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The configuration space of almost regular polygons

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Abstract. For a given angle θ, consider the configuration space C_n of equilateral n-gons in $\mathbf{R}^3$ whose bond angles are equal to θ except for two successive ones. We show that when $n \geq 8$ and θ is sufficiently close to the inner angle $\frac{n-2}{n}\pi$ of the regular n-gon, C_n is homeomorphic to the $(n-4)$-dimensional sphere S^{n-4}.

1. Introduction

Configuration spaces of n-gons in the Euclidean space $\mathbf{R}^d$ have been studied from a topological, an algorithmic or a kinematic viewpoint (see, for example, [3], [9], [11], [12], [13], [14], [15], [17], [19]). In this paper, we fix an integer $n \geq 5$ and an angle θ with $\frac{n-3}{n-1}\pi < \theta < \frac{n-2}{n}\pi$, which we call the *fixed bond angle*, and consider the *configuration space* $C_n = C_n(\theta)$ of *equilateral n-gons* in $\mathbf{R}^3$ whose bond angles are equal to θ except for two successive ones.

We give a precise definition of C_n. An *n-gon* is a graph embedded in $\mathbf{R}^3$ with vertices $v_0, v_1, \ldots, v_{n-1}$ and bonds $\beta_1, \beta_2, \ldots, \beta_{n-1}, \beta_0$, where β_i connects v_{i-1} and v_i $(i = 1, 2, \ldots, n-1)$. (Indices are considered modulo n whenever we treat an n-gon.) We call the vector $\boldsymbol{\beta}_i := v_i - v_{i-1}$ the *i-th bond vector*. An n-gon is said to be *equilateral* if all of its bonds have the same length, say 1. The bond angle of an n-gon at the vertex v_i is defined to be the angle between the vectors $-\boldsymbol{\beta}_i$ and $\boldsymbol{\beta}_{i+1}$. We assume that every such equilateral n-gon is normalized so that $v_0 = (0, 0, 0)$, $v_{n-1} = (-1, 0, 0)$ and $v_{n-2} = (\cos\theta - 1, \sin\theta, 0)$. Then the configuration space $C_n(\theta)$ is defined as follows.

Definition 1 ([6], [7], [8]). For $k = 1, \ldots, n-2$, let $f_k : (\mathbf{R}^3)^{n-3} \to \mathbf{R}$ be the function defined by

$$f_k(v_1, \ldots, v_{n-3}) = \frac{1}{2}(\|\boldsymbol{\beta}_k\| - 1).$$

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For $k = 1, \dots, n-3$, let $g_k : (\mathbf{R}^3)^{n-3} \to \mathbf{R}$ be the function defined by

$$g_1(v_1, \dots, v_{n-3}) = \langle -\boldsymbol{\beta}_0, \boldsymbol{\beta}_1 \rangle - \cos\theta,$$
$$g_k(v_1, \dots, v_{n-3}) = \langle -\boldsymbol{\beta}_{k+1}, \boldsymbol{\beta}_{k+2} \rangle - \cos\theta \qquad (k = 2, \dots, n-3).$$

Here $\langle\, , \rangle$ denotes the standard inner product in $\mathbf{R}^3$ and $\|\boldsymbol{x}\|$ the standard norm $\sqrt{\langle \boldsymbol{x}, \boldsymbol{x} \rangle}$. The configuration space $C_n = C_n(\theta)$ is defined by as follows:

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

The maps f_k, g_k are called *rigidity maps*, and they determine bond lengths and angles of the n-gon in C_n. The n-gons in C_n are equilateral n-gons in $\mathbf{R}^3$ with n vertices such that the bond angles are all equal to the given angle θ except for the two successive bond angles at the vertices v_1 and v_2.

We have been interested in a mathematical model of n-membered ringed hydrocarbon molecules, and obtained the following results in [7]. If $n = 5$ and $\theta = \frac{7}{12}\pi$, the average of bond angles of 5-membered ringed hydrocarbon molecules, then $C_n(\theta)$ is homeomorphic to S^{n-4}. If $n = 6, 7$ and the fixed bond angle is tetrahedral angle $\theta = \cos^{-1}\left(-\frac{1}{3}\right)$, the standard bond angle of the carbon atom, then $C_n(\theta)$ is homeomorphic to S^{n-4}. Moreover, these results were generalized in [6] as follows. If $n = 5, 6, 7$ and the bond angle θ satisfies $\frac{n-4}{n-2}\pi < \theta < \frac{n-2}{n}\pi$, then $C_n(\theta)$ is homeomorphic to S^{n-4}. If $n = 8$ and the bond angle θ satisfies $\frac{5}{7}\pi \le \theta < \frac{3}{4}\pi$, then $C_n(\theta)$ is homeomorphic to S^{n-4}.

The purpose of this paper is to prove the following generalization of the results in [6] for all $n \ge 5$.

Theorem 1. *For each integer $n \ge 5$, there exists θ_0 such that the configuration space $C_n(\theta)$ is homeomorphic to the $(n-4)$-dimensional sphere S^{n-4} for every bond angle θ with $\theta_0 < \theta < (n-2)\pi/n$.*

Since the case where $5 \le n \le 8$ is already treated in the pervious papers, we assume $n > 8$ throughout the paper.

This paper is arranged as follows. Section 2 is devoted to preliminaries for the proof of Theorem 1. Section 3 is devoted to the proof of Theorem 1.

2. Preliminaries

Lemma 1. *Let n be an integer greater than 8. Then there exists θ_1 such that any n-gon in $C_n = C_n(\theta)$ satisfies the following* (a)–(d) *for any bond angle θ with $\theta_1 < \theta < (n-2)\pi/n$.*

(a) *Any n-gon in C_n does not contain the local configurations of three successive bonds β_2, β_3 and β_4 with the relation $\boldsymbol{\beta}_3 + \boldsymbol{\beta}_4 = \gamma\boldsymbol{\beta}_2$, where $\gamma = \pm\sqrt{2 - 2\cos\theta}$ as in Figs.* 1 *and* 2.

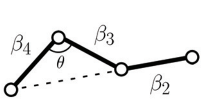

Fig. 1. The forbidden local configuration (a) for $\gamma > 0$

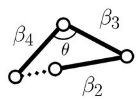

Fig. 2. The forbidden local configuration (a) for $\gamma < 0$

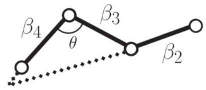

Fig. 3. The forbidden local configuration (b) for $\delta > 0$

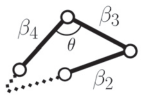

Fig. 4. The forbidden local configuration (b) for $\delta < 0$

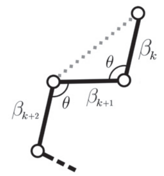

Fig. 5. The forbidden local configuration (c) with $\boldsymbol{\beta}_k = \boldsymbol{\beta}_{k+2}$

(b) *Any n-gon in C_n does not contain the local configurations of three successive bonds β_2, β_3 and β_4 with the relation $\boldsymbol{\beta}_3 - \lambda\boldsymbol{\beta}_4 = \delta\boldsymbol{\beta}_2$, where $\lambda = 2\cos\theta$ and $\delta = \pm\sqrt{1+2\lambda^2}$ as in Figs.* 3 *and* 4.

(c) *Any n-gon in C_n does not contain the local configurations of three successive bonds β_k, β_{k+1}, β_{k+2} $(k \neq 0, 1, 2)$ with the bond angles θ and with the relation $\boldsymbol{\beta}_k = \boldsymbol{\beta}_{k+2}$ as in Fig.* 5, *where indices are considered modulo n.*

(d) *Any n-gon in C_n cannot be contained in a plane.*

We call a local configuration described in (a), (b) or (c) in the above lemma a *forbidden local configuration*.

Proof. We draw a regular n-sided polygon in the xy plane as in Figs. 6, 7, 9 and 10. Let P be the plane which intersects the xy plane vertically in the dotted line, and fix a unit normal vector v to this plane as in Figs. 6, 7, 9 and 10.

When n is odd, we fix the bond $\beta_{(n+3)/2}$ as in Figs. 6 and 9 and consider all of the polygonal lines consisting of the bonds $\beta_{(n+3)/2}, \dots, \beta_3$. When n is even, we fix the bond $\beta_{(n+4)/2}$ as in Figs. 7 and 10 and consider all of the polygonal lines consisting of the bonds $\beta_{(n+4)/2}, \dots, \beta_3$. Let $\mathrm{Arm}(\theta)$ denote such a non-closed polygonal line with the bond angle θ.

Let δ_k denote the dihedral angle between the planes defined by bond pairs $\{\beta_{k-1}, \beta_k\}$ and $\{\beta_k, \beta_{k+1}\}$ respectively for $k = 4, 5, \dots, \left[\frac{n+2}{2}\right]$, where $[x]$ denotes the largest integer less than or equal to x. Let $\mathrm{pArm}(\theta)$ denote the non-closed polygonal line with the bond angle θ where all dihedral angles δ_k are 0. Note that $\mathrm{pArm}(\theta)$ is planar. Observe that, when the bond angle between the bonds

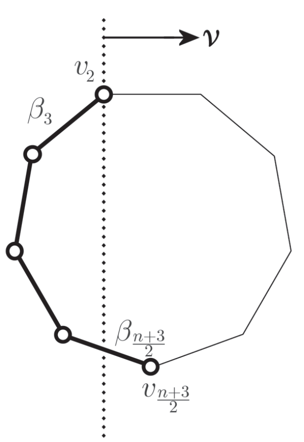

Fig. 6. pArm$\left(\frac{n-2}{n}\pi\right)$ when n is odd ($n = 9$)

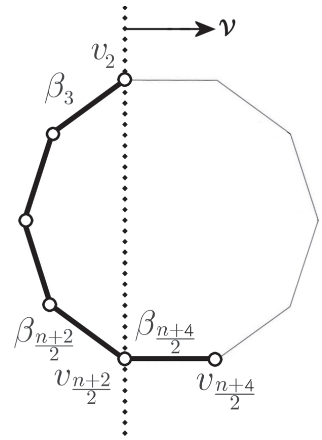

Fig. 7. pArm$\left(\frac{n-2}{n}\pi\right)$ when n is even ($n = 10$)

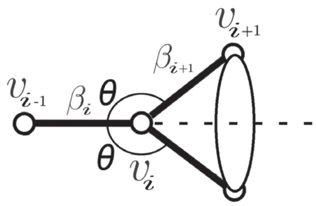

Fig. 8. All positions of v_{i+1} on the cone

β_i and β_{i+1} is equal to θ, the vertex v_{i+1} is on the cone centered on β_i with the apex at v_i as in Fig. 8.

First, we consider the case where the bond angle θ is $\frac{n-2}{n}\pi$. Then the vertex v_2 is contained in the plane P only when the non-closed polygonal line is congruent to pArm$\left(\frac{n-2}{n}\pi\right)$ in Figs. 6 and 7. By applying the same argument to the "right" side to n-gons in $C_n\left(\frac{n-2}{n}\pi\right)$, we see that any n-gon in $C_n\left(\frac{n-2}{n}\pi\right)$ is congruent to the regular n-polygon in the plane.

Next, assume that $\theta < \frac{n-2}{n}\pi$. Then Arm$(\theta)$ can intersect the plane P. We take a sufficiently small $\varepsilon > 0$ with $1 - 2\varepsilon > 0$. Then there exists θ_ε with $\theta_\varepsilon < \frac{n-2}{n}\pi$ such that the vertex v_2 is contained in the plane $P + \varepsilon \cdot v = \{p + \varepsilon \cdot v \mid p \in P\}$ only when Arm(θ_ε) is congruent to pArm(θ_ε) as in Figs. 9 and 10.

In other words, the distance from v_2 to $P + v$ is greater than or equal to $1 - \varepsilon$, and equal to $1 - \varepsilon$ only when Arm(θ_ε) is congruent to pArm(θ_ε) as in Figs. 9 and 10. Hence, for any Arm(θ), the distance from v_2 to $P + v$ is greater than $1 - \varepsilon$ when $\theta_\varepsilon < \theta < \frac{n-2}{n}\pi$.

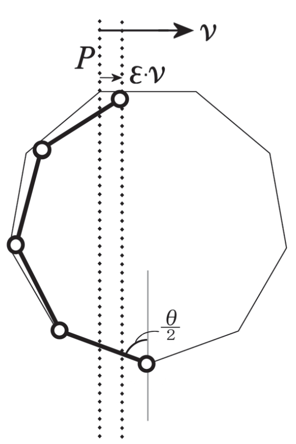

Fig. 9. pArm(θ_ε) when n is odd $(n = 9)$

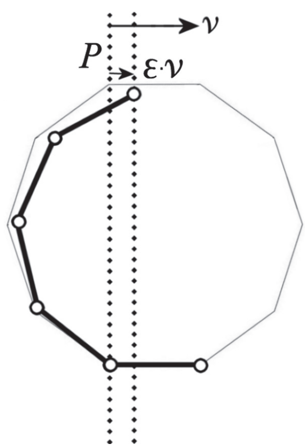

Fig. 10. pArm(θ_ε) when n is even $(n = 10)$

Now we consider the non-closed polygonal line with the bond angle θ which consists of $n-1$ number of the bonds $\beta_3, \beta_4, \ldots, \beta_{n-1}, \beta_0, \beta_1$. By using the above argument for the end point v_1, we see that, when the non-closed polygonal line with the bond angle θ_ε forms a part of the boundary of a convex polygon, the distance along v between v_1 and v_2 is greater than or equal to $1 - 2\varepsilon$ (cf. [5, p. 147, Corollary 8.2.4]). Hence, for any non-closed polygonal line with the bond angle θ, the distance along v between v_1 and v_2 is greater than $1 - 2\varepsilon$ when $\theta_\varepsilon < \theta < \frac{n-2}{n}\pi$.

(a) We now prove the assertion (a).

Case (a-1) $\gamma > 0$. We add the bond β_2 to Arm(θ) at v_2 to form the local configuration in Fig. 1. We replace the two bonds β_2 and β_3 with a new bond which connects v_1 to v_3. Let $\bar{\beta}_{(2,3)}$ denote this new bond. As mentioned above, the distance from v_2 to $P + v$ attains the minimum only when the resulting non-closed polygonal line with the bond $\bar{\beta}_{(2,3)}$ has a planar configuration where all dihedral angles are 0. Note that this planar configuration is obtained by adding β_2 to pArm(θ) at v_2 as in Fig. 1.

When $\theta = \frac{n-2}{n}\pi$, for pArm$\left(\frac{n-2}{n}\pi\right)$ with the added bond β_2 as in Fig. 1, we have $\langle \boldsymbol{\beta}_2, v \rangle < 1$ with some computations. Then the distance from v_1 to $P + v$ is equal to $1 - \langle \boldsymbol{\beta}_2, v \rangle$ (> 0). We put $\varepsilon = \frac{1}{4}(1 - \langle \boldsymbol{\beta}_2, v \rangle)$. We see that a bond angle θ'_{a_+} can be chosen so that, for any pArm(θ) with the added bond β_2 as in Fig. 1, $\langle \boldsymbol{\beta}_2, v \rangle$ is less than $1 - 3\varepsilon$ when $\theta'_{a_+} < \theta < \frac{n-2}{n}\pi$.

Now we consider the non-closed polygonal line which consists of bonds $\beta_3, \beta_4, \ldots, \beta_{n-1}, \beta_0, \beta_1$, and add the bond β_2 to the non-closed polygonal line at v_2 to form the local configuration in Fig. 1. We put $\theta_{a_+} = \max\{\theta'_{a_+}, \theta_\varepsilon\}$.

When $\theta_{a_+} < \theta < \frac{n-2}{n}\pi$, the distance from the vertex v_1 of β_2 to $P + (1-\varepsilon) \cdot v$ is greater than ε (>0). Hence the polygonal line with the added bond β_2 as in Fig. 1 cannot form an n-gon when $\theta_{a_+} < \theta < \frac{n-2}{n}\pi$.

Case (a-2) $\gamma < 0$. We add the bond β_2 to $\mathrm{Arm}(\theta)$ at v_2 to form the local configuration in Fig. 2. We replace the union of the two bonds β_2 and β_3 with a new bond which connects v_1 to v_3. Let $\bar{\beta}_{(2,3)}$ denote this new bond. As mentioned above, the distance from v_2 to $P + v$ attains the minimum only when the resulting non-closed polygonal line with the bond $\bar{\beta}_{(2,3)}$ has a planar configuration where all dihedral angles are 0. Note that this planar configuration is obtained by adding β_2 to $\mathrm{pArm}(\theta)$ at v_2 as in Fig. 2.

When $\theta = \frac{n-2}{n}\pi$, for $\mathrm{pArm}\left(\frac{n-2}{n}\pi\right)$ with the added bond β_2 as in Fig. 2, we have $\langle \boldsymbol{\beta}_2, v\rangle < 0$ with some computations. Then the distance from v_1 to $P + v$ is greater than 1. We see that a bond angle, θ'_{a_-} can be chosen so that, for any $\mathrm{pArm}(\theta)$ with the added bond β_2 as in Fig. 2, $\langle \boldsymbol{\beta}_2, v\rangle < 0$ when $\theta'_{a_-} < \theta < \frac{n-2}{n}\pi$.

Now we consider the non-closed polygonal line which consists of bonds $\beta_3, \beta_4, \dots, \beta_{n-1}, \beta_0, \beta_1$, add the bond β_2 to the non-closed polygonal line at v_2 to form the local configuration in Fig. 2. We put $\varepsilon = \frac{1}{3}$ and $\theta_{a_-} = \max\{\theta'_{a_-}, \theta_\varepsilon\}$. When $\theta_{a_-} < \theta < \frac{n-2}{n}\pi$, the distance from the vertex v_1 of β_2 to $P + (1-\varepsilon) \cdot v$ is greater than ε (>0). Hence the polygonal line with the added bond β_2 as in Fig. 2 cannot form an n-gon when $\theta_{a_-} < \theta < \frac{n-2}{n}\pi$.

(b) We now prove the assertion (b).

Case (b-1) $\delta > 0$. We add the bond β_2 to $\mathrm{Arm}(\theta)$ at v_2 to form the local configuration in Fig. 3.

When $\theta = \frac{n-2}{n}\pi$, for $\mathrm{pArm}\left(\frac{n-2}{n}\pi\right)$ with the added bond β_2 as in Fig. 3, we have $\langle \boldsymbol{\beta}_2, v\rangle < 1$ with some computations. Then the distance from v_1 to $P + v$ is equal to $1 - \langle \boldsymbol{\beta}_2, v\rangle$ (>0).

By an argument similar to the case $\gamma > 0$ of (a), we can take θ_{b_+} so that any n-gon in C_n does not have the local configuration as in Fig. 3 when $\theta_{b_+} < \theta < \frac{n-2}{n}\pi$.

Case (b-2) $\delta < 0$. We add the bond β_2 to $\mathrm{Arm}(\theta)$ at v_2 to form the local configuration in Fig. 4.

When $\theta = \frac{n-2}{n}\pi$, for $\mathrm{pArm}\left(\frac{n-2}{n}\pi\right)$ with the added bond β_2 as in Fig. 4, we have $\langle \boldsymbol{\beta}_2, v\rangle < 0$ with some computations. Then the distance from v_1 to $P + v$ is greater than 1.

By an argument similar to that in the case $\gamma < 0$ of (a), we can take θ_{b_-} so that any n-gon in C_n does not have the local configuration as in Fig. 4 when $\theta_{b_-} < \theta < \frac{n-2}{n}\pi$.

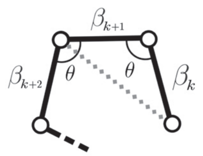

Fig. 11. A planar local configuration of the three successive bonds

(c) We consider the non-closed polygonal line with the bond angle θ consisting of the bonds $\beta_3, \beta_4, \dots, \beta_{n-1}, \beta_0, \beta_1$. Assume that the non-closed polygonal line has one or more planar local configurations as in Fig. 5. Now, we choose the three successive bonds β_k, β_{k+1} and β_{k+2} having a planar local configuration as in Fig. 5. We replace the union of the two bonds β_k and β_{k+1} with a new bond which connects v_{k-1} to v_{k+1} along the dotted line in Fig. 5 or 11. Let $\bar{\beta}_{(k,k+1)}$ denote this new bond. When the bond angle between β_{k+2} and $\bar{\beta}_{(k,k+1)}$ is equal to $\frac{\pi+\theta}{2}$, the non-closed polygonal line having the local configuration of Fig. 5 can be identified with the non-closed polygonal line of $n-2$ bonds obtained by replacing the union of the two bonds β_k and β_{k+1} with the bond $\bar{\beta}_{(k,k+1)}$. Note that the end points of the non-closed polygonal line are v_1 and v_2.

We consider the distance between the end points v_1 and v_2 of the non-closed polygonal line obtained by replacing the union of the two bonds β_k and β_{k+1} with the bond $\bar{\beta}_{(k,k+1)}$. As mentioned above, when the non-closed polygonal line obtained by replacing the union of β_k and β_{k+1} with the bond $\bar{\beta}_{(k,k+1)}$ forms a part of the boundary of the convex $(n-1)$-sided polygon, the distance between v_1 and v_2 attains the minimum.

On the other hand, the distance between v_1 and v_2 of the original non-closed polygonal line attains the minimum when the original non-closed polygonal line forms a part of the boundary of a convex n-sided polygon.

Then the three successive bonds β_k, β_{k+1} and β_{k+2} have a planar local configuration as in Fig. 11.

The non-closed polygonal line having the local configuration of Fig. 11 can be identified with the non-closed polygonal line of $n-2$ bonds obtained by replacing the union of the two bonds β_k and β_{k+1} with the bond $\bar{\beta}_{(k,k+1)}$ when the bond angle between β_{k+2} and $\bar{\beta}_{(k,k+1)}$ is equal to $\frac{-\pi+3\theta}{2}$. Note that the resulting non-closed polygonal line forms a part of the boundary of a convex $(n-1)$-sided polygon when the bond angle between β_{k+2} and $\bar{\beta}_{(k,k+1)}$ is equal to $\frac{-\pi+3\theta}{2}$ and the original non-closed polygonal line forms a part of the boundary of a convex n-sided polygon.

By applying Cauchy's arm lemma ([4, p. 229]) to convex $(n-1)$-sided polygons with a bond $\bar{\beta}_{(k,k+1)}$, we see that the distance between v_1 and v_2 is a monotonically increasing function of the bond angle between β_{k+2} and $\bar{\beta}_{(k,k+1)}$.

The distance between v_1 and v_2 is 1 when $\theta = \frac{n-2}{n}\pi$ and the bond angle between β_{k+2} and $\bar{\beta}_{(k,k+1)}$ is equal to $\frac{-\pi+3\theta}{2}$. Then the distance between v_1 and v_2 is greater than 1 when $\theta = \frac{n-2}{n}\pi$ and the bond angle between β_{k+2} and $\bar{\beta}_{(k,k+1)}$ is equal to $\frac{\pi+\theta}{2}$.

We can take $\theta(k)$ so that, for any angle θ with $\theta(k) < \theta < \frac{n-2}{n}\pi$, the distance between v_1 and v_2 is greater than 1 when the bond angle between β_{k+2} and $\bar{\beta}_{(k,k+1)}$ is equal to $\frac{\pi+\theta}{2}$. By taking $\theta_c = \max_k\{\theta(k)\}$, the proof of Lemma 1 (c) is completed.

(d) Let θ_c be the angle in Lemma 1 (c) and consider n-gons in $C_n(\theta)$ when $\theta_c < \theta < \frac{n-2}{n}\pi$. We assume that there is an n-gon contained in a plane. By forgetting the bond β_2 from the n-gon, we have a non-closed polygonal line with the end points v_1, v_2. By Lemma 1 (c), the three successive bonds form a planar local configuration as in Fig. 11. If the bond angle θ is not equal to $\frac{n-2}{n}\pi$, the distance between v_1 and v_2 is not equal to 1. By contradiction, the proof of Lemma 1 (d) is completed.

By taking $\theta_1 = \max\{\theta_{a_+}, \theta_{a_-}, \theta_{b_+}, \theta_{b_-}, \theta_c\}$, the proof of Lemma 1 is completed. $\square$

3. The proof of Theorem 1

By Lemma 1, we show the following Proposition 1:

Proposition 1. *Let θ_0 be the maximum of the angle θ_1 in Lemma 1 and the solutions of the following equations:*

$$\frac{\sin(mx)}{\sin x} = 1 - 2\cos x \qquad (1 \le m \le n-6,\ \pi/2 < x < (n-2)\pi/n).$$

Then the configuration space C_n is an orientable closed $(n-4)$-dimensional submanifold of $\mathbf{R}^{3n-9}$ if the bond angle θ satisfies $\theta_0 < \theta < (n-2)\pi/n$.

Proof. First, note that θ_0 can be determined from the Chebyshev polynomials of second kind $\frac{\sin(mx)}{\sin x} = \sum_{j=0}^{[(m-1)/2]} {}_mC_{2j+1}(\cos x)^{m-2j-1}(\cos^2 x - 1)^j$, where $[y]$ denotes the largest integer less than or equal to y. We define $F : (\mathbf{R}^3)^{n-3} \to \mathbf{R}^{2n-5}$ by $F = (f_1, \dots, f_{n-2}, g_1, \dots, g_{n-3})$. Then $C_n = F^{-1}(\{\mathrm{O}\})$ for $\mathrm{O} = (0, \dots, 0) \in \mathbf{R}^{2n-5}$.

We show that $\mathrm{O} \in \mathbf{R}^{2n-5}$ is a regular value of F. It suffices to prove that gradient vectors $(\operatorname{grad} f_1)_p, \dots, (\operatorname{grad} f_{n-2})_p$, $(\operatorname{grad} g_1)_p, \dots, (\operatorname{grad} g_{n-3})_p$ are linearly independent for any $p \in F^{-1}(\{\mathrm{O}\}) = C_n$, 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 as follows:

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

Here $\mathbf{0} = (0, 0, 0)$ and $\boldsymbol{\beta}_k$ $(k = 0, \ldots, n-1)$ denote the bond vectors of the n-gon corresponding to $p \in C_n$.

Assume that the gradient vectors $(\mathrm{grad}\ f_1)_p, \ldots, (\mathrm{grad}\ f_{n-2})_p$, $(\mathrm{grad}\ g_1)_p, \ldots,$ $(\mathrm{grad}\ g_{n-3})_p$ are linearly dependent. Then, for some $(c_1, \ldots, c_{2n-5}) \neq (0, \ldots, 0)$, we have a linear relation:

$$\sum_{i=1}^{n-2} c_i (\mathrm{grad}\ f_i)_p + \sum_{i=1}^{n-3} c_{i+n-2} (\mathrm{grad}\ g_i)_p = (\mathbf{0}, \ldots, \mathbf{0}). \tag{$*$}$$

In what follows, we show, by using Lemma 1 (a), (b), (c), that, under this assumption, all vertices of the n-gon corresponding to p are contained in a single plane. Since two successive bond vectors not including $\boldsymbol{\beta}_2$ are linearly independent, we get $c_2 \neq 0$. The first 1×3 block of the linear combination $(*)$ implies that the bond vectors $\boldsymbol{\beta}_0$, $\boldsymbol{\beta}_1$ and $\boldsymbol{\beta}_2$ are contained in a single plane. The second 1×3 block of the linear combination $(*)$ implies that the bond vectors $\boldsymbol{\beta}_2$, $\boldsymbol{\beta}_3$ and $\boldsymbol{\beta}_4$ are contained in a single plane.

We show by induction $c_k \neq 0$ $(n+1 \leq k \leq 2n-5)$. First, we observe $c_{n+1} \neq 0$. In fact, the second and the third 1×3 blocks of the linear combination $(*)$ imply $c_{n+1} \neq 0$ by Lemma 1 (a). Then the bond vectors $\boldsymbol{\beta}_3$, $\boldsymbol{\beta}_4$ and $\boldsymbol{\beta}_5$ are contained in a single plane.

We study c_ℓ $(n+1 \leq \ell \leq k)$. Assume that $c_\ell \neq 0$ $(n+1 \leq \ell \leq k-1)$. Then the bond vectors $\boldsymbol{\beta}_0, \boldsymbol{\beta}_1, \ldots, \boldsymbol{\beta}_{k-n+3}$ are contained in a single plane. Observe, by using Lemma 1 (c), the relation $\boldsymbol{\beta}_i + \lambda \boldsymbol{\beta}_{i+1} + \boldsymbol{\beta}_{i+2} = \mathbf{0}$ $(\lambda = 2\cos\theta)$

when $\boldsymbol{\beta}_i$, $\boldsymbol{\beta}_{i+1}$, $\boldsymbol{\beta}_{i+2}$ are contained in a single plane for $i \neq 0, 1, 2$. The third 1×3 block of the linear combination $(*)$ implies the equality $(c_3 + c_n)\boldsymbol{\beta}_3 - (c_4 + c_n)\boldsymbol{\beta}_4 + c_{n+1}\boldsymbol{\beta}_5 = \mathbf{0}$ with some computations.

Since $\boldsymbol{\beta}_3$, $\boldsymbol{\beta}_4$, $\boldsymbol{\beta}_5$ are contained in a single plane, we have the following relations for the coefficients:

$$c_{n+1} = c_3 + c_n, \tag{$R_{n+1,1}$}$$

$$c_4 = -c_n - \lambda c_{n+1}. \tag{$R_{n+1,2}$}$$

With some computations, the $(j - n + 2)$-th 1×3 block of the linear combination $(*)$ implies the equality

$$(-c_{j-2})\boldsymbol{\beta}_{j-n+1} + (c_{j-n+2} + c_{j-1})\boldsymbol{\beta}_{j-n+2} - (c_{j-n+3} + c_{j-1})\boldsymbol{\beta}_{j-n+3} + c_j\boldsymbol{\beta}_{j-n+4} = \mathbf{0}.$$

We have the following relations $(R_{j,1})$ and $(R_{j,2})$ among the coefficients of $\boldsymbol{\beta}_{j-n+2}$ and $\boldsymbol{\beta}_{j-n+3}$, respectively:

$$c_j = \lambda c_{j-2} + c_{j-1} + c_{j-n+2}, \tag{$R_{j,1}$}$$

$$c_{j-n+3} = c_{j-2} - c_{j-1} - \lambda c_j. \tag{$R_{j,2}$}$$

We fix ℓ with $n + 2 \leq \ell \leq k$. By adding the equalities $(R_{j,1})$ and $(R_{j,2})$ for $n + 1 \leq j \leq \ell$, we have $c_\ell = -\lambda c_{\ell-1} - c_{\ell-2} + (1 + \lambda)c_n + c_3$ $(n + 2 \leq \ell \leq k)$. Put $d = (1 + \lambda)c_n + c_3$. With some computations, we obtain the recurrence relations $(c_\ell - \alpha_1 c_{\ell-1}) = \alpha_2(c_{\ell-1} - \alpha_1 c_{\ell-2}) + d$, where α_1 and α_2 denote the two solutions of $x^2 + \lambda x + 1 = 0$. Note that $\alpha_1 + \alpha_2 = -\lambda$ and $\alpha_1\alpha_2 = 1$. From these recurrence relations, we have the following two equalities:

$$(c_k - \alpha_1 c_{k-1}) = \alpha_2^{k-n-1}(c_{n+1} - \alpha_1 c_n) + d(\alpha_2^{k-n-2} + \alpha_2^{k-n-3} + \cdots + 1),$$
$$(c_k - \alpha_2 c_{k-1}) = \alpha_1^{k-n-1}(c_{n+1} - \alpha_2 c_n) + d(\alpha_1^{k-n-2} + \alpha_1^{k-n-3} + \cdots + 1).$$

We prove that $c_k \neq 0$. Now, we assume to the contrary that $c_k = 0$. We put $m = k - n - 1$ $(1 \leq m \leq n - 6)$. By using the above two equalities and $c_{n+1} = c_n + c_3$, we obtain $Ac_3 + Bc_n = 0$. Here, $A = (\alpha_2^{m+1} - \alpha_1^{m+1}) + (\alpha_2^m - \alpha_1^m) + \cdots + (\alpha_2 - \alpha_1)$ and $B = \{(\alpha_2^{m+1} - \alpha_1^{m+1}) + (\alpha_2^{m-1} - \alpha_1^{m-1}) + \cdots + (\alpha_2 - \alpha_1)\} + \lambda\{(\alpha_2^m - \alpha_1^m) + \cdots + (\alpha_2 - \alpha_1)\}$. It is easy to see that $A = \lambda B$. If $A \neq 0$ and $B \neq 0$, then we have $\lambda c_3 + c_n = 0$. The second 1×3 block of the linear combination $(*)$ implies the equality $c_2\boldsymbol{\beta}_2 - c_3\boldsymbol{\beta}_3 + c_n\boldsymbol{\beta}_4 = \mathbf{0}$. Since $\lambda c_3 + c_n = 0$, we have $c_2\boldsymbol{\beta}_2 = c_3(\boldsymbol{\beta}_3 - \lambda\boldsymbol{\beta}_4)$. Hence we obtain $A = B = 0$ from Lemma 1 (b). Note that $(\alpha_2^{m+1} - \alpha_1^{m+1}) + (\alpha_2^m - \alpha_1^m) + \cdots + (\alpha_2 - \alpha_1)$ $= \frac{1}{1+\lambda}(\alpha_2^{m+1} - \alpha_1^{m+1}) + (\alpha_2 - \alpha_1) - (\alpha_2^{m+2} - \alpha_1^{m+2})$. With some more computations, we have $B = \frac{1}{1+\lambda}\{-(\alpha_2^m - \alpha_1^m) + (1 + \lambda)(\alpha_2 - \alpha_1)\}$.

On the other hand, it is easy to check the following equality:

$$\frac{\alpha_2^m - \alpha_1^m}{\alpha_2 - \alpha_1} = \frac{1}{2^{m-1}} \sum_{j=0}^{[(m-1)/2]} {}_mC_{2j+1}(-\lambda)^{m-2j-1}(\lambda^2 - 1)^j$$
$$= \sum_{j=0}^{[(m-1)/2]} {}_mC_{2j+1}(\cos\theta)^{m-2j-1}(\cos^2\theta - 1)^j,$$

where $[y]$ denotes the largest integer less than or equal to y. From the Chebyshev polynomials of second kind, we obtain $\frac{\alpha_2^m - \alpha_1^m}{\alpha_2 - \alpha_1} = \frac{\sin(m\theta)}{\sin\theta}$. By the definition of θ_0, we have $\frac{\sin(m\theta)}{\sin\theta} \neq 1 - 2\cos\theta$ $(\theta_0 < \theta)$. Thus we obtain $B \neq 0$, and $c_k \neq 0$ by contradiction. Therefore, all vertices of the n-gon corresponding to p are contained in a single plane. This contradicts Lemma 1 (d). As a result, the gradient vectors $(\operatorname{grad} f_1)_p, \dots, (\operatorname{grad} f_{n-2})_p$, $(\operatorname{grad} g_1)_p, \dots, (\operatorname{grad} g_{n-3})_p$ are linearly independent for any $p \in C_n$. The proof of Proposition 1 is completed. □

Proof of Theorem 1. We first show that C_n is non-empty when $n > 8$. Consider the non-closed polygonal line with the bond angle θ which consists of the bonds $\beta_3, \beta_4, \dots, \beta_{n-1}, \beta_0, \beta_1$. For $k = 4, 5, \dots, n-1, 0$, let δ_k denote the dihedral angle between the planes defined by the bond pairs $\{\beta_{k-1}, \beta_k\}$ and $\{\beta_k, \beta_{k+1}\}$ respectively, where all indices are considered modulo n. The distance between v_1 and v_2 is a continuous function of the dihedral angles $\delta_4, \delta_5, \dots, \delta_{n-1}, \delta_0$. If the non-closed polygonal line is contained in the boundary of a convex polygon, that is, all dihedral angles δ_k are 0, then the distance between v_1 and v_2 is less than 1 because $\frac{n-3}{n-1}\pi < \theta < \frac{n-2}{n}\pi$. If the non-closed polygonal line has the maximum span as in [1], [2], that is, all dihedral angles δ_k are π, then the distance between v_1 and v_2 is greater than 1. Since the distance between v_1 and v_2 is a continuous function, the distance between v_1 and v_2 can be 1. Hence C_n is non-empty.

Let θ_0 be the angle in Proposition 1 and consider the configuration space C_n of n-gons having the bond angle θ with $\theta_0 < \theta < \frac{n-2}{n}\pi$. We define $h : \mathbf{R} \times (\mathbf{R} - \{0\})^2 \times (\mathbf{R}^3)^{n-4} \to \mathbf{R}$ by $h(v_1, \dots, v_{n-3}) = \frac{x_2}{\sqrt{x_2^2 + x_3^2}}$, where $v_1 = (x_1, x_2, x_3)$. Recall the extension of Reeb's theorem that a smooth connected closed manifold M is homeomorphic to a sphere if M admits a smooth function f with only two critical points (see [16, p. 25, REMARK 1], [18, p. 380, Lemma 1]).

We show that $h|_{C_n}$ is a differentiable function on C_n with only two critical points. Note that $p \in C_n$ is a critical point of $h|_{C_n}$ if and only if there exist $a_i \in \mathbf{R}$ such that $(\operatorname{grad} h)_p = \sum_{i=1}^{n-2} a_i (\operatorname{grad} f_i)_p + \sum_{i=1}^{n-3} a_{i+n-2}(\operatorname{grad} g_i)_p$ (cf. [10]). We can easily check that $(\operatorname{grad} h)_p = \left(0, \frac{x_3^2}{\sin^3\theta}, -\frac{x_2x_3}{\sin^3\theta}, 0, \dots, 0\right)$. 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 have

$a_2 \neq 0$ 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 argument in the proof of Proposition 1, there exists a bond angle, such that, for the configuration of the n-gon corresponding to a critical point $p \in C_n = C_n(\theta)$, the vertices v_i $(i = 1, \dots, n-1)$ are contained in the plane $\mathrm{Span}\langle \boldsymbol{\beta}_2, \boldsymbol{\beta}_3 \rangle = \mathrm{Span}\langle \boldsymbol{\beta}_2, \dots, \boldsymbol{\beta}_{n-1} \rangle$.

By forgetting the bond β_2 from the n-gon, we have a non-closed polygonal line with the end points v_1, v_2. Since the three successive bonds with the bond angle θ form a planar local configuration as in Fig. 11 by Lemma 1 (c), the vertices $v_2, \dots, v_{n-1}$ are uniquely determined. If three bonds β_{n-1}, β_0 and β_1 have a planar local configuration as in Fig. 11, the distance between v_1 and v_2 is less than 1. If three bonds β_{n-1}, β_0 and β_1 have a planar local configuration as in Fig. 5, the distance between v_1 and v_2 is greater than 1. We replace the union of the two bonds β_0 and β_1 with a new bond which connects v_{n-1} to v_1. Let $\bar{\beta}_{(0,1)}$ denote this new bond. We see that the resulting non-closed polygonal line forms a part of the boundary of a convex $(n-1)$-sided polygon. By applying Cauchy's arm lemma, we obtain that the distance between v_1 and v_2 is a monotonically increasing continuous function of the bond angle between β_{n-1} and $\bar{\beta}_{(0,1)}$. When the distance between v_1 and v_2 is 1, the bond angle between β_{n-1} and $\bar{\beta}_{(0,1)}$ is uniquely determined. Thus the vertex v_1 is uniquely determined and we can see, by using the restriction of the bond angle and length, that there are precisely two possible positions for the vertex v_0. These two are mirror symmetric with respect to the plane $\mathrm{Span}\langle \boldsymbol{\beta}_2, \boldsymbol{\beta}_3 \rangle$. As a result, we have just two configurations of n-gons corresponding to the critical points. The proof of Theorem 1 is completed. □

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References

[1] Benbernou N., Fixed-angle polygonal chains: locked chains and the maximum span [Undergraduate thesis], Smith College, Northampton, Mass, USA, 2006.

[2] Benbernou N. and O'Rourke J., On the maximum span of fixed-angle chains, in Proceedings of the 18th Canadian Conference on Computational Geometry, Kingston, Canada, August (2006) 14–16.

[3] Crippen G. M. and Havel T. F., Distance Geometry and Molecular Conformation, Wiley, New York, 1988.

[4] Cromwell P. R., Polyhedra, Cambridge University Press, 1999.

[5] Demaine E. D. and O'Rourke J., Geometric Folding Algorithms: Linkages, Origami, Polyhedra, Cambridge University Press, 2007.

[6] Goto S., Hemmi Y., Komatsu K. and Yagi J., The closed chains with spherical configuration spaces, Hiroshima Math. J. **42** (2012), 253–266.
[7] Goto S. and Komatsu K., The configuration space of a model for ringed hydrocarbon molecules, Hiroshima Math. J. **42** (2012), 115–126.
[8] Goto S., Komatsu K. and Yagi J., A remark on the configuration space of a model for ringed hydrocarbon molecules, Kochi J. Math. **7** (2012), 89–96.
[9] Havel T. F., Some examples of the use of distances as coordinates for Euclidean geometry, J. Symbolic Computation **11** (1991), 579–593.
[10] Kamiya H., Weighted trace functions as examples of Morse functions, Jour. Fac. Sci. Shinshu Univ. **7** (1971), 85–96.
[11] Kamiyama Y., On the level set of a function with degenerate minimum point, International Journal of Mathematics and Mathematical Sciences, (2015), 6 pages.
[12] Kapovich M. and Millson J., On the moduli space of polygons in the Euclidean plane, J. Diff. Geom. **42** (1995), 430–464.
[13] Lenhart W. J. and Whitesides S. H., Reconfiguring closed polygonal chains in Euclidean d-space, Jour. Discrete Comput. Geom. **13** (1995), 123–140.
[14] Milgram R. J. and Trinkle J. C., Complete path planning for closed kinematic chains with spherical joints, Internat. J. Robotics Res. **21** (2002), 773–789.
[15] Milgram R. J. and Trinkle J. C., The geometry of configuration spaces for closed chains in two and three dimensions, Homology, Homot., Appl. **6** (2004), 237–267.
[16] Milnor J., Morse Theory, Princeton University Press, Princeton, 1969.
[17] O'Hara J., The configuration space of equilateral and equiangular hexagons, Osaka Journal of Mathematics **50** (2013), 477–489.
[18] Rosen R., A weak form of the star conjecture for manifolds, Abstract 570-28, Notices Amer. Math. Soc. **7** (1960), 380.
[19] Shimamoto D. and Vanderwaart C., Spaces of polygons in the plane and Morse theory, American Math. Month. **112** (2005), 289–310.

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