pi$. Since $w_1, \dots, w_7$ are in xy-plane, we put $w_1 = (a, b, 0)$. From the restriction of the bond length, we have $\|w_2 - w_1\| = 1$. Moreover, from the restriction of the bond angle, we have $\|w_7 - w_1\| = \sqrt{2 - 2\cos\theta}$. Then, we have two solutions $(\alpha_1, \beta_1, 0)$ or $(\alpha_2, \beta_2, 0)$ of a pair of equations in α and β: $\alpha^2 + \beta^2 = 2 - 2\cos\theta$, $(\alpha - a)^2 + (\beta - b)^2 = 1$, since the discriminant of the quadratic equation with respect to α or β obtained from the pair of equations is no less than 0 respectively. We put $w_0 = (-\cos\theta, x\sin\theta, y\sin\theta)$ $(x^2 + y^2 = 1)$. From $\|w_1 - w_0\| = (\alpha + \cos\theta)^2 + (\beta - x\sin\theta)^2 + (y\sin\theta)^2 = 1$ we have $x = \frac{(\alpha+\cos\theta)^2 + \beta^2 - \cos^2\theta}{2\beta\cos\theta}$. Note that there is only one solution of (α, β) that satisfies $|x| \le 1$. The other solution gives $|x| > 1$. Then, we can represent the coordinate of $w_0 = (x_1, x_2, x_3)$ by the following:

$$\begin{aligned}
x_1 &= -\cos\theta,\\
x_2 &= (\alpha^2 + \beta^2 + 2\alpha\cos\theta)/2\beta,\\
x_3 &= \pm\sqrt{1 - \cos^2\theta - x^2\sin^2\theta}.
\end{aligned}$$

Thus the coordinate of w_1 is uniquely decided, since either of solutions $(a_1, b_1, 0)$ or $(a_2, b_2, 0)$ satisfies $\cos^2\theta + x^2\sin^2\theta > 1$.

Hence the vertices $v_1, v_2, \dots, v_{n-1}$ are uniquely determined and just two positions of the vertex v_0 are determined for original closed chains with vertices $\{v_0, v_1, \dots, v_{n-1}\}$. Then we have just two configurations of closed chains corresponding to the critical points. These two are mirror symmetric with respect to the plane $\mathrm{Span}\langle \beta_2, \beta_3 \rangle$. Hence we obtain that $h|C_n$ has only two critical points. In fact, we can see Figs 11, 12, 13 and 14 for the critical configurations. We choose viewpoints in order to see easily configurations. □

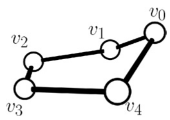

Fig. 11. $n = 5$ $(\theta = \frac{7}{12}\pi)$

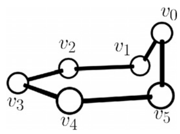

Fig. 12. $n = 6$ $(\theta = \cos^{-1}(-\frac{1}{3}))$

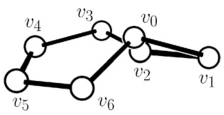

Fig. 13. $n = 7$ $(\theta = \cos^{-1}(-\frac{1}{3}))$

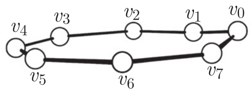

Fig. 14. $n = 8$ $(\theta = \cos^{-1}(-\frac{7}{10}))$

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