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The configuration space of a model for ringed hydrocarbon molecules

Dedicated to Professor Takao Matumoto on his sixtieth birthday

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Abstract. We give a mathematical model of n-membered ringed hydrocarbon molecules, and study the topology of a configuration space C_n of the model. Under the bond angle conditions required for ringed molecules, we prove that C_n is homeomorphic to $(n-4)$-dimensional sphere S^{n-4} when $n = 5, 6, 7$. This result gives an appropriate explanation of the configuration space of n-membered ringed hydrocarbon molecules when $n = 5, 6$.

1. Introduction

Due to [1], representative samples of 5- and 6-membered ringed hydrocarbon molecules were retrieved from the Cambridge Structural Database. By principal-component analysis, the configuration space of 5- or 6-membered ringed hydrocarbon molecules is regarded as the circle S^1 or the 2-dimensional sphere S^2, respectively. When $n \geq 7$, what shapes become configuration spaces havn't been specified.

As a mathematical model of n-membered ringed hydrocarbon molecules, we consider closed chains in $\mathbf{R}^3$ with rigidity ([3], [4], [8], [13]). In Mathematics, the study of configurations of closed chains has been considered from a topological, an algorithmic or a kinematic viewpoint. See, for example ([2], [5], [7], [9], [10], [11], [14], [16]).

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

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

DEFINITION 1. We define $f_k : (\mathbf{R}^3)^{n-3} \to \mathbf{R}$ by $f_k(v_1,\dots,v_{n-3}) = \frac{1}{2}(\|\beta_k\| - 1)$ for $k = 1,\dots,n-2$, and $g_k : (\mathbf{R}^3)^{n-3} \to \mathbf{R}$ by $g_1(v_1,\dots,v_{n-3}) = \langle -\beta_0, \beta_1\rangle - \cos\theta$, $g_k(v_1,\dots,v_{n-3}) = \langle -\beta_{k+1}, \beta_{k+2}\rangle - \cos\theta$ for $k = 2,\dots,n-3$, where $\langle\,,\rangle$ denotes the standard inner product in $\mathbf{R}^3$ and the standard norm $\|x\| = \sqrt{\langle x, x\rangle}$. We call θ a *bond angle*.

Then the configuration space C_n is defined by the following;

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

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

When $n = 5$, we assume that θ is equal to $\frac{7}{12}\pi$ that is the average of bond angles of 5-membered ringed hydrocarbon molecules. When $n = 6, 7$, we assume that θ is equal to tetrahedral angle $\cos^{-1}\left(-\frac{1}{3}\right)$ that is the standard bond angle of the carbon atom. Note that C_n is not the empty set. C_n actually includes the closed chains in Figs. 7, 8 and 9 of §3.

The above model gives an appropriate explanation of the result that the configuration space of n-membered ringed hydrocarbon molecules is regarded as the $(n-4)$-dimensional sphere when $n = 5, 6$. We obtain the following theorem:

THEOREM 1. *The configuration space C_n is homeomorphic to $(n-4)$-dimensional sphere S^{n-4} when $n = 5, 6, 7$.*

For $n \geq 8$, there exists some bond angle θ such that closed chains satisfy the properties mentioned in §2 if we choose a bond angle larger than the tetrahedral angle $\cos^{-1}(-1/3)$. Then there might be a possibility that it serve as a simulation model of the conformation of the molecule.

However, we are interested in the possibility of approximating larger macrocyclic molecules by smaller ones (e.g. $n = 5, 6, 7$) as we did in [3], [4] and [13].

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

In the following sections, we assume that $\theta = \frac{7}{12}\pi$ when $n = 5$ and that $\theta = \cos^{-1}\left(-\frac{1}{3}\right)$ when $n = 6, 7$.

2. Preliminaries

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

Lemma 1. *When $n = 5, 6, 7$, closed chains in the configuration space C_n satisfies the following properties* (1)–(3)*:*

(1) *Any closed chain in C_n does not have the local configurations of successive three bonds β_k, β_{k+1} and β_2 $(k = 0, 3)$ with the relation $\beta_k + \beta_{k+1} = \lambda\beta_2$ for any nonzero λ as in Figs.* 1, 2, 3 *and* 4.

(2) *Any closed chain in C_n does not have the local configurations of successive three bonds β_k, β_{k+1}, β_{k+2} with bond angles θ and the relation $\beta_k = \beta_{k+2}$ as in Fig.* 5*, where all indices are modulo n. In particular, the rotation around the axis β_k does not admit a full 2π-radian roll for $k \neq 1, 2, 3$.*

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

(3) *All vertices do not be on one plane for each closed chain in C_n.*

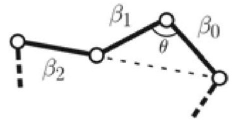

Fig. 1. (1) the forbidden local configuration for $k = 0$ and $\lambda > 0$

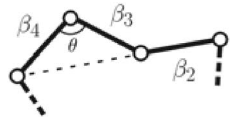

Fig. 2. (1) the forbidden local configuration for $k = 3$ and $\lambda > 0$

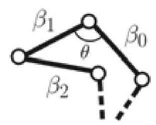

Fig. 3. (1) the forbidden local configuration for $k = 0$ and $\lambda < 0$

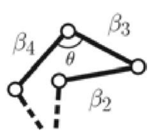

Fig. 4. (1) the forbidden local configuration for $k = 3$ and $\lambda < 0$

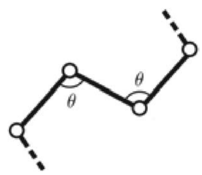

Fig. 5. (2) the forbidden local configuration $\beta_k = \beta_{k+2}$

Proof. (1) First, we give the proof in the case where $k = 0$ and $\lambda > 0$. By a similar argument we can treat the case where $k = 3$ and $\lambda > 0$. We consider a non-closed chain which consists of four bonds β_{n-1}, β_0, β_1 and β_2. Assume that a part of this chain forms the local configuration as in Fig. 1. Then, the distance between v_{n-2} and v_2 has the minimal value $\sqrt{1 + (1 - 2c)^2 + (1 - 2c)\sqrt{2 - 2c}}$ (> 2), where $c = \cos\theta$, for $n = 5$, and $\frac{1}{3}\sqrt{34 + 10\sqrt{6}}$ (> 2.54) for $n = 6, 7$.

For $n=5$, we do not get any closed chains in C_5 from the above non-closed chain by adding a bond β_3 even if we forget the restriction of the bond angle at v_3.

For $n=6$, we do not get any closed chains in C_6 from the above non-closed chain by adding two bonds β_3, β_4 since the distance between v_2 and v_4 is equal to $\frac{2\sqrt{6}}{3}$ (<2) by the restriction of the bond angle at v_3.

When a non-closed chain consists of three bonds with the length 1 and the bond angle θ, we see that the distance between the end-points has the maximal value $\frac{\sqrt{57}}{3}$ (<2.52). So, we do not get any closed chains in C_7 from the above non-closed chain by adding three bonds β_3, β_4, β_5.

Hence any closed chain in C_n $(n=5,6,7)$ does not have the local configurations as in Figs. 1 and 2.

Next, we give the proof in the case where $k=0$ and $\lambda<0$. By a similar argument we can treat the case where $k=3$ and $\lambda<0$.

For $n=5$, we consider a non-closed chain which consists of three bonds β_0, β_1, and β_2. Assume that this chain forms the local configuration as in Fig. 3. The distance between v_{n-1} and v_2 is equal to $\sqrt{2-2\cos\theta}-1$ for $n=5$. So, we do not get any closed chains in C_5 from the above non-closed chain by adding two bonds β_3, β_4 since the distance between v_2 and v_4 is equal to $\sqrt{2-2\cos\theta}$ by the restriction of the bond angle at v_3.

For $n=6,7$, we consider a non-closed chain which consists of four bonds β_{n-1}, β_0, β_1, and β_2. Assume that a part of this chain forms the local configuration as in Fig. 3. Then, the distance between v_{n-2} and v_2 has the maximal value $\frac{1}{3}\sqrt{66-18\sqrt{2}}$ (<1.6) for $n=6,7$.

For $n=6$, we do not get any closed chains in C_6 from the above non-closed chain by adding two bonds β_3, β_4 since the distance between v_2 and v_4 is equal to $\frac{2\sqrt{6}}{3}$ (>1.6) by the restriction of the bond angle at v_3.

When a non-closed chain consists of three bonds with the length 1 and the bond angle θ, we see that the distance between the end-points has the minimal value $\frac{5}{3}$ (>1.6). So, we do not get any closed chains in C_7 from the above non-closed chain by adding three bonds β_3, β_4, β_5.

Hence any closed chain in C_n $(n=5,6,7)$ does not have the local configurations as in Figs. 3 and 4.

(2) For $n=5$, we consider a non-closed chain which consists of three bonds β_{k-1}, β_k, and β_{k+1}. Assume that this chain forms the local configuration as in Fig. 5. The distance between v_{k-2} and v_{k+1} is equal to $\sqrt{5-4\cos\theta}$ (>2.4) for $n=5$. So, we do not get any closed chains in C_5 from the above non-closed chain by adding successive two bonds since the distance between the end-points is at most 2.

For $n=6,7$, we consider a non-closed chain which consists of five bonds

β_{k-2}, β_{k-1}, β_k, β_{k+1} and β_{k+2}. Assume that the part β_{k-1}, β_k, β_{k+1} of this chain forms the local configuration as in Fig. 5.

If the bond angles at v_{k-2} and v_{k+1} are θ, the distance between the end-points has the minimal value 3.

For $n = 6$, we do not get any closed chains in C_6 from the above non-closed chain by adding one bond with the length 1.

For $n = 7$, we do not get any closed chains in C_7 from the above non-closed chain by adding successive two bonds since the distance between v_{k-3} and v_{k+2} is at most 2.

If the bond angle at one of v_{k-2} and v_{k+1} isn't θ, we have the part of the non-closed chain, which consists of 4 bonds with the bond angles θ. Because the distance between the end-points in this part has the minimal value $\frac{8}{3}$, we see that the distance between v_{k-3} and v_{k+2} has the minimal value $\frac{5}{3}$ (> 1.66).

For $n = 6$, we do not get any closed chains in C_6 from the above non-closed chain by adding one bond with the length 1.

For $n = 7$, we do not get any closed chains in C_7 from the above non-closed chain by adding successive two bonds since the distance between the end-points is equal to $\frac{2\sqrt{6}}{3}$ (< 1.64) by the restriction of the included bond angle.

Hence any closed chain in C_n ($n = 5, 6, 7$) does not have the local configurations as in Fig. 5.

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

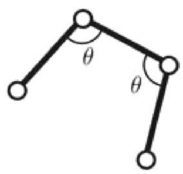

Fig. 6. the planar local configuration of the succcessive three bonds

Then we can explicitly calculate of the distance between v_1 and v_2 in the non-closed chain. When $n = 5$, the distance between v_1 and v_2 is equal to $-2\cos\theta\sqrt{2 - 2\cos\theta}$ (< 0.9). When $n = 6$, the distance between v_1 and v_2 is equal to $\frac{1}{9}$ (< 1). When $n = 7$, the distance between v_1 and v_2 is equal to $\frac{10\sqrt{6}}{27}$ (< 0.91).

Since the distance between v_1 and v_2 is shorter than 1, all vertices do not be on one plane for each closed chain in C_n. $\square$

By Lemma 1 we obtain the following proposition:

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

PROOF. 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 $C_n = F^{-1}(\{O\})$ for $O = (0, \dots, 0) \in \mathbf{R}^{2n-5}$.

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

$$
\begin{aligned}
(\text{grad}\, f_1)_p &= (\beta_1, 0, \dots\dots, 0),\\
&\ \vdots\\
(\text{grad}\, f_k)_p &= (0, \dots, 0, -\beta_k, \beta_k, 0, \dots, 0),\\
&\ \vdots\\
(\text{grad}\, f_{n-2})_p &= (0, \dots\dots, 0, -\beta_{n-2}),\\
(\text{grad}\, g_1)_p &= (-\beta_0, 0, \dots\dots, 0),\\
&\ \vdots\\
(\text{grad}\, g_k)_p &= (0, \dots, 0, \beta_{k+2}, \beta_{k+1} - \beta_{k+2}, -\beta_{k+1}, 0, \dots, 0),\\
&\ \vdots\\
(\text{grad}\, g_{n-4})_p &= (0, \dots, 0, \beta_{n-2}, \beta_{n-3} - \beta_{n-2}),\\
(\text{grad}\, g_{n-3})_p &= (0, \dots\dots, 0, \beta_{n-1}),
\end{aligned}
$$

where β_k denotes the bond vectors of the closed chain corresponding to $p \in C_n$, $0 = (0, 0, 0)$.

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

Now we will show that all vertices of the closed chain corresponding to p are on one plane by using Lemma 1 (1), (2) in what follows. Let $v_0, v_1, \dots, v_{n-1}$ denote the vertices of the closed chain corresponding to p. Since two successive bond vectors β_k, β_{k+1} are linearly independent for $k \neq 1, 2$, we get that $c_2 \neq 0$. Then the first 1×3 blocks of gradient vectors implies that the vertices v_0, v_1, v_2 and v_{n-1} are on one plane and the second 1×3 blocks of gradient vectors implies that the vertices v_1, v_2, v_3 and v_4 are on one plane.

When $n = 6, 7$, by Lemma 1 (1) the second and third 1×3 blocks of gradient vectors implies that $c_{n+1} \neq 0$. Then the vertices v_2, v_3, v_4 and v_5 are on one plane.

When $n = 7$, the vertices $v_1, v_2, \dots, v_5$ are on one plane by the above argument.

If $\beta_2 = \pm\beta_4$, then $\beta_k = -\beta_{k+2}$ by Lemma 1 (2) and the distance between v_1 and v_5 is equal to $\frac{2}{3}$. So, we do not get any closed chains in C_7 from the above non-closed chain by adding successive three bonds since the distance between the end-points has the minimal value $\frac{5}{3}$. Thus we see that $\beta_2 \neq \pm\beta_4$, and get that $c_3 \neq 0$. Due to the forbidden local configuration of Fig. 5 in Lemma 1 (2), We have the relation $3\beta_3 - 2\beta_4 + 3\beta_5 = 0$. By using $c_3 \neq 0$ and this relation, the third and fourth 1×3 blocks of gradient vectors implies that $c_9 \neq 0$. Then the vertices v_3, v_4, v_5 and v_6 are on one plane.

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

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

Remark 1. *For $n \geq 8$ and $\theta = \cos^{-1}\left(-\frac{1}{3}\right)$, some closed chains in C_n have forbidden local configurations of* Lemma 1 (1), (2). *So, we cannot apply the proof of Proposition* 1 *to the $n \geq 8$ cases.*

3. The proof of Theorem 1

We define $h : (\mathbf{R}^3)^{n-3} \to \mathbf{R}$ by $h(v_1, \dots, v_{n-3}) = \frac{x_2}{\sqrt{x_2^2 + x_3^2}}$, where $v_1 = (x_1, x_2, x_3)$. Due to [12, p. 25, Remark 1], [15, p. 380, Lemma 1] we have the extension of Reeb's theorem that M is homeomorphic to a sphere if M is a compact manifold and f is a differentiable function on M with only two critical points.

We show that $h|C_n$ is a differentiable function on C_n with only two critical points. Due to [6] for a function on a manifold embedded in Euclidean space, $p \in C_n$ is a critical point of $h|C_n$ for $h : (\mathbf{R}^3)^{n-3} \to \mathbf{R}$ if and only if there exist $a_i \in \mathbf{R}$ such that $(\mathrm{grad}\, h)_p = \sum_{i=1}^{n-2} a_i (\mathrm{grad}\, f_i)_p + \sum_{i=1}^{n-3} a_{i+n-2} (\mathrm{grad}\, g_i)_p$. We can easily check that $(\mathrm{grad}\, h)_p = \left(0, \frac{x_3^2}{\sin^3\theta}, -\frac{x_2 x_3}{\sin^3\theta}, 0, \dots, 0\right)$. Note that the first

1×3 block $\left(0, \frac{x_3^2}{\sin^3 \theta}, -\frac{x_2 x_3}{\sin^3 \theta}\right)$ is orthogonal to β_0 and β_1. So, we see that $a_2 \neq 0$ if $(\mathrm{grad}\, h)_p = \sum_{i=1}^{n-2} a_i (\mathrm{grad}\, f_i)_p + \sum_{i=1}^{n-3} a_{i+n-2} (\mathrm{grad}\, g_i)_p$. By the same argument as the proof of Proposition 1 in § 2, we obtain that the configuration of the closed chain corresponding to a critical point p satisfies that the vertices v_i $(i = 1, \dots, n-1)$ are on one plane $\mathrm{Span}\langle \beta_2, \beta_3 \rangle = \mathrm{Span}\langle \beta_2, \dots, \beta_{n-1} \rangle$.

We transform the closed chains by the congruent transformation that maps v_{n-1}, v_{n-2} and v_{n-3} to $(0,0,0)$, $(-1,0,0)$ and $(\cos\theta - 1, \sin\theta, 0)$ in this order, and we denote the image of v_k as w_k. This congruent transformation can be expressed by the composition of a translation and a rotation around z-axis and a rotation around x-axis. Because the vertices w_i $(i = 1, \dots, n-1)$ are in the xy-plane, it becomes easy to find the coordinates of the vertices w_i concretely.

$\underline{n = 5}$:

By the definition of w_i, we have the coordinates of vertices:

$$w_2 = (\cos\theta - 1, \sin\theta, 0),$$
$$w_3 = (-1, 0, 0),$$
$$w_4 = (0, 0, 0),$$

where $\cos\theta = \frac{-\sqrt{6}+\sqrt{2}}{4}$.

Since $w_1, \dots, w_4$ are in xy-plane, we put $w_1 = (a, b, 0)$. By the restriction of the bond length, we see that $\|w_2 - w_1\| = 1$. By the restriction of the bond angle at w_0, we see that $\|w_4 - w_1\| = \sqrt{2 - 2\cos\theta}$. Then $(x, y) = (a, b)$ is a solution of a pair of equations: $x^2 + y^2 = 2 - 2\cos\theta$, $(x + 1 - \cos\theta)^2 + (y - \sin\theta)^2 = 1$. Because of the existence of w_0, the coordinate of w_1 is uniquely determined as follows:

$$a = \frac{1}{4}\left(-3 + \sqrt{2} - \sqrt{6} + \sqrt{-7 - 8\sqrt{2} + 8\sqrt{3} + 4\sqrt{6}}\right),$$
$$b = (1 - \cos\theta)a + \frac{1}{2} - \cos\theta.$$

We put $w_0 = (x_1, x_2, x_3)$. By the restriction of the bond angle at w_4, we see that $x_1 = -\cos\theta$. Then $(y, z) = (x_2, x_3)$ is a solution of a pair of equations: $\cos^2\theta + y^2 + z^2 = 1$, $(a + \cos\theta)^2 + (b - y)^2 + z^2 = 1$. The coordinate of w_0 is determined as follows:

$$x_1 = -\cos\theta,$$
$$x_2 = (1 - \cos\theta + a\cos\theta)/b,$$
$$x_3 = \pm\sqrt{1 - x_1^2 - x_2^2}.$$

$\underline{n = 6}$:

Since $w_1, \dots, w_5$ are in xy-plane, we can calculate the coordinate of w_2 concretely by the restriction of the bond angle at w_3. Note that $\cos\theta = -1/3$. We have the coordinates of vertices:

$$\begin{aligned} w_2 &= (-5/9, 10\sqrt{2}/9, 0), \\ w_3 &= (\cos\theta - 1, \sin\theta, 0) = (-4/3, 2\sqrt{2}/3, 0), \\ w_4 &= (-1, 0, 0), \\ w_5 &= (0, 0, 0). \end{aligned}$$

Since $w_1, \dots, w_5$ are in xy-plane, we put $w_1 = (a, b, 0)$. By the restriction of the bond length, we see that $\|w_2 - w_1\| = 1$. By the restriction of the bond angle at w_0, we see that $\|w_5 - w_1\| = \sqrt{2 - 2\cos\theta}$. Then $(x, y) = (a, b)$ is a solution of a pair of equations: $x^2 + y^2 = 2 - 2\cos\theta$, $(x + 5/9)^2 + (y - 10\sqrt{2}/9)^2 = 1$. Because of the existence of w_0, the coordinate of w_1 is uniquely determined as follows:

$$a = \frac{4}{9}, \quad b = \frac{10\sqrt{2}}{9}.$$

We put $w_0 = (x_1, x_2, x_3)$. By the restriction of the bond angle at w_5, we see that $x_1 = -\cos\theta$. Then $(y, z) = (x_2, x_3)$ is a solution of a pair of equations: $\cos^2\theta + y^2 + z^2 = 1$, $(a + \cos\theta)^2 + (b - y)^2 + z^2 = 1$. The coordinate of w_0 is determined as follows:

$$\begin{aligned} x_1 &= -\cos\theta = \frac{1}{3}, \\ x_2 &= (1 - \cos\theta + a\cos\theta)/b = \frac{8\sqrt{2}}{15}, \\ x_3 &= \pm\sqrt{1 - x_1^2 - x_2^2} = \frac{2\sqrt{2}}{5}. \end{aligned}$$

For $n = 6$ the vertex w_1 have comparatively simple coordinates.

$\underline{n = 7}$:

Since $w_1, \dots, w_6$ are in xy-plane, we can calculate the coordinate of w_2, w_3 concretely by the restriction of the bond angle at w_3, w_4. Note that $\cos\theta = -1/3$. We have the coordinates of vertices:

$$\begin{aligned} w_2 &= (8/27, 20\sqrt{2}/27, 0), \\ w_3 &= (-5/9, 10\sqrt{2}/9, 0), \end{aligned}$$

$$w_4 = (\cos\theta - 1, \sin\theta, 0) = (-4/3, 2\sqrt{2}/3, 0),$$

$$w_5 = (-1, 0, 0),$$

$$w_6 = (0, 0, 0).$$

Since $w_1, \dots, w_6$ are in xy-plane, we put $w_1 = (a, b, 0)$. By the restriction of the bond length, we see that $\|w_2 - w_1\| = 1$. By the restriction of the bond angle at w_0, we see that $\|w_6 - w_1\| = \sqrt{2 - 2\cos\theta}$. Then $(x, y) = (a, b)$ is a solution of a pair of equations: $x^2 + y^2 = 2 - 2\cos\theta$, $(x - 8/27)^2 + (y - 20\sqrt{2}/27)^2 = 1$. Because of the existence of w_0, the coordinate of w_1 is uniquely determined as follows:

$$a = \frac{1}{432}(154 + 5\sqrt{6574}), \quad b = \frac{1}{432}(385\sqrt{2} - 2\sqrt{3287}).$$

We put $w_0 = (x_1, x_2, x_3)$. By the restriction of the bond angle at w_6, we see that $x_1 = -\cos\theta$. Then $(y, z) = (x_2, x_3)$ is a solution of a pair of equations: $\cos^2\theta + y^2 + z^2 = 1$, $(a + \cos\theta)^2 + (b - y)^2 + z^2 = 1$. The coordinate of w_0 is determined as follows:

$$x_1 = \frac{1}{3},$$

$$x_2 = (1 - \cos\theta + a\cos\theta)/b = (-a + 4)/3b,$$

$$x_3 = \pm\sqrt{1 - x_1^2 - x_2^2}.$$

Thus the vertices $v_1, v_2, \dots, v_{n-1}$ are uniquely determined and just two positions of the vertex v_0 are determined for original closed chains with vertices $\{v_0, v_1, \dots, v_{n-1}\}$. Then we have just two configurations of closed chains corresponding to the critical points. These two are mirror symmetric with respect to the plane $\mathrm{Span}\langle\beta_2, \beta_3\rangle$. Hence we obtain that $h|C_n$ has only two critical points. See Figs. 7, 8, and 9 for the critical configurations. We note that when $n = 6$, configurations of closed chains corresponding to critical points have reflection symmetry in the plane, through v_0 and v_3, perpendicular to $\mathrm{Span}\langle\beta_2, \beta_3\rangle$ as in Fig. 8.

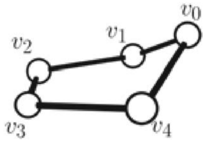

Fig. 7. $n = 5$

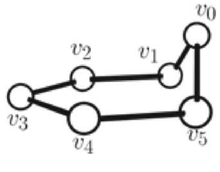

Fig. 8. $n = 6$

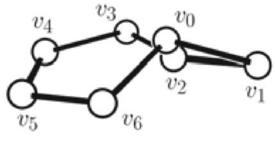

Fig. 9. $n = 7$

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