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On the existence of a rotational closed chain

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Abstract

The set of closed chains is called the configuration space of the closed chains. Let $M_n^n(\theta)$ be the configuration space of equilateral and equiangular closed chains with the bond angle θ and n-vertices, and $M_n^{n-2}(\theta)$ the configuration space of equilateral closed chains with n-vertices whose $n-2$ bond angles are the same θ except for successive two angles. In this paper, we study the condition of n for which $M_n^n\left(\frac{\pi}{2}\right)$ or $M_n^{n-2}\left(\cos^{-1}\left(-\frac{1}{3}\right)\right)$ has a rotational closed chain. This results give a geometrical approach for the study of the topology of $M_n^n\left(\frac{\pi}{2}\right)$ or $M_n^{n-2}\left(\cos^{-1}\left(-\frac{1}{3}\right)\right)$.

1 Introduction and Main Theorem

A *closed chain* is defined to be a spatial graph in $\mathbf{R}^3$ consisting of vertices $v_0, v_1, \ldots, v_{n-1}$ and bonds $\beta_0, \beta_1, \beta_2, \ldots, \beta_{n-1}$, where β_i connects v_i with v_{i-1}, and β_0 is the edge connecting v_0 with v_{n-1}. Let $\boldsymbol{\beta}_i$ denotes the *bond vector* $v_i - v_{i-1}$, where $i = 1, 2, \ldots, n$ and $v_n = v_0$. For a closed chain, we prepare the following definitions: the *bond length* for the bond β_i is defined to be the distance between v_i and v_{i-1}, a *bond angle* is defined to be the angle between two adjacent bonds, the *dihedral angle* for three bond vectors $\boldsymbol{\beta}_i, \boldsymbol{\beta}_{i+1}$ and $\boldsymbol{\beta}_{i+2}$ is defined to be the angle between two planes; one is spanned by the two bond vectors $\boldsymbol{\beta}_i$ and $\boldsymbol{\beta}_{i+1}$ and the other is spanned by the two bond vectors $\boldsymbol{\beta}_{i+1}$ and $\boldsymbol{\beta}_{i+2}$. In particular, dihedral angles have important roles to determine closed chains. A closed chain is called a *rotational closed chain* if it has a rotatable bond, that is the dihedral angles of the bond can take any value. In this paper, we impose the following condition for a closed chain :

Assumption 1. *We fix θ with $0 \leq \theta < \pi$. Assume that all bond lengths of a closed chain with n-vertices are 1. The closed chain satisfies either of the following conditions (1)-(3):*

(1) $\langle -\boldsymbol{\beta}_j, \boldsymbol{\beta}_{j+1} \rangle = \cos\theta \quad (j = 0, 1, 2, \ldots, n-1)$

(2) $\langle -\boldsymbol{\beta}_j, \boldsymbol{\beta}_{j+1} \rangle = \cos\theta \quad (j = 1, 2, \ldots, n-1)$

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(3) $\langle -\boldsymbol{\beta}_j, \boldsymbol{\beta}_{j+1}\rangle = \cos\theta \quad (j = 1, 2, \ldots, n-2)$

Here, $\boldsymbol{\beta}_0, \boldsymbol{\beta}_1, \ldots, \boldsymbol{\beta}_{n-1}$ *denote bond vectors of the closed chain, and* $\boldsymbol{\beta}_n = \boldsymbol{\beta}_0$*.*

Throughout this paper, we fix three vertices v_1, v_2 and v_3 to $v_1 = (0,0,0)$, $v_2 = (1,0,0)$ and $v_3 = (1-\cos\theta, \sin\theta, 0)$ respectively. The set of closed chains is called the *configuration space* of the closed chains.

Notation. *If the closed chain satisfies the condition (1), the closed chain is equilateral and equiangular with the bond angle* θ*. In generally, the configuration space of such closed chains is denoted by* $M_n^n(\theta)$*.*

If the closed chain satisfies the condition (2), the closed chain is equilateral whose $n-1$ *bond angles are* θ *except for* $\angle v_1 v_0 v_{n-1}$*. The configuration space of such closed chains is denoted by* $M_n^{n-1}(\theta)$*.*

If the closed chain satisfies the condition (3), the closed chain is equilateral whose $n-2$ *bond angles are* θ *except for* $\angle v_1 v_0 v_{n-1}$ *and* $\angle v_0 v_{n-1} v_{n-2}$*. The configuration space of such closed chains is denoted by* $M_n^{n-2}(\theta)$*.*

Many researchers have studied the structure of the configuration space consisting of such closed chains. In [**?**], they considered closed chains in $M_n^{n-2}(\theta)$ as a mathematical model of cycroalkenes, and showed that the configuration space $M_n^{n-2}(\theta)$ is homeomorphic to S^{n-4}, when θ is the standard bond angle, and $n = 5, 6, 7$. Here, if $n = 5$ the standard bond angle is given by $\frac{7}{12}\pi$, and if $n \geq 6$ the standard bond angle is given by $\cos^{-1}\left(-\frac{1}{3}\right)$. More generally, if the bond angle θ is sufficiently close to $\frac{n-2}{n}\pi$, the configuration space $M_n^{n-2}(\theta)$ is homeomorphic to S^{n-4}, for $n \geq 5$ ([**?**, **?**]). Here, the bond angle of the n-regular polygon is $\frac{n-2}{n}\pi$. On the other hand, many researchers are also interested in the study of the topology of $M_n^n(\theta)$. When $n = 6$ and 7, the topological types of $M_n^n(\theta)$ are classified in [**?**] and [**?**] respectively, for generic θ.

The study of rotational closed chains in $M_n^n(\theta)$ (resp. $M_n^{n-2}(\theta)$) is to relate the study of the topology of $M_n^n(\theta)$ (resp. $M_n^{n-2}(\theta)$), since the fundamental group of $M_n^n(\theta)$ (resp. $M_n^{n-2}(\theta)$) is non-trivial if $M_n^n(\theta)$ (resp. $M_n^{n-2}(\theta)$) has a rotational closed chain (see [**?**]). Recently, in [**?**], we studied reversibility of a polyhedral annulus of even isosceles right triangles. This result implies that there is a rotational equilateral and equiangular $2n$-closed chain with the bond angle $\frac{\pi}{2}$, for $n \geq 2$. In this paper, we study the condition of n for which $M_n^n\left(\frac{\pi}{2}\right)$ or $M_n^{n-2}\left(\cos^{-1}\left(-\frac{1}{3}\right)\right)$ has a rotational closed chain. Our Theorem is the following:

Theorem 2. *(1) Assume that the fixed bond angle is* $\cos^{-1}(-\frac{1}{3})$*. When* $n = 5, 6, 7$*,* $M_n^{n-2}(\theta)$ *dose not have rotational closed chains. If* $n \geq 8$*,* $M_n^{n-2}(\theta)$ *has a rotational closed chain.*

(2) Assume that the fixed bond angle is $\frac{\pi}{2}$*. When* $n = 5, 6, 7$*,* $M_n^n(\theta)$ *dose not have rotational closed chains. If* $n \geq 8$ *and* $n \neq 9$*,* $M_n^n(\theta)$ *has a rotational closed chain.*

2 Proof of Theorem 2 (1)

In this section, we give a proof of Theorem 2 (1). Throughout this section, we assume $\theta = \cos^{-1}\left(-\frac{1}{3}\right)$. Note that if a straight chain has a rotatable bond β_i $(1 \leq i \leq n)$, the three bond vectors $\boldsymbol{\beta}_{i-1}, \boldsymbol{\beta}_i$ and $\boldsymbol{\beta}_{i+1}$ of the straight chain form a planar local configuration as in Fig. 1, where $\beta_n = \beta_0$ and $\beta_{n+1} = \beta_1$.

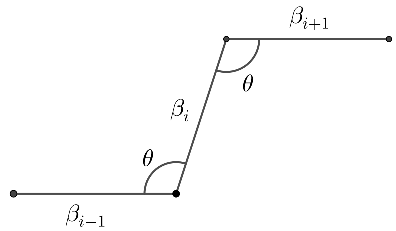

Figure 1: A forbidden local configuration

However, if $n = 5, 6, 7$, from Lemma 1 (2) stated in [?], any closed chain in $M_n^{n-2}(\theta)$ does not have local configurations as in Fig. 1. This implies that, when $n = 5, 6, 7$, $M_n^{n-2}(\theta)$ dose not have rotational closed chains.

In what follows, for $n \geq 8$, we construct a rotational closed chain in $M_n^{n-2}(\theta)$ to show Theorem 2 (1). We refer to Theorem A and B stated in [?].

Lemma 3 ([?])**.** *Let n is a positive integer with $n \geq 4$.*
If n is odd, we have $M_n^{n-1}(\theta) \neq \varnothing$ if and only if $\theta \in \left[\frac{\pi}{n}, \frac{n-2}{n}\pi\right]$.
If n is even, we have $M_n^{n-1}(\theta) \neq \varnothing$ if and only if $\theta \in \left[0, \frac{n-2}{n}\pi\right]$

We fix a positive integer n with $n \geq 8$. From Lemma 3, when $\theta = \cos^{-1}\left(-\frac{1}{3}\right)$, we obtain $M_{n-2}^{n-3}(\theta) \neq \varnothing$. By attaching the parallel stacked two bonds to a closed chain in $M_{n-2}^{n-3}(\theta)$ as in Fig. 2, we get a rotational closed chain in $M_n^{n-2}(\theta)$. More precisely, we need to rename the bonds of the new rotational closed chain so that the rotational closed chain is contained in $M_n^{n-2}(\theta)$. We give an example of the case $n = 8$ as in Fig. 3. The dihedral angles of a rotatable bond β_2 can take any value.

Remark 4. *Fix a positive integer n with $n \geq 5$. It is easy to see that for the case $n = 5$ we have $M_{n-2}^{n-3} \neq \varnothing$ if and only if $\theta = \frac{\pi}{3}$. From Lemma 3, one can verify that if n is odd and $n \geq 7$, we have $M_{n-2}^{n-3}(\theta) \neq \varnothing$ if and only if $\theta \in \left[\frac{\pi}{n-2}, \frac{n-4}{n-2}\pi\right]$ and that if n is even and $n \geq 6$, we have $M_{n-2}^{n-3}(\theta) \neq \varnothing$ if and only if $\theta \in \left[0, \frac{n-4}{n-2}\pi\right]$. For such θ, by using the above method, we can construct a rotational closed chain in $M_n^{n-2}(\theta)$.*

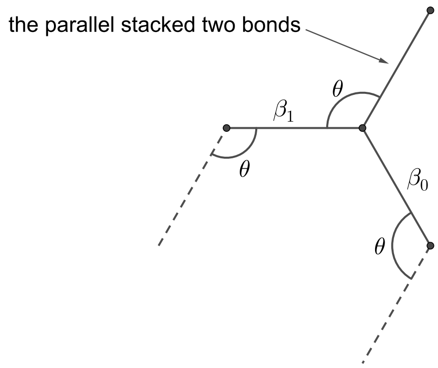

Figure 2: A rotational closed chain in $M_n^{n-2}(\theta)$

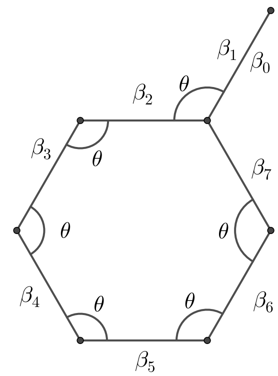

Figure 3: The case of a rotational closed chain in $M_8^6(\theta)$

3 Proof of Theorem 2 (2)

In this section, we prove Theorem 2 (2). Throughout this section, we assume $\theta = \frac{\pi}{2}$. We begin the following Lemma.

Lemma 5. *Assume that $n = 5, 6, 7$. Any closed chain in $M_n^n(\theta)$ does not have the local configurations as in Fig. 4.*

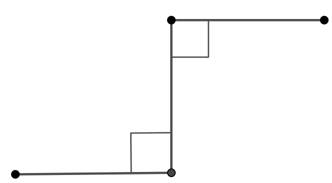

Figure 4: A forbidden local configuration

Proof. Assume that a closed chain in $M_n^n(\theta)$ has a local configuration as in Fig. 4 for $n = 5, 6, 7$. Without loss of generality, we can assume that the three bonds β_2, β_3 and β_4 of the closed chain form the configuration as in Fig. 5 or 6.

Firstly, we consider the case of $n = 5$. Then v_0 and v_4 are $(0, y, z)$ and $(2, 1, 0)$ respectively, where $y^2 + z^2 = 1$ (see Fig. 5).

Then the distance between v_0 and v_4 is given by $\sqrt{2^2 + (1-y)^2 + z^2}$. From $\|\boldsymbol{\beta}_0\| = 1$, we have the equation $\sqrt{2^2 + (1-y)^2 + z^2} = 1$. However, we see

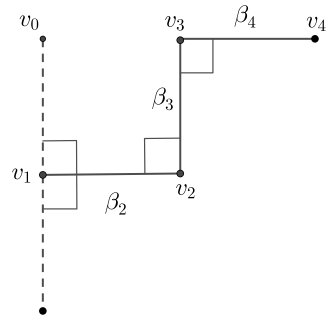

Figure 5: A forbidden local configuration when the case of $n = 5$

$\sqrt{2^2 + (1-y)^2 + z^2} \geq \sqrt{2^2} = 2 > 1$. This contradicts that a closed chain in $M_5^5(\theta)$ has a local configuration as in Fig. 4.

Secondly, we consider the case $n = 6$. Then v_0 and v_5 are given by $(0, y_1, z_1)$ and $(2, 1 + y_2, z_2)$ respectively, where $y_1^2 + z_1^2 = 1$ and $y_2^2 + z_2^2 = 1$ (see Fig. 6).

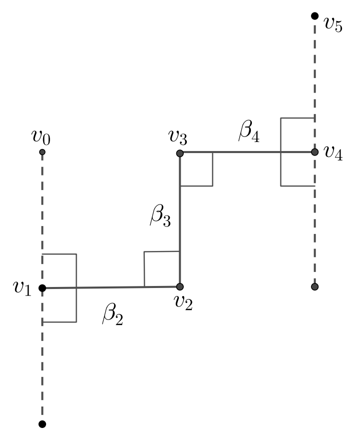

Figure 6: A forbidden local configuration when the case of $n = 6$ and $n = 7$

So, the distance between v_0 and v_5 is $\sqrt{2^2 + (1 + y_2 - y_1)^2 + (z_2 - z_1)^2}$. Since $\|\boldsymbol{\beta}_0\| = 1$, we see the equation $\sqrt{2^2 + (1 + y_2 - y_1)^2 + (z_2 - z_1)^2} = 1$. But, it is easy to see that $\sqrt{2^2 + (1 + y_2 - y_1)^2 + (z_2 - z_1)^2} \geq \sqrt{2^2} = 2 > 1$. This contradicts that a closed chain in $M_6^6(\theta)$ has a local configuration as in Fig. 4.

Finally, we consider the case $n = 7$. Then v_0 and v_5 are given by $(0, y_1, z_1)$ and $(2, 1 + y_2, z_2)$ respectively, where $y_1^2 + z_1^2 = 1$ and $y_2^2 + z_2^2 = 1$ (see Fig. 6). The distance between v_0 and v_5 is $\sqrt{2^2 + (1 + y_2 - y_1)^2 + (z_2 - z_1)^2}$. From the restriction of the bond angle $\angle v_5v_6v_0$, we have $\|v_0 - v_5\| = \sqrt{2}$, which implies that the equation $\sqrt{2^2 + (1 + y_2 - y_1)^2 + (z_2 - z_1)^2} = \sqrt{2}$ (see Fig. 7).

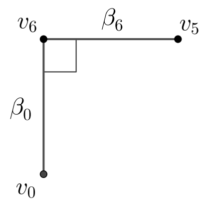

Figure 7: A local configuration consisting of β_0 and β_6

However, one can verify that $\sqrt{2^2 + (1 + y_2 - y_1)^2 + (z_2 - z_1)^2} \geq \sqrt{2^2} = 2 > \sqrt{2}$. This contradicts that a closed chain in $M_7^7(\theta)$ has a local configuration as in Fig. 4. □

If the dihedral angles of a rotatable bond β_i ($1 \leq i \leq n$) can take any value, the three bond vectors $\boldsymbol{\beta}_{i-1}, \boldsymbol{\beta}_i$ and $\boldsymbol{\beta}_{i+1}$ form a local configuration as in Fig. 4, where $\beta_n = \beta_0$ and $\beta_{n+1} = \beta_1$. But, from Lemma 5, we see that any closed chain in $M_n^n(\theta)$ does not have the local configuration as in Fig. 4, when $n = 5, 6, 7$.

Next, we assume that $n \geq 8$ and $n \neq 9$. From now on, we construct a rotational closed chain in $M_n^n(\theta)$ to prove Theorem 2 (2). We recall Theorem A and B stated in [**?**].

Lemma 6 ([**?**])**.** *Let n is a positive integer with $n \geq 4$ and $n \neq 5$.*
If n is odd, we have $M_n^n(\theta) \neq \varnothing$ if and only if $\theta \in \left[\frac{\pi}{n}, \frac{n-2}{n}\pi\right]$.
If n is even, we have $M_n^n(\theta) \neq \varnothing$ if and only if $\theta \in \left[0, \frac{n-2}{n}\pi\right]$

By Lemma 6, when $\theta = \frac{\pi}{2}$, we obtain $M_{n-4}^{n-4}(\theta) \neq \varnothing$. By attaching the four bonds β_a, β_b, β_c and β_d to a closed chain in $M_{n-4}^{n-4}(\theta)$ as in Fig. 8, we get a rotational closed chain in $M_n^n(\theta)$. In fact, the closed chain has a rotatable bond β_i, where $i = a, d$. (see Fig. 8). More precisely, we also need to rename the bonds of the new rotational closed chain so that the rotational closed chain is contained in $M_n^n(\theta)$.

We give an example of the case $n = 8$ as in Fig. 9. Note that the dihedral angles of a rotatable bond β_i can take any value, where $i = 3, 6$ and $\boldsymbol{\beta}_8 = \boldsymbol{\beta}_0$.

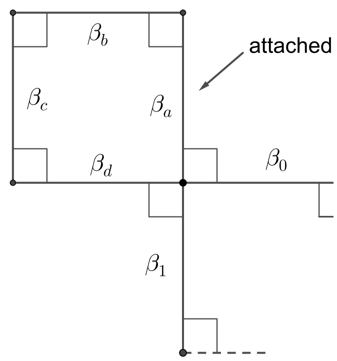

Figure 8: A rotational closed chain in $M_n^n(\theta)$

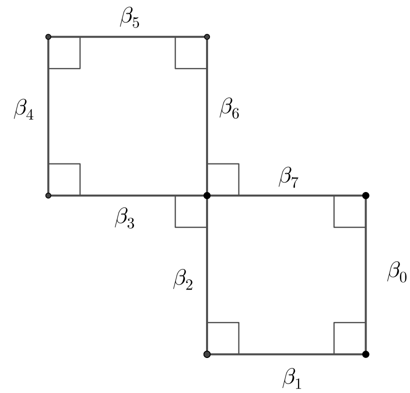

Figure 9: The case of a rotational closed chain in $M_8^8(\theta)$

Remark 7. *When $n = 9$, we cannot apply the above method to determine whether $M_9^9\left(\frac{\pi}{2}\right)$ has a rotational closed chain. In fact, since, from Theorem A in [**?**], $M_5^5(\theta) \neq \varnothing$ if and only if $\theta = \frac{\pi}{5}$ or $\frac{3}{5}\pi$, we have $M_5^5\left(\frac{\pi}{2}\right) = \varnothing$.*

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