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THE CONFIGURATION SPACE OF A MODEL FOR 5-MEMBERED STRAIGHT-CHAIN HYDROCARBON MOLECULES PARAMETRIZED BY CHAIN LENGTHS

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Abstract. We provide a mathematical model of n-membered straight-chain hydrocarbon molecules. The configuration space of the model is parametrized by chain lengths. By assuming the bond angle conditions required for hydrocarbon molecules, we determine the topological types of fibers of the configuration space of the model by chain lengths when $n = 5$.

1. Introduction

A *straight chain* with n vertices is defined to be a graph in $\mathbf{R}^3$ with vertices $\{v_0, v_1, \ldots, v_{n-1}\}$ and bonds $\{\beta_1, \beta_2, \ldots, \beta_{n-1}\}$, where β_i connects v_{i-1} with v_i ($i = 1, 2, \ldots, n-1$). A *bond angle* is defined to be the angle between two adjacent bonds. The *chain length* of a straight chain with n vertices $\{v_0, v_1, \ldots, v_{n-1}\}$ is defined to be the distance between v_0 and v_{n-1}. For simplicity, $\boldsymbol{\beta}_i$ denotes the *bond vector* $v_i - v_{i-1}$, where $i = 1, 2, \ldots, n-1$.

We consider straight chains in $\mathbf{R}^3$ with rigidity as a mathematical model of straight-chain hydrocarbon molecules. Organic synthesis chemists are interested in lengths of flexible hydrocarbon chains with a straight-chain part because they have important significance in terms of chemical properties. For instance, it was reported that the observed lengths of the flexible hydrocarbon chains of receptor blockers are related directly to their inhibitory effect on the activity of an asthma chemical mediator ([1]). To detect the change in chain length, we consider the set, which is called the configuration space, of all such straight chains, and study the topology of fibers of the configuration space by chain lengths.

Definition 1. *We fix θ with $0 \le \theta < \pi$, and put three vertices $v_1 = (-1, 0, 0)$, $v_2 = (0, 0, 0)$, $v_3 = (-\cos\theta, \sin\theta, 0)$. We define functions $f_k : (\mathbf{R}^3)^{n-3} \to \mathbf{R}$ by $f_k(v_0, \check{v}_1, \check{v}_2, \check{v}_3, v_4, \ldots, v_{n-1}) = \frac{1}{2}(\|\boldsymbol{\beta}_k\|^2 - 1)$ for $k = 1, 4, \cdots, n-1$, and $g_k : (\mathbf{R}^3)^{n-3} \to \mathbf{R}$ by $g_k(v_0, \check{v}_1, \check{v}_2, \check{v}_3, v_4, \ldots, v_{n-1}) = \langle -\boldsymbol{\beta}_k, \boldsymbol{\beta}_{k+1}\rangle - \cos\theta$ for $k = 1,$*

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$3, \cdots, n-2$, *where* $\langle\ ,\ \rangle$ *denotes the standard inner product in* $\mathbf{R}^3$ *and* $\|\cdot\|$ *the standard norm* $\|\boldsymbol{x}\| = \sqrt{\langle \boldsymbol{x}, \boldsymbol{x}\rangle}$, *and* $\check{v_i}$ $(i = 1, 2, 3)$ *means that* v_i *removes from* $(v_0, v_1, \cdots, v_{n-1})$, *e.g.* $(v_0, \check{v_1}, \check{v_2}, \check{v_3}, v_4) = (v_0, v_4)$, $(v_0, \check{v_1}, \check{v_2}, \check{v_3}, v_4, v_5) = (v_0, v_4, v_5)$ *and* $(v_0, \check{v_1}, \check{v_2}, \check{v_3}, v_4, v_5, v_6) = (v_0, v_4, v_5, v_6)$. *Then we define the configuration space* $M(n)$ *of straight chains with rigidity by the following:*

$$M(n) = \left\{ p = (v_0, \check{v_1}, \check{v_2}, \check{v_3}, v_4, \ldots, v_{n-1}) \in (\mathbf{R}^3)^{n-3} \;\middle|\; \begin{array}{l} f_i(p) = g_j(p) = 0 \\ i = 1, 4, \cdots, n-1 \\ j = 1, 3, \ldots, n-2 \end{array} \right\}.$$

f_i and g_j are called *rigidity maps*, which determine the bond lengths and angles of any chain in $M(n)$. Note that a straight chain in $M(n)$ is an equilateral and equiangular straight chain with n vertices and bond lengths 1. The dihedral angle for three bond vectors $\boldsymbol{\beta}_k, \boldsymbol{\beta}_{k+1}$ and $\boldsymbol{\beta}_{k+2}$ is the angle between two planes that consist of the plane spanned by the two vectors $\boldsymbol{\beta}_k$ and $\boldsymbol{\beta}_{k+1}$ and the plane spanned by the two vectors $\boldsymbol{\beta}_{k+1}$ and $\boldsymbol{\beta}_{k+2}$. Because the straight chains in $M(n)$ are parametrized by dihedral angles with the angular range of 2π, we see that $M(n)$ is $(n-3)$-dimensional torus T^{n-3}. We consider the fibers of $M(n)$ by chain lengths. For convenience, we put the bond vector $v_0 - v_{n-1} = \boldsymbol{\beta}_0$.

Definition 2. *We put a positive real number* ℓ, *and set* $f_0^\ell : (\mathbf{R}^3)^{n-3} \to \mathbf{R}$ *by* $f_0^\ell(v_0, v_4, \cdots, v_{n-1}) = \frac{1}{2}(\|\boldsymbol{\beta}_0\|^2 - \ell)$. *We define the fiber* $M_\ell(n)$ *of* $M(n)$ *by the following:*

$$M_\ell(n) = \{p \in M(n) \mid f_0^\ell(p) = 0\}.$$

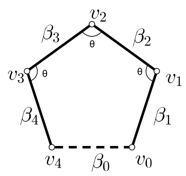
Note that $M_\ell(n)$ is the set which consists of straight chains in $M(n)$ whose chain length is ℓ. So we see that $M(n) = \bigcup_\ell M_\ell(n)$. In particular, when $\ell = 1$, we can regard $M_\ell(n)$ as the configuration space of the model of n-membered ringed hydrocarbon molecules in [2], [3] and [4]. In this paper, we assume that the bond angle θ is equal to the tetrahedral angle $\cos^{-1}(-\frac{1}{3})$ which is the standard bond angle of the saturated carbon atom, and study the topology of the fiber $M_\ell(n)$ of $M(n) = T^{n-3}$ for any chain length ℓ. When $n = 3, 4$, the fiber $M_\ell(n)$ is simple. In fact, we can easily verify that the topological types of $M_\ell(3)$ of $M(3)$ are one point set if $\ell = \sqrt{\frac{8}{3}}$ and the empty set if $\ell \neq \sqrt{\frac{8}{3}}$. And, the topological types of $M_\ell(4)$ of $M(4) = T^1 = S^1$ are two point set if $\frac{5}{3} < \ell < \frac{\sqrt{57}}{3}$, one point set if $\ell = \frac{5}{3}$ or $\frac{\sqrt{57}}{3}$ and the empty set if $\ell < \frac{5}{3}$ or $\frac{\sqrt{57}}{3} < \ell$.

When $n = 5$, we obtain the following theorem:

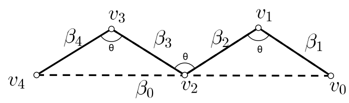
Theorem 3. *Let* ℓ *be a positive real number. The topological type of the fiber* $M_\ell(5)$ *of* $M(5) = T^2$ *is given by the following:*

(1) *If* $\ell = \frac{4}{3}\sqrt{\frac{2}{3}}$ *or* $4\sqrt{\frac{2}{3}}$, $M_\ell(5)$ *is one point set,*
(2) *If* $\frac{4}{3}\sqrt{\frac{2}{3}} < \ell < \frac{8}{3}$ *or* $\frac{8}{3} < \ell < 4\sqrt{\frac{2}{3}}$, $M_\ell(5)$ *is homeomorphic to a circle* S^1,
(3) *If* $\ell = \frac{8}{3}$, $M_\ell(5)$ *is homeomorphic to a union of two circles that intersect at two points,*
(4) *If* $\ell < \frac{4}{3}\sqrt{\frac{2}{3}}$ *or* $4\sqrt{\frac{2}{3}} < \ell$, $M_\ell(5)$ *is the empty set.*

Remark. Hydrocarbon molecules have three basic structures: ringed chains, straight chains, and branched chains. In [6], Jun O'Hara studied the configuration space of equilateral and equiangular spatial hexagons for any bond angle, as a mathematical model of 6-membered ringed hydrocarbon molecules.



(a)



(b)

FIG. 1. The configuration corresponding to one point.

When $\ell = \frac{4}{3}\sqrt{\frac{2}{3}}$ (resp. $4\sqrt{\frac{2}{3}}$) we have the configuration as in Fig. 1 (a) (resp. (b)) as the straight chain corresponding to one point. So we can easily verify Theorem 3 (1) and (4). In Section 2 we will give a proof of Theorem 3 (2) by the similar argument to [3]. In Section 3 we prove Theorem 3 (3) by giving explicit expressions of all the possible shapes (cf. [6]).

2. Proof of Theorem 3 (2)

In this section we assume $\frac{4}{3}\sqrt{\frac{2}{3}} < \ell < \frac{8}{3}$, $\frac{8}{3} < \ell < 4\sqrt{\frac{2}{3}}$. We first prove the following proposition.

Proposition 4. $M_\ell(5)$ *is an orientable closed* 1*-dimensional submanifold of* $\mathbf{R}^5$.

We show the following lemma for the proof of Proposition 4:

Lemma 5.

(1) *All vertices cannot be in one plane for each straight chain in* $M_\ell(5)$.
(2) $M_\ell(5)$ *is not the empty set.*

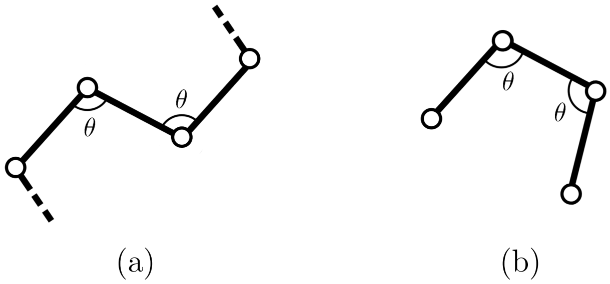


FIG. 2. Local planar configurations of the successive three bonds.

Proof of Lemma 5. (1) We assume that for a straight chain in $M_\ell(5)$ all vertices are in one plane. Since the straight chain has local configurations as in Fig. 2 (a) or (b), the straight chain is one of the four types as in Fig. 3.

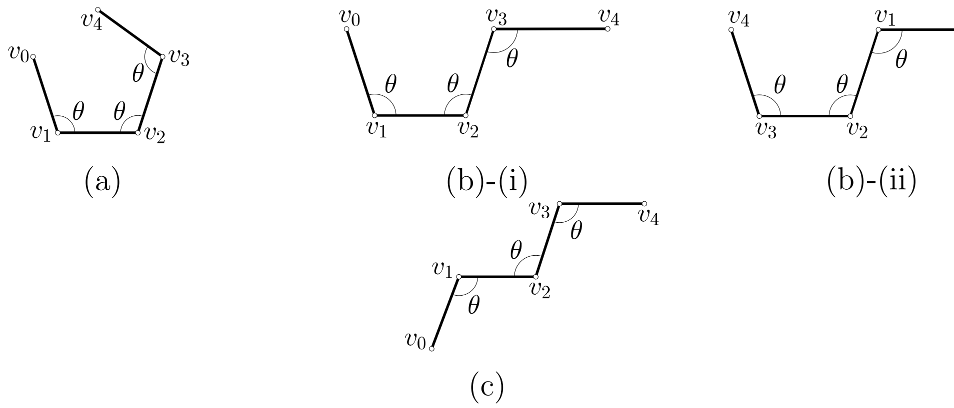


FIG. 3. Four types of local planar configurations.

By calculating, chain lengths of four straight chains as in Fig. 3 are $\frac{4}{3}\sqrt{\frac{2}{3}}$ in the case of Fig. 3 (a), $\frac{8}{3}$ in the case of Fig. 3 (b)-(i), $\frac{8}{3}$ in the case of Fig. 3 (b)-(ii) and $4\sqrt{\frac{2}{3}}$ in the case of Fig. 3 (c). This means that any straight chain of $M_\ell(5)$ cannot be in one plane.

(2) We consider all straight chains in $M(5)$. We define a function $d : M(5) \to \mathbf{R}$ by $d(v_0, v_4) = \|v_0 - v_4\|$. We note that d is continuous with respect to v_0 and v_4. From the proof of (1), if we have a configuration as in Fig. 3 (a) (resp. (c)), the value of $d(v_0, v_4)$ is equal to $\frac{4}{3}\sqrt{\frac{2}{3}}$ (resp. $4\sqrt{\frac{2}{3}}$). From the connectedness of $M(5)$, the configuration space $M_\ell(5)$ is not the empty set. $\square$

Under the above preparation, we prove Proposition 4. From now on, f_0^ℓ is simply denoted by f_0 when ℓ is fixed.

Proof of Proposition 4. We define $F : (\mathbf{R}^3)^2 \to \mathbf{R}^5$ as $F = (f_1, f_0, f_4, g_1, g_3)$. Then we see $M_\ell(5) = F^{-1}(\{\boldsymbol{O}\})$ for $\boldsymbol{O} = (0, \ldots, 0) \in \mathbf{R}^5$. By the regular value theorem, we show that $\boldsymbol{O} \in \mathbf{R}^5$ is a regular value of F. Due to [5], it is sufficient to prove that the gradient vectors (grad $f_1)_p$, (grad f_0), (grad $f_4)_p$, (grad $g_1)_p$ and (grad $g_3)_p$ are linearly independent for any $p \in F^{-1}(\{\boldsymbol{O}\}) = M_\ell(5)$, where (grad $f)_p = \left(\frac{\partial f}{\partial x_j}(p)\right)_j$. Using the zero vector $\mathbf{0} = (0, 0, 0)$ and the bond vectors $\boldsymbol{\beta}_k$ $(k = 0, \ldots, 4)$ of the straight chain corresponding to $p \in M_\ell(5)$, we decompose the gradient vectors of f_k and g_k into 1×3 blocks as follows:

$$
\begin{aligned}
(\text{grad } f_1)_p &= (\ -\boldsymbol{\beta}_1, \quad \mathbf{0}\ ), \\
(\text{grad } f_0)_p &= (\quad \boldsymbol{\beta}_0, -\boldsymbol{\beta}_0), \\
(\text{grad } f_4)_p &= (\quad \mathbf{0}, \quad\ \boldsymbol{\beta}_4), \\
(\text{grad } g_1)_p &= (\quad \boldsymbol{\beta}_2, \quad \mathbf{0}\ ), \\
(\text{grad } g_3)_p &= (\quad \mathbf{0}, \ -\boldsymbol{\beta}_3).
\end{aligned}
$$

We assume that the gradient vectors (grad $f_1)_p$, (grad $f_0)_p$, (grad $f_4)_p$, (grad $g_1)_p$ and (grad $g_3)_p$ are linearly dependent. This means $c_k \neq 0$ and $c_1(\text{grad } f_1)_p + c_2(\text{grad } f_0)_p + c_3(\text{grad } f_4)_p + c_4(\text{grad } g_1)_p + c_5(\text{grad } g_3)_p = (\mathbf{0}, \mathbf{0})$ for some k. We then have the bond vector relations:

$$
\begin{aligned}
-c_1\boldsymbol{\beta}_1 + c_2\boldsymbol{\beta}_0 + c_4\boldsymbol{\beta}_2 &= 0, \\
-c_2\boldsymbol{\beta}_0 + c_3\boldsymbol{\beta}_4 - c_5\boldsymbol{\beta}_3 &= 0.
\end{aligned}
$$

Let v_0, v_1, v_2, v_3 and v_4 denote the vertices of the straight chain corresponding to $p \in M_\ell(5)$. Because two successive bond vectors $\boldsymbol{\beta}_k$ and $\boldsymbol{\beta}_{k+1}$ are linearly independent for $k \neq 0, 4$, we get $c_2 \neq 0$. So the bond vector relation $-c_1\boldsymbol{\beta}_1 + c_2\boldsymbol{\beta}_0 + c_4\boldsymbol{\beta}_2 = 0$ implies that the vertices v_0, v_1, v_2 and v_4 are in one plane, and the bond vector relation $-c_2\boldsymbol{\beta}_0 + c_3\boldsymbol{\beta}_4 - c_5\boldsymbol{\beta}_3 = 0$ implies that the vertices v_0, v_2, v_3 and v_4 are in one plane. This means that all vertices of the straight chain are in one plane. However this contradicts Lemma 5 (1).

Thus, since $\boldsymbol{O} \in \mathbf{R}^5$ is a regular value of F, $M_\ell(5)$ is an orientable closed 1-dimensional submanifold of $\mathbf{R}^5$. $\square$

We define a differential function $h : (\mathbf{R}^3)^2 - \{\boldsymbol{O}\} \to \mathbf{R}$ derived from the dihedral angle for $\boldsymbol{\beta}_1, \boldsymbol{\beta}_2, \boldsymbol{\beta}_3$ by $h(v_0, v_4) = \frac{y_0}{\sqrt{y_0^2 + z_0^2}}$, where $v_0 = (x_0, y_0, z_0)$ and $\boldsymbol{O} \in (\mathbf{R}^3)^2$.

Proposition 6. *$h|M_\ell(5)$ has two critical points.*

Proof. Due to [5] $p \in M_\ell(5)$ is a critical point of $h|M_\ell(5)$ for $h : (\mathbf{R}^3)^2 \to \mathbf{R}$ if and only if there exist $a_i \in \mathbf{R}$ $(i = 1, 2, 3, 4, 5)$ such that (grad $h)_p = a_1(\text{grad } f_1)_p + a_2(\text{grad } f_0)_p + a_3(\text{grad } f_4)_p + a_4(\text{grad } g_1)_p + a_5(\text{grad } g_3)_p$. We can easily check that

$(\text{grad } h)_p = \left(0, \frac{27z_0^2}{16\sqrt{2}}, -\frac{27y_0z_0}{16\sqrt{2}}, 0, 0, 0\right)$. Note that the first 1×3 block $\left(0, \frac{27z_0^2}{16\sqrt{2}}, -\frac{27y_0z_0}{16\sqrt{2}}\right)$ is orthogonal to $\boldsymbol{\beta}_1$ and $\boldsymbol{\beta}_2$. So, we see that $a_2 \neq 0$ if $(\text{grad } h)_p = a_1(\text{grad } f_1)_p + a_2(\text{grad } f_0)_p + a_3(\text{grad } f_4)_p + a_4(\text{grad } g_1)_p + a_5(\text{grad } g_3)_p$. By the same argument as the proof of Proposition 4, the vertices v_0, v_2, v_3 and v_4 of the straight chain corresponding to a critical point p are in one plane Span $\langle \beta_3, \beta_4\rangle =$ Span $\langle \beta_3, \beta_4, \beta_0\rangle$. We transform the straight chain by the congruent transformation that maps v_2, v_3 and v_4 to $(0,0,0)$, $(1,0,0)$ and $(\frac{4}{3}, \frac{2\sqrt{2}}{3}, 0)$ in this order, and denote the image of v_k as w_k. Since w_0, w_2, w_3 and w_4 are in xy-plane, we put $w_0 = (\alpha, \beta, 0)$. From the restriction of the bond length and bond angle, we have $\|w_0 - w_4\| = \sqrt{(\alpha - \frac{4}{3})^2 + (\beta - \frac{2\sqrt{2}}{3})^2} = \ell$, $\|w_2 - w_0\| = \sqrt{\alpha^2 + \beta^2} = \sqrt{\frac{8}{3}}$. Remark that the two solution pairs $(\alpha_\pm, \beta_\pm)$ of the two equations $(\alpha - \frac{4}{3})^2 + (\beta - \frac{2\sqrt{2}}{3})^2 = \ell^2$, $\alpha^2 + \beta^2 = \frac{8}{3}$ are given by $(\alpha_\pm, \beta_\pm) = (\frac{1}{24}(32 - 6\ell^2 \pm \sqrt{6}\sqrt{\ell^2(32 - 3\ell^2)}), \frac{1}{24}(16\sqrt{2} - 3\sqrt{2}\ell^2 \mp 2\sqrt{3\ell^2(32 - 3\ell^2)}))$ (double sign in same order). Note that $\alpha_\pm$ and $\beta_\pm$ are real numbers when $\frac{4}{3}\sqrt{\frac{2}{3}} < \ell < \frac{8}{3}$ or $\frac{8}{3} < \ell < 4\sqrt{\frac{2}{3}}$, and that $\alpha_\pm$ and $\beta_\pm$ are determined by ℓ. We denote the coordinate $(\alpha, \beta, 0)$ of w_0 as $(\alpha_\pm, \beta_\pm, 0)$, and put $w_1 = (-\frac{1}{3}, x\frac{2\sqrt{2}}{3}, y\frac{2\sqrt{2}}{3})$ $(x^2 + y^2 = 1)$. From $\|w_0 - w_1\|^2 = (\alpha_\pm + \frac{1}{3})^2 + (\beta_\pm - x\frac{2\sqrt{2}}{3})^2 + (y\frac{2\sqrt{2}}{3})^2 = 1$ and $x^2 + y^2 = 1$ we see that $x = \frac{4+\alpha_\pm}{2\sqrt{2}\beta_\pm}$.

Claim 7. *We see that* $(\frac{4+\alpha_-}{2\sqrt{2}\beta_-})^2 < 1$ *and* $(\frac{4+\alpha_+}{2\sqrt{2}\beta_+})^2 > 1$ *if* ℓ *satisfies* $\frac{4}{3}\sqrt{\frac{2}{3}} < \ell < \frac{8}{3}$, *and that* $(\frac{4+\alpha_+}{2\sqrt{2}\beta_+})^2 < 1$ *and* $(\frac{4+\alpha_-}{2\sqrt{2}\beta_-})^2 > 1$ *if* ℓ *satisfies* $\frac{8}{3} < \ell < 4\sqrt{\frac{2}{3}}$.

Proof of Claim 7. We see that $(\frac{4+\alpha_\pm}{2\sqrt{2}\beta_\pm})^2 > 1$ (resp. < 1) if and only if $(2\sqrt{2}\beta_\pm)^2 - (4+\alpha_\pm)^2 > 0$ (resp. < 0). Since $(2\sqrt{2}\beta_\pm)^2 - (4+\alpha_\pm)^2 = \pm\frac{\sqrt{32-3\ell^2}}{96}(-64+9\ell^2)(2\sqrt{6}\ell \pm \sqrt{32 - 3\ell^2})$ (double sign corresponds), we have only to check the factors of the right side are positive or negative.

First, we assume that $\frac{4}{3}\sqrt{\frac{2}{3}} < \ell < \frac{8}{3}$. When $\frac{4}{3}\sqrt{\frac{2}{3}} < \ell < \frac{8}{3}$, we have that $(-64 + 9\ell^2) < 0$ and $2\sqrt{6}\ell + \sqrt{32 - 3\ell^2} > 0$. Then, we get that $(2\sqrt{2}\beta_+)^2 - (4 + \alpha_+)^2 = \frac{\sqrt{32-3\ell^2}}{96}(-64 + 9\ell^2)(2\sqrt{6}\ell + \sqrt{32 - 3\ell^2}) < 0$. Meanwhile, we can see that $2\sqrt{6}\ell - \sqrt{32 - 3\ell^2} = \frac{27\ell^2-32}{2\sqrt{6}\ell+\sqrt{32-3\ell^2}} > 0$. Then, we get $(2\sqrt{2}\beta_-)^2 - (4 + \alpha_-)^2 = -\frac{\sqrt{32-3\ell^2}}{96}(-64 + 9\ell^2)(2\sqrt{6}\ell - \sqrt{32 - 3\ell^2}) > 0$. Hence, we get $(\frac{4+\alpha_-}{2\sqrt{2}\beta_-})^2 < 1$ and $(\frac{4+\alpha_+}{2\sqrt{2}\beta_+})^2 > 1$ if $\frac{4}{3}\sqrt{\frac{2}{3}} < \ell < \frac{8}{3}$.

Secondly, we assume that ℓ satisfies $\frac{8}{3} < \ell < 4\sqrt{\frac{2}{3}}$. When ℓ satisfies $\frac{8}{3} < \ell < 4\sqrt{\frac{2}{3}}$, we have that $(-64 + 9\ell^2) > 0$ and $2\sqrt{6}\ell + \sqrt{32 - 3\ell^2} > 0$. Then, we get that $(2\sqrt{2}\beta_+)^2 - (4 + \alpha_+)^2 = \frac{\sqrt{32-3\ell^2}}{96}(-64 + 9\ell^2)(2\sqrt{6}\ell + \sqrt{32 - 3\ell^2}) > 0$. Meanwhile, we can see that $2\sqrt{6}\ell - \sqrt{32 - 3\ell^2} = \frac{27\ell^2-32}{2\sqrt{6}\ell+\sqrt{32-3\ell^2}} > 0$. Then, we get that $(2\sqrt{2}\beta_-)^2 -$

$(4+\alpha_-)^2 = -\frac{\sqrt{32-3\ell^2}}{96}(-64+9\ell^2)(2\sqrt{6}\ell - \sqrt{32-3\ell^2}) < 0$. Hence, we get that $(\frac{4+\alpha_+}{2\sqrt{2}\beta_+})^2 < 1$ and $(\frac{4+\alpha_-}{2\sqrt{2}\beta_-})^2 > 1$ if $\frac{8}{3} < \ell < 4\sqrt{\frac{2}{3}}$.

The proof of Claim 7 is completed. □

From Claim 7, when $\frac{4}{3}\sqrt{\frac{2}{3}} < \ell < \frac{8}{3}$ or $\frac{8}{3} < \ell < 4\sqrt{\frac{2}{3}}$, either $(\alpha_+, \beta_+, 0)$ or $(\alpha_-, \beta_-, 0)$ satisfies $1 - x^2 > 0$. So, we can represent the coordinate of $w_1 = (x_1, y_1, z_1)$ by the following:

$$\begin{aligned} x_1 &= -1/3, \\ y_1 &= (4+\alpha)/3\beta, \\ z_1 &= \pm 2\sqrt{2(1-x^2)}/3, \end{aligned}$$

where $(\alpha, \beta) = (\alpha_-, \beta_-)$ or (α_+, β_+). The vertices v_2, v_3, v_4 and v_0 are determined uniquely and just two positions of the vertex v_1 are determined for the original straight chains with vertices $\{v_4, v_3, v_2, v_1, v_0\}$. We then have only two configurations of straight chains corresponding to the critical points. They are mirror symmetric with respect to the plane Span $\langle \beta_3, \beta_4 \rangle$. Thus $h|M_\ell(5)$ has only two critical points. For instance, the critical configuration is shown in Fig. 4. We choose a viewpoint in order to see easily configuration.

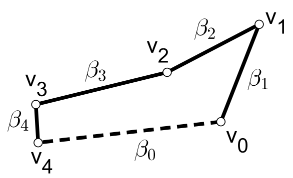


FIG. 4. A critical configuration.

□

By Proposition 6 $M_\ell(5)$ is connected. Thus, $M_\ell(5)$ is homeomorphic to a circle S^1.

Remark 8. $M_\ell(5)$ is also diffeomorphic to a circle.

3. Proof of Theorem 3 (3)

When $\ell = \frac{8}{3}$ there are straight chains corresponding to singular points (see Fig. 5). So, we need to give explicit expressions of all the possible shapes.

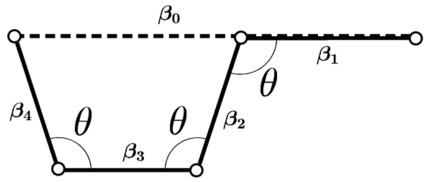


FIG. 5. A singular configuration in one plane.

Let $\tilde{S}$ be a union of two circles that intersect at two points. We consider a straight chain in $M_\ell(5)$. The coordinates of v_0 and v_4 are $v_0 = (-\frac{4}{3}, \frac{2\sqrt{2}}{3}\cos\theta_1, \frac{2\sqrt{2}}{3}\sin\theta_1)$ and $v_4 = (\frac{4(1-2\cos\theta_2)}{9}, \frac{2\sqrt{2}(4+\cos\theta_2)}{9}, \frac{2\sqrt{2}}{3}\sin\theta_2)$, where $0 \le \theta_1, \theta_2 \le 2\pi$. We note that v_0 and v_4 depend on θ_1 and θ_2 respectively. Since v_1, v_2 and v_3 are fixed, any straight chain in $M_\ell(5)$ is determined by the positions of v_0 and v_4 in the straight chain. So we denote by $[v_0, v_4]$ a straight chain in $M_\ell(5)$. From $\|\boldsymbol{\beta}_0\|^2 = \|v_0 - v_4\|^2 = (-\frac{4}{3} - \frac{4(1-2\cos\theta_2)}{9})^2 + (\frac{2\sqrt{2}}{3}\cos\theta_1 - \frac{2\sqrt{2}(4+\cos\theta_2)}{9})^2 + (\frac{2\sqrt{2}}{3}(\sin\theta_1 - \sin\theta_2))^2 = (\frac{8}{3})^2$, we have $(4+\cos\theta_2)\cos\theta_1 + (3\sin\theta_2)\sin\theta_1 = -(1+4\cos\theta_2)$. Since we see $\cos^2\theta_1 + \sin^2\theta_1 = 1$ and $1-\cos^2\theta_2 \ge 0$, we get $\cos\theta_1 = \frac{-(1+4\cos\theta_2)(4+\cos\theta_2)\mp 6\sqrt{6}\sin\theta_2\sqrt{1-\cos^2\theta_2}}{(4+\cos\theta_2)^2+(3\sin\theta_2)^2}$ and $\sin\theta_1 = \frac{-3\sin\theta_2(1+4\cos\theta_2)\pm 2\sqrt{6}(4+\cos\theta_2)\sqrt{1-\cos^2\theta_2}}{(4+\cos\theta_2)^2+(3\sin\theta_2)^2}$ (double sign corresponds). Thus the coordinate of $v_0 = (x_0, y_0, z_0)$ is given by the following:

$$
\begin{aligned}
x_0 &= -4/3, \\
y_0 &= \frac{-2\sqrt{2}(1+4\cos\theta_2)(4+\cos\theta_2) \mp 24\sqrt{3}\sin\theta_2\sqrt{1-\cos^2\theta_2}}{3((4+\cos\theta_2)^2 + (3\sin\theta_2)^2)}, \\
z_0 &= \frac{-6\sqrt{2}\sin\theta_2(1+\cos\theta_2) \pm 8\sqrt{3}(4+\cos\theta_2)\sqrt{1-\cos^2\theta_2}}{3((4+\cos\theta_2)^2 + (3\sin\theta_2)^2)}.
\end{aligned}
$$

When $\theta_2 \ne 0, \pi, 2\pi$ we have $1-\cos^2\theta_2 = (1-\cos\theta_2)(1+\cos\theta_2) > 0$. So we obtain two straight chains in $M_\ell(5)$ for θ_2 ($\ne 0, \pi, 2\pi$). Therefore, $\{[v_0, v_4] \mid 0 < \theta_2 < \pi\}$ and $\{[v_0, v_4] \mid \pi < \theta_2 < 2\pi\}$ correspond to two disjoint arcs. Since $\{[v_0, v_4] \mid \theta_2 = \pi\}$ and $\{[v_0, v_4] \mid \theta_2 = 0, 2\pi\}$ are one point, we have $\{[v_0, v_4] \mid \theta_2 = 0\} \cup \{[v_0, v_4] \mid 0 < \theta_2 < \pi\} \cup \{[v_0, v_4] \mid \theta_2 = \pi\} \cup \{[v_4, v_0] \mid \pi < \theta_2 < 2\pi\} \cup \{[v_0, v_4] \mid \theta_2 = 2\pi\} \cong \tilde{S}$. Thus the configuration space $M_\ell(5)$ is homeomorphic to a union of two circles that intersect at two points.

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