The configuration space of almost regular polygons

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Abstract. For a given angle $\theta$, consider the configuration space $C_n$ of equilateral $n$-gons in $\mathbb{R}^3$ whose bond angles are equal to $\theta$ except for two successive ones. We show that when $n \geq 8$ and $\theta$ is sufficiently close to the inner angle $\frac{n}{2}$ 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 $\mathbb{R}^d$ 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 $\theta$ with $\frac{n-1}{n} \pi < \theta < \frac{n-2}{n} \pi$, which we call the fixed bond angle, and consider the configuration space $C_n = C_n(\theta)$ of equilateral $n$-gons in $\mathbb{R}^3$ whose bond angles are equal to $\theta$ except for two successive ones.

We give a precise definition of $C_n$. An $n$-gon is a graph embedded in $\mathbb{R}^3$ with vertices $v_0, v_1, \ldots, v_{n-1}$ and bonds $\beta_1, \beta_2, \ldots, \beta_{n-1}, \beta_0$, where $\beta_i$ 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 $\beta_i := v_i - v_{i-1}$ 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 $-\beta_i$ and $\beta_{i+1}$. We assume that every such equilateral $n$-gon is normalized so that $v_0 = (0, 0, 0)$, $v_n = (-1, 0, 0)$ 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 $f_k : (\mathbb{R}^3)^{n-3} \to \mathbb{R}$ be the function defined by

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

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

\[
g_1(v_1, \ldots, v_{n-3}) = \langle \beta_0, \beta_1 \rangle - \cos \theta, \quad g_k(v_1, \ldots, v_{n-3}) = \langle \beta_{k+1}, \beta_{k+2} \rangle - \cos \theta \quad (k = 2, \ldots, n - 3).
\]

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

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

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 $\mathbb{R}^3$ with $n$ vertices such that the bond angles are all equal to the given angle $\theta$ 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 $\theta = \frac{\pi}{3} \pi$, the average of bond angles of 5-membered ringed hydrocarbon molecules, then $C_5(\theta)$ is homeomorphic to $S^{n-4}$. If $n = 6, 7$ and the fixed bond angle is tetrahedral angle $\theta = \cos^{-1}\left(-\frac{1}{2}\right)$, 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 $\theta$ satisfies $\frac{\pi}{n-2} \pi < \theta < \frac{n-3}{n} \pi$, then $C_n(\theta)$ is homeomorphic to $S^{n-4}$. If $n = 8$ and the bond angle $\theta$ satisfies $\frac{\pi}{4} \pi \leq \theta < \frac{3}{2} \pi$, 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 $n \geq 5$.

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

Since the case where $5 \leq n \leq 8$ 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 $\theta_1$ such that any $n$-gon in $C_n = C_n(\theta)$ satisfies the following (a)–(d) for any bond angle $\theta$ 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 $\beta_2, \beta_3$, and $\beta_4$ with the relation $\beta_3 + \beta_4 = \gamma \beta_2$, where $\gamma = \pm \sqrt{2 - 2 \cos \theta}$ as in Figs. 1 and 2.
Any n-gon in $C_n$ does not contain the local configurations of three successive bonds $b_2, b_3$ and $b_4$ with the relation $b_3 \sim b_4 = \delta b_2$, where $\delta = \pm \sqrt{1 + 2 \lambda^2}$ as in Figs. 3 and 4.

Any n-gon in $C_n$ does not contain the local configurations of three successive bonds $b_k, b_{k+1}, b_{k+2}$ ($k \neq 0, 1, 2$) with the bond angles $\theta$ and with the relation $b_k = b_{k+2}$ as in Fig. 5, where indices are considered modulo $n$.

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 $\nu$ to this plane as in Figs. 6, 7, 9 and 10.

When $n$ is odd, we fix the bond $b_{(n+3)/2}$ as in Figs. 6 and 9 and consider all of the polygonal lines consisting of the bonds $b_{(n+3)/2}, \ldots, b_3$. When $n$ is even, we fix the bond $b_{(n+4)/2}$ as in Figs. 7 and 10 and consider all of the polygonal lines consisting of the bonds $b_{(n+4)/2}, \ldots, b_3$. Let $\text{Arm}(\theta)$ denote such a non-closed polygonal line with the bond angle $\theta$.

Let $\delta_k$ denote the dihedral angle between the planes defined by bond pairs \{\(b_{k-1}, b_k\)\} and \{\(b_k, b_{k+1}\)\} respectively for $k = 4, 5, \ldots, \left[\frac{n+2}{2}\right]$, where $\left[\frac{x}{y}\right]$ denotes the largest integer less than or equal to $x$. Let $\text{pArm}(\theta)$ denote the non-closed polygonal line with the bond angle $\theta$ where all dihedral angles $\delta_k$ are 0. Note that $\text{pArm}(\theta)$ is planar. Observe that, when the bond angle between the bonds
\[ b_i + 1 \] is equal to \( y \), the vertex \( v_{i+1} \) is on the cone centered on \( b_i \) with the apex at \( v_i \) as in Fig. 8.

First, we consider the case where the bond angle \( y \) 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 \( p \text{Arm} \left( \frac{n-2}{n} \pi \right) \) 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 \( y < \frac{n-2}{n} \pi \). Then \( \text{Arm}(\theta) \) can intersect the plane \( P \). We take a sufficiently small \( \varepsilon > 0 \) with \( 1 - 2\varepsilon > 0 \). Then there exists \( \theta_{\varepsilon} \) 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 \( \text{Arm}(\theta_{\varepsilon}) \) is congruent to \( p \text{Arm}(\theta_{\varepsilon}) \) 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 \( \text{Arm}(\theta_{\varepsilon}) \) is congruent to \( p \text{Arm}(\theta_{\varepsilon}) \) as in Figs. 9 and 10. Hence, for any \( \text{Arm}(\theta) \), the distance from \( v_2 \) to \( P + v \) is greater than \( 1 - \varepsilon \) when \( \theta_{\varepsilon} < \theta < \frac{n-2}{n} \pi \).
Now we consider the non-closed polygonal line with the bond angle \( \theta \) 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 \( \phi \) forms a part of the boundary of a convex polygon, the distance along \( \nu \) 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 \( \theta \), the distance along \( \nu \) between \( v_1 \) and \( v_2 \) is greater than \( 1 - 2\varepsilon \) when \( \phi < \theta < \frac{n-2}{n} \pi \).

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

Case (a-1) \( \gamma > 0 \). We add the bond \( \beta_2 \) to \( \text{Arm}(\theta) \) at \( v_2 \) to form the local configuration in Fig. 1. We replace the two bonds \( \beta_2 \) and \( \beta_3 \) with a new bond which connects \( v_1 \) to \( v_3 \). Let \( \tilde{\beta}_{(2,3)} \) denote this new bond. As mentioned above, the distance from \( v_2 \) to \( P + \nu \) attains the minimum only when the resulting non-closed polygonal line with the bond \( \tilde{\beta}_{(2,3)} \) has a planar configuration where all dihedral angles are 0. Note that this planar configuration is obtained by adding \( \beta_2 \) to \( \text{pArm}(\theta) \) at \( v_2 \) as in Fig. 1.

When \( \theta = \frac{n-2}{n} \pi \), for \( \text{pArm}(\frac{n-2}{n} \pi) \) with the added bond \( \beta_2 \) as in Fig. 1, we have \( \langle \beta_2, \nu \rangle < 1 \) with some computations. Then the distance from \( v_1 \) to \( P + \nu \) is equal to \( 1 - \langle \beta_2, \nu \rangle \) (\( > 0 \)). We put \( \varepsilon = \frac{1}{4}(1 - \langle \beta_2, \nu \rangle) \). We see that a bond angle \( \theta_{\alpha_{\varepsilon}} \) can be chosen so that, for any \( \text{pArm}(\theta) \) with the added bond \( \beta_2 \) as in Fig. 1, \( \langle \beta_2, \nu \rangle \) is less than \( 1 - 3\varepsilon \) when \( \theta_{\alpha_{\varepsilon}} < \theta < \frac{n-2}{n} \pi \).

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 \( \beta_2 \) to the non-closed polygonal line at \( v_2 \) to form the local configuration in Fig. 1. We put \( \theta_{\alpha_{\varepsilon}} = \max\{\theta_{\alpha_{\varepsilon}}, \theta_{\varepsilon}\} \).
When $\theta_a < \theta < \frac{n-2}{n}\pi$, the distance from the vertex $v_1$ of $\beta_2$ to $P + (1 - \varepsilon) \cdot v$ is greater than $\varepsilon$ $(>0)$. Hence the polygonal line with the added bond $\beta_2$ 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 $\beta_2$ to $\text{Arm}(\theta)$ at $v_2$ to form the local configuration in Fig. 2. We replace the union of the two bonds $\beta_2$ and $\beta_3$ with a new bond which connects $v_1$ to $v_3$. Let $\tilde{\beta}_{(2,3)}$ 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 $\tilde{\beta}_{(2,3)}$ has a planar configuration where all dihedral angles are $0$. Note that this planar configuration is obtained by adding $\beta_2$ to $p\text{Arm}(\theta)$ at $v_2$ as in Fig. 2.

When $\theta = \frac{n-2}{n}\pi$, for $p\text{Arm}(\frac{n-2}{n}\pi)$ with the added bond $\beta_2$ as in Fig. 2, we have $\langle \beta_2, v \rangle < 0$ with some computations. Then the distance from $v_1$ to $P + v$ is greater than $1$. We see that a bond angle, $\theta_a'$, can be chosen so that, for any $p\text{Arm}(\theta)$ with the added bond $\beta_2$ as in Fig. 2, $\langle \beta_2, v \rangle < 0$ when $\theta_a' < \theta < \frac{n-2}{n}\pi$.

Now we consider the non-closed polygonal line which consists of bonds $\beta_3, \beta_4, \ldots, \beta_{n-1}, \beta_0, \beta_1$, add the bond $\beta_2$ to the non-closed polygonal line at $v_2$ to form the local configuration in Fig. 2. We put $\varepsilon = \frac{1}{n}$ and $\theta_a' = \max\{\theta_a', \theta_2\}$. When $\theta_a < \theta < \frac{n-2}{n}\pi$, the distance from the vertex $v_1$ of $\beta_2$ to $P + (1 - \varepsilon) \cdot v$ is greater than $\varepsilon$ $(>0)$. Hence the polygonal line with the added bond $\beta_2$ 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 $\beta_2$ to $\text{Arm}(\theta)$ at $v_2$ to form the local configuration in Fig. 3.

When $\theta = \frac{n-2}{n}\pi$, for $p\text{Arm}(\frac{n-2}{n}\pi)$ with the added bond $\beta_2$ as in Fig. 3, we have $\langle \beta_2, v \rangle < 1$ with some computations. Then the distance from $v_1$ to $P + v$ is equal to $1 - \langle \beta_2, v \rangle$ $(>0)$.

By an argument similar to the case $\gamma > 0$ of (a), we can take $\theta_{b_+}$ 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 $\beta_2$ to $\text{Arm}(\theta)$ at $v_2$ to form the local configuration in Fig. 4.

When $\theta = \frac{n-2}{n}\pi$, for $p\text{Arm}(\frac{n-2}{n}\pi)$ with the added bond $\beta_2$ as in Fig. 4, we have $\langle \beta_2, v \rangle < 0$ 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 $\theta_{b_-}$ so that any $n$-gon in $C_n$ does not have the local configuration as in Fig. 4 when $\theta_{b_-} < \theta < \frac{n-2}{n}\pi$. 
(c) We consider the non-closed polygonal line with the bond angle $\theta$ consisting of the bonds $\beta_3, \beta_4, \ldots, \beta_{n-1}, \beta_0, \beta_1$. 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 $\beta_k, \beta_{k+1}$ and $\beta_{k+2}$ having a planar local configuration as in Fig. 5. We replace the union of the two bonds $\beta_k$ and $\beta_{k+1}$ 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 $\beta_{k+2}$ 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 $\beta_k$ and $\beta_{k+1}$ 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 $\beta_k$ and $\beta_{k+1}$ with the bond $\bar{\beta}_{(k,k+1)}$. As mentioned above, when the non-closed polygonal line obtained by replacing the union of $\beta_k$ and $\beta_{k+1}$ 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 $\beta_k, \beta_{k+1}$ and $\beta_{k+2}$ 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 $\beta_k$ and $\beta_{k+1}$ with the bond $\bar{\beta}_{(k,k+1)}$ when the bond angle between $\beta_{k+2}$ 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 $\beta_{k+2}$ 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 $\beta_{k+2}$ and $\bar{\beta}_{(k,k+1)}$. 

![Fig. 11. A planar local configuration of the three successive bonds](image-url)
The distance between \(v_1\) and \(v_2\) is 1 when \(\theta = \frac{n-2}{n} \pi\) and the bond angle between \(\beta_{k+2}\) and \(\beta_{(k,k+1)}\) 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 \(\beta_{k+2}\) and \(\beta_{(k,k+1)}\) is equal to \(\frac{\pi + \theta}{2}\).

We can take \(\theta(k)\) so that, for any angle \(\theta\) 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 \(\beta_{k+2}\) and \(\beta_{(k,k+1)}\) 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 \(\theta_c\) 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 \(\beta_3\) 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 \(\theta\) 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 \(\theta_1 = \max \{\theta_{a_1}, \theta_{a_2}, \theta_{b_1}, \theta_{b_2}, \theta_c\}\), 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 \(\theta_0\) be the maximum of the angle \(\theta_1\) in Lemma 1 and the solutions of the following equations:

\[
\frac{\sin(mx)}{\sin x} = 1 - 2 \cos x \quad (1 \leq m \leq n - 6, \pi/2 < x < (n - 2)\pi/n).
\]

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

**Proof.** First, note that \(\theta_0\) can be determined from the Chebyshev polynomials of second kind \(\frac{\sin(mx)}{\sin x} = \sum_{j=0}^{[m/2]} (-1)^j mC_{2j+1}(\cos x)^{m-2j-1}(\cos^2 x - 1)^j\), where \([y]\) denotes the largest integer less than or equal to \(y\). We define \(F : (\mathbb{R}^3)^{n-3} \to \mathbb{R}^{2n-5}\) by \(F = (f_1, \ldots, f_{n-2}, g_1, \ldots, g_{n-3})\). Then \(C_n = F^{-1}(\{O\})\) for \(O = (0, \ldots, 0) \in \mathbb{R}^{2n-5}\).

We show that \(O \in \mathbb{R}^{2n-5}\) is a regular value of \(F\). It suffices to prove that gradient vectors \((\text{grad} f_1)_p, \ldots, (\text{grad} f_{n-2})_p, (\text{grad} g_1)_p, \ldots, (\text{grad} g_{n-3})_p\) are linearly independent for any \(p \in F^{-1}(\{O\}) = C_n\), where \((\text{grad} f)_p = \left(\frac{\partial f_j}{\partial x_j}(p)\right)\). It is convenient to decompose the gradient vectors of \(f_k\) and \(g_k\) into \(1 \times 3\) blocks as follows:
(\text{grad } f_1)_p = (\beta_1, 0, \ldots, 0),
\vdots
(\text{grad } f_k)_p = (0, \ldots, 0, -\beta_k, \beta_k, 0, \ldots, 0),
\vdots
(\text{grad } f_{n-2})_p = (0, \ldots, 0, -\beta_{n-2}),
(\text{grad } g_1)_p = (-\beta_0, 0, \ldots, 0),
\vdots
(\text{grad } g_k)_p = (0, \ldots, 0, \beta_{k+2}, \beta_{k+1} - \beta_{k+2}, -\beta_{k+1}, 0, \ldots, 0),
\vdots
(\text{grad } g_{n-4})_p = (0, \ldots, 0, \beta_{n-2}, \beta_{n-3} - \beta_{n-2}),
(\text{grad } g_{n-3})_p = (0, \ldots, 0, 0).

Here $0 = (0, 0, 0)$ and $\beta_k$ ($k = 0, \ldots, n-1$) denote the bond vectors of the $n$-gon corresponding to $p \in C_n$.

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

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

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 $\beta_2$ are linearly independent, we get $c_2 \neq 0$. The first $1 \times 3$ block of the linear combination (*) implies that the bond vectors $\beta_0$, $\beta_1$ and $\beta_2$ are contained in a single plane. The second $1 \times 3$ block of the linear combination (*) implies that the bond vectors $\beta_2$, $\beta_3$ and $\beta_4$ 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 $1 \times 3$ blocks of the linear combination (*) imply $c_{n+1} \neq 0$ by Lemma 1 (a). Then the bond vectors $\beta_3$, $\beta_4$ and $\beta_5$ are contained in a single plane.

We study $c_\ell$ ($n + 1 \leq \ell \leq k$). Assume that $c_\ell \neq 0$ ($n + 1 \leq \ell \leq k - 1$). Then the bond vectors $\beta_0, \beta_1, \ldots, \beta_{k-n+3}$ are contained in a single plane. Observe, by using Lemma 1 (c), the relation $\beta_\ell + \lambda \beta_{\ell+1} + \beta_{\ell+2} = 0$ ($\lambda = 2 \cos \theta$)
when \( \beta_i, \beta_{i+1}, \beta_{i+2} \) are contained in a single plane for \( i \neq 0,1,2 \). The third \( 1 \times 3 \) block of the linear combination (*) implies the equality \((c_3 + c_n)\beta_3 - (c_4 + c_n)\beta_4 + c_{n+1}\beta_5 = 0 \) with some computations.

Since \( \beta_3, \beta_4, \beta_5 \) are contained in a single plane, we have the following relations for the coefficients:

\[
c_{n+1} = c_3 + c_n, \quad (R_{n+1,1})
\]
\[
c_4 = -c_n - \lambda c_{n+1}. \quad (R_{n+1,2})
\]

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

\[
(-c_{j-2})\beta_{j-n+1} + (c_{j-n+2} + c_{j-1})\beta_{j-n+2} - (c_{j-n+3} + c_{j-1})\beta_{j-n+3} + c_j\beta_{j-n+4} = 0.
\]

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

\[
c_j = \lambda c_{j-2} + c_{j-1} + c_{j-n+2}, \quad (R_{j,1})
\]
\[
c_{j-n+3} = c_{j-2} - c_{j-1} - \lambda c_j. \quad (R_{j,2})
\]

We fix \( \ell \) 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 \((c_\ell - x_1 c_{\ell-1}) = x_2(c_{\ell-1} - x_1 c_{\ell-2}) + d\), where \( x_1 \) and \( x_2 \) denote the two solutions of \( x^2 + \lambda x + 1 = 0 \). Note that \( x_1 + x_2 = -\lambda \) and \( x_1 x_2 = 1 \). From these recurrence relations, we have the following two equalities:

\[
(c_k - x_1 c_{k-1}) = x_2^{k-1}(c_{n+1} - x_1 c_n) + d(x_2^{k-2} + x_2^{k-3} + \cdots + 1),
\]
\[
(c_k - x_2 c_{k-1}) = x_1^{k-1}(c_{n+1} - x_2 c_n) + d(x_1^{k-2} + x_1^{k-3} + \cdots + 1).
\]

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 \( Ac_2 + Bc_n = 0 \). Here, \( A = (x_2^{m+1} - x_1^{m+1}) + (x_2^m - x_1^m) + \cdots + (x_2 - x_1) \) and \( B = \{(x_2^{m+1} - x_1^{m+1}) + (x_2^{m-1} - x_1^{m-1}) + \cdots + (x_2 - x_1)\} + \lambda\{(x_2^{m} - x_1^{m}) + \cdots + (x_2 - x_1)\} \). 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 \( 1 \times 3 \) block of the linear combination (*) implies the equality \( c_2\beta_2 - c_3\beta_3 + c_4\beta_4 = 0 \). Since \( \lambda c_3 + c_n = 0 \), we have \( c_2\beta_2 = c_3(\beta_3 - \lambda \beta_4) \). Hence we obtain \( A = 0 \) from Lemma 1 (b). Note that \( (x_2^{m+1} - x_1^{m+1}) + (x_2^m - x_1^m) + \cdots + (x_2 - x_1) = \frac{1}{1 + \lambda}(x_2^{m+1} - x_1^{m+1}) + (x_2 - x_1) - (x_2^{m+2} - x_1^{m+2}) \). With some more computations, we have \( B = \frac{1}{1 + \lambda}\{-(x_2^m - x_1^m) + (1 + \lambda)(x_2 - x_1)\} \).

On the other hand, it is easy to check the following equality:
\[
\frac{x_2^m - x_1^m}{x_2 - x_1} = \frac{1}{2^{m-1}} \sum_{j=0}^{\lfloor (m-1)/2 \rfloor} mC_{2j+1}(-\lambda)^{m-2j-1}(\lambda^2 - 1)^j
\]

\[
= \sum_{j=0}^{\lfloor (m-1)/2 \rfloor} mC_{2j+1}(\cos \theta)^{m-2j-1}(\cos^2 \theta - 1)^j,
\]

where \( \lfloor y \rfloor \) denotes the largest integer less than or equal to \( y \). From the Chebyshev polynomials of second kind, we obtain \( \frac{x_2^m - x_1^m}{x_2 - x_1} = \frac{\sin(m\theta)}{\sin \theta} \). By the definition of \( \theta_0 \), 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 \( \text{grad } f_1 p, \ldots, \text{grad } f_{n-2} p, \text{grad } g_1 p, \ldots, \text{grad } g_{n-3} p \) 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 \( \theta \) which consists of the bonds \( \beta_2, \beta_4, \ldots, \beta_{n-1}, \beta_0, \beta_1 \). For \( k = 4, 5, \ldots, n - 1, 0 \), let \( \delta_k \) 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 \( \delta_4, \delta_5, \ldots, \delta_{n-1}, \delta_0 \). If the non-closed polygonal line is contained in the boundary of a convex polygon, that is, all dihedral angles \( \delta_k \) 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 \( \delta_k \) are \( \pi \), 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 \( \theta_0 \) be the angle in Proposition 1 and consider the configuration space \( C_n \) of \( n \)-gons having the bond angle \( \theta \) with \( \theta_0 < \theta < \frac{n-2}{n} \pi \). We define \( h : \mathbb{R} \times (\mathbb{R} - \{ 0 \})^2 \times (\mathbb{R}^3)^{n-4} \to \mathbb{R} \) by \( h(v_1, \ldots, v_{n-3}) = \sqrt{x_1^2 + x_2^2} \), 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 \( a_i \in \mathbb{R} \) such that \( (\text{grad } h)_p = \sum_{i=1}^{n-2} a_i (\text{grad } f_i)_p + \sum_{i=1}^{n-3} a_{i+n-2} (\text{grad } g_i)_p \) (cf. [10]). We can easily check that \( (\text{grad } h)_p = \left( 0, \frac{x_1^2}{\sin^2 \theta} - \frac{x_2 x_3}{\sin^3 \theta}, 0, \ldots, 0 \right) \). Note that the first \( 1 \times 3 \) block \( \left( 0, \frac{x_1^2}{\sin^2 \theta}, -\frac{x_2 x_3}{\sin^3 \theta} \right) \) is orthogonal to \( \beta_0 \) and \( \beta_1 \). So, we have
$a_2 \neq 0$ if $(\text{grad } h)_p = \sum_{i=1}^{n-2} a_i(\text{grad } f_i)_p + \sum_{i=1}^{n-3} a_{i+n-2}(\text{grad } g_i)_p$. 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 $v_i$ $(i = 1, \ldots, n-1)$ are contained in the plane $\text{Span} \langle \beta_2, \beta_3 \rangle = \text{Span} \langle \beta_2, \ldots, \beta_{n-1} \rangle$.

By forgetting the bond $\beta_2$ 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 $\theta$ form a planar local configuration as in Fig. 11 by Lemma 1 (c), the vertices $v_2, \ldots, v_{n-1}$ are uniquely determined. If three bonds $\beta_{n-1}, \beta_0$ and $\beta_1$ have a planar local configuration as in Fig. 11, the distance between $v_1$ and $v_2$ is less than 1. If three bonds $\beta_{n-1}, \beta_0$ and $\beta_1$ 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 $\beta_0$ and $\beta_1$ with a new bond which connects $v_{n-1}$ to $v_1$. Let $\beta(0,1)$ 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 $\beta_{n-1}$ and $\beta(0,1)$. When the distance between $v_1$ and $v_2$ is 1, the bond angle between $\beta_{n-1}$ and $\beta(0,1)$ 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 $\text{Span} \langle \beta_2, \beta_3 \rangle$. 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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