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THE SQUARED CHAIN LENGTH FUNCTION OF 5 OR 6-MEMBERED STRAIGHT-CHAINS WITH THE TETRAHEDRAL BOND ANGLE

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ABSTRACT. We provide straight-chains with the tetrahedral bond angle $\cos^{-1}(-1/3)$ as a mathematical model of n-membered straight-chain hydrocarbon molecules. We study the squared chain length function on the configuration space of the model and determine the critical points with planar configurations when $n = 5, 6$.

1. Introduction

A *straight chain* with n vertices is defined to be a graph in $\mathbf{R}^3$ with vertices $\{v_0, v_1, \dots, v_{n-1}\}$ and bonds $\{\beta_1, \beta_2, \dots, \beta_{n-1}\}$, where β_i connects v_{i-1} with v_i ($i = 1, 2, \dots, n-1$). A *bond angle* is defined to be the angle between two adjacent bonds of a straight chain. In the following, we assume that bond angles are the tetrahedral angle $\cos^{-1}(-\frac{1}{3})$, which is the standard bond angle of the saturated carbon atom. The *chain length* of a straight chain with n vertices $\{v_0, v_1, \dots, v_{n-1}\}$ is defined to be the distance between v_0 and v_{n-1}. For simplicity, $\boldsymbol{\beta}_i$ denotes the *bond vector* $v_i - v_{i-1}$, where $i = 1, 2, \dots, n-1$.

We consider straight chains in $\mathbf{R}^3$ with rigidity as a mathematical model of straight-chain hydrocarbon molecules.

Definition 1.1. We fix $\theta = \cos^{-1}(-1/3)$ and put three vertices $v_0 = (0,0,0)$, $v_1 = (\sqrt{2/3}, -\sqrt{1/3}, 0)$, $v_2 = (2\sqrt{2/3}, 0, 0)$.

We define functions $f_k : (\mathbf{R}^3)^{n-3} \to \mathbf{R}$ by $f_k(v_3, v_4, \dots, v_{n-1}) = \frac{1}{2}(\|\boldsymbol{\beta}_k\|^2 - 1)$ for $k = 3, 4, \cdots, n-1$, and $g_k : (\mathbf{R}^3)^{n-3} \to \mathbf{R}$ by $g_k(v_3, v_4, \dots, v_{n-1}) = \langle -\boldsymbol{\beta}_k, \boldsymbol{\beta}_{k+1} \rangle - \cos\theta$ for $k = 2, 3, \cdots, n-2$, where $\langle\ ,\ \rangle$ denotes the standard inner product in $\mathbf{R}^3$ and $\|\cdot\|$ the standard norm $\|\boldsymbol{x}\| = \sqrt{\langle \boldsymbol{x}, \boldsymbol{x} \rangle}$. Then we define the *configuration space*

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$M(n)$ of straight chains with rigidity by the following:

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

f_i and g_j are called *rigidity maps*, which determine the bond lengths and angles of any chain in $M(n)$. So, a straight chain in $M(n)$ is an equilateral and equiangular straight chain with n vertices and the bond angles θ and bond lengths 1. The dihedral angle for three bond vectors $\boldsymbol{\beta}_k, \boldsymbol{\beta}_{k+1}$ and $\boldsymbol{\beta}_{k+2}$ is the angle between two planes that consist of the plane spanned by the two vectors $\boldsymbol{\beta}_k$ and $\boldsymbol{\beta}_{k+1}$ and the plane spanned by the two vectors $\boldsymbol{\beta}_{k+1}$ and $\boldsymbol{\beta}_{k+2}$. Because the straight chains in $M(n)$ are parametrized by dihedral angles with the angular range of 2π, we see that $M(n)$ is $(n-3)$-dimensional torus T^{n-3}. We define the function $h : (\mathbf{R}^3)^{n-3} \to \mathbf{R}$ by $h(v_3, v_4, \ldots, v_{n-1}) = \|v_0 - v_{n-1}\|^2$, and call the restriction $h|M(n)$ the squared chain length function on $M(n)$. For convenience, we put a virtual bond $\boldsymbol{\beta}_n = v_0 - v_{n-1}$ without the bond angle restriction. Then, we have $h(v_3, \ldots, v_{n-1}) = \|\boldsymbol{\beta}_n\|^2$.

In [3], we determine the topological types of fibers of the configuration space by chain lengths when $n = 5$. In [1] and [2], we prove that $(h|M(n))^{-1}(1)$ is diffeomorphic to $(n-4)$-dimensional sphere S^{n-4} when $n = 5, 6, 7$. We regard $(h|M(n))^{-1}(1)$ as the configuration space of the model of n-membered ringed hydrocarbon molecules.

If the successive three bonds of a straight chain in $M(n)$ are in one plane, these form a planar local configuration in Fig. 1 or 2. Let $c(k)$ denote a planar local configuration in Fig. 1 of the successive three bonds $\boldsymbol{\beta}_k, \boldsymbol{\beta}_{k+1}, \boldsymbol{\beta}_{k+2}$ and $z(k)$ denote a planar local configuration in Fig. 2 of the successive three bonds $\boldsymbol{\beta}_k, \boldsymbol{\beta}_{k+1}, \boldsymbol{\beta}_{k+2}$.

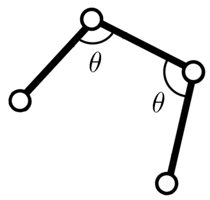

FIG. 1. a planar local configuration $c(k)$

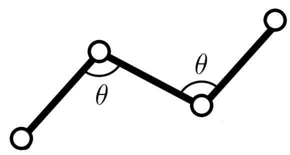

FIG. 2. a planar local configuration $z(k)$

To detect the change in chain length, we study the squared chain length function on the configuration space and determine the critical points corresponding to chains which have planar configurations.

Theorem 1.1. *When $n = 5$, the critical values of the squared chain length function $h|M(n)$ are $\frac{32}{27}$, $\frac{64}{9}$ and $\frac{32}{3}$. All critical points have planar configurations. The critical points corresponding to chains which have planar configurations is given by the following:*

(1) *If a critical value is $\frac{32}{27}$, then a critical point is non-degenerate and has an index 0 and a chain corresponding to the critical point has a planar configuration with $c(1)$, $c(2)$.*
(2) *If a critical value is $\frac{64}{9}$, then two critical points are non-degenerate and have an index 1 and chains corresponding to two critical points have planar configurations with $c(1)$, $z(2)$ and with $z(1)$, $c(2)$.*
(3) *If a critical value is $\frac{32}{3}$, then a critical point is degenerate and a chain corresponding to the critical point has a planar configuration with $z(1)$, $z(2)$.*

Note that Theorem 1.1 explains the result of [3] from a Morse theoretic viewpoint.

Theorem 1.2. *When $n = 6$, the critical values of the squared chain length function $h|M(n)$ are $\frac{1}{81}$, $\frac{107}{27}$, $\frac{89}{3}$, $\frac{275}{27}$, $\frac{49+20\sqrt{6}}{9}$, $\frac{121}{9}$ and 17. The critical points with the critical values except for $\frac{49+20\sqrt{6}}{9}$ have planar configurations. The critical points corresponding to chains which have planar configurations is given by the following:*

(1) *If a critical value is $\frac{1}{81}$, then a critical point is non-degenerate and has an index 0 and a chain corresponding to the critical point has a planar configuration with $c(1)$, $c(2)$, $c(3)$.*
(2) *If a critical value is $\frac{107}{27}$, then two critical points are non-degenerate and have an index 1 and chains corresponding to two critical points have planar configurations with $c(1)$, $c(2)$, $z(3)$ and with $z(1)$, $c(2)$, $c(3)$.*
(3) *If a critical value is $\frac{89}{3}$, then two critical points are non-degenerate and have an index 1 and chains corresponding to two critical points have planar configurations with $c(1)$, $z(2)$, $z(3)$ and with $c(1)$, $z(2)$, $c(3)$.*
(4) *If a critical value is $\frac{275}{27}$, then a critical point is non-degenerate and has an index 1 and a chain corresponding to the critical point has a planar configuration with $z(1)$, $z(2)$, $c(3)$.*
(5) *If a critical value is $\frac{121}{9}$, then a critical point is non-degenerate and has an index 2 and a chain corresponding to the critical point has a planar configuration with $z(1)$, $c(2)$, $z(3)$.*
(6) *If a critical value is 17, then a critical point is non-degenerate and has an index 3 and a chain corresponding to the critical point has a planar configuration with $z(1)$, $z(2)$, $z(3)$.*

Note that by Theorems 1.1 and 1.2, all planar configurations appear in the critical points when $n = 5, 6$.

In Theorem 1.2, note that chains corresponding to two critical points have non-planar configurations with $c(3)$ as in Fig. 3 and its mirror image with respect to xy-plane when a critical value is $\frac{49+20\sqrt{6}}{9}$.

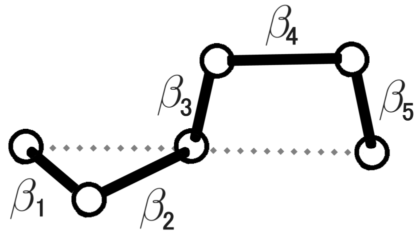

FIG. 3. a non-planar configuration with $c(3)$

2. The proofs of Theorems 1.1 and 1.2

Proof of Theorem 1.1. Due to [4] for a function on a manifold embedded in Euclidean space, $p \in M(n)$ is a critical point of $h|M(n)$ for $h : (\mathbf{R}^3)^{n-3} \to \mathbf{R}$ if and only if $(\text{grad } h)_p = \sum_{i=3}^{n-1} a_i(\text{grad } f_i)_p + \sum_{j=2}^{n-2} b_j(\text{grad } g_j)_p$ for some nonzero a_i, where $(\text{grad } f)_p = \left(\frac{\partial f}{\partial x_k}(p)\right)_k$. It is convenient to decompose gradient vectors of f_i, g_j and h into 1×3 blocks. We have the following forms:

$$\begin{aligned}
(\text{grad } f_3)_p &= (\boldsymbol{\beta}_3, \mathbf{0}),\\
(\text{grad } f_4)_p &= (-\boldsymbol{\beta}_4, \boldsymbol{\beta}_4),\\
(\text{grad } g_2)_p &= (-\boldsymbol{\beta}_2, \mathbf{0}),\\
(\text{grad } g_3)_p &= (\boldsymbol{\beta}_3 - \boldsymbol{\beta}_4, -\boldsymbol{\beta}_3),\\
(\text{grad } h)_p &= (\mathbf{0}, -2\boldsymbol{\beta}_5),
\end{aligned}$$

where $\boldsymbol{\beta}_k$ denotes bond vectors of the closed chain corresponding to $p \in M(5)$, $\mathbf{0} = (0,0,0)$.

We assume that $p \in M(n)$ is a critical point of $h|M(n)$. So, $(\text{grad } h)_p = \sum_{i=3}^{n-1} a_i(\text{grad } f_i)_p + \sum_{j=2}^{n-2} b_j(\text{grad } g_j)_p$ for some nonzero a_i, b_j. The first 1×3 blocks of gradient vectors implies the equation $(-b_2)\boldsymbol{\beta}_2 + (a_3+b_3)\boldsymbol{\beta}_3 + (-a_4-b_3)\boldsymbol{\beta}_4 = 0$. The second 1×3 blocks of gradient vectors implies the equation $-b_3\boldsymbol{\beta}_3 + a_4\boldsymbol{\beta}_4 = -2\boldsymbol{\beta}_5$. Then, we have the following case (a) or (b) for the configuration corresponding to the critical point $p \in M(5)$ of $h|M(5)$:

(a) $\boldsymbol{\beta}_1, \boldsymbol{\beta}_2, \ldots, \boldsymbol{\beta}_5$ are in one plane,

(b) $\boldsymbol{\beta}_3, \ldots, \boldsymbol{\beta}_5$ are in one plane and $b_2 = 0$, $a_3 = a_4 = -b_3$.

In the case (b), we have the relation $\boldsymbol{\beta}_5 = \frac{b_3}{2}(\boldsymbol{\beta}_3 + \boldsymbol{\beta}_4)$. With some computations, we obtain that the chain has a planar configuration with $z(1)$, $z(2)$.

Now, we check up all the planar configurations of chains.

If a chain has a planar configuration with $c(1)$, $c(2)$ (Theorem 1.1 (1)), we have the relation $\boldsymbol{\beta}_5 = -\frac{10}{9}\boldsymbol{\beta}_3 + \frac{2}{3}\boldsymbol{\beta}_4$. Then, a squared chain length is $\frac{32}{27}$ and we see that $b_3 = -\frac{20}{9}$ and $a_4 = -\frac{4}{3}$.

If a chain has a planar configuration with $c(1)$, $z(2)$ (Theorem 1.1 (2)), we have the relation $\boldsymbol{\beta}_5 = -\frac{8}{3}\boldsymbol{\beta}_4$. Then, a squared chain length is $\frac{64}{9}$ and we see that $b_3 = 0$ and $a_4 = \frac{16}{3}$.

If a chain has a planar configuration with $z(1)$, $c(2)$ (Theorem 1.1 (2)), we have the relation $\boldsymbol{\beta}_5 = -\frac{8}{3}\boldsymbol{\beta}_3$. Then, a squared chain length is $\frac{64}{9}$ and we see that $b_3 = -\frac{16}{3}$ and $a_4 = 0$.

If a chain has a planar configuration with $z(1)$, $z(2)$ (Theorem 1.1 (3)), we have the relation $\boldsymbol{\beta}_5 = -2\boldsymbol{\beta}_3 - 2\boldsymbol{\beta}_4$. Then, a squared chain length is $\frac{32}{3}$ and we see that $b_3 = -4$ and $a_4 = 4$.

Note that we have the relation $3\boldsymbol{\beta}_k - 2\boldsymbol{\beta}_{k+1} + 3\boldsymbol{\beta}_{k+2} = 0$ for a planar local configuration $c(k)$ (Fig. 1) and $\boldsymbol{\beta}_k = \boldsymbol{\beta}_{k+2}$ for a planar local configuration $z(k)$ (Fig. 2). When a chain has a planar configuration, we can calculate a_3, b_2 concretely from the relation of the first 1×3 blocks. Then, we can see that $(\mathrm{grad}\ h)_p = \sum_{i=3}^{4} a_i(\mathrm{grad}\ f_i)_p + \sum_{j=2}^{3} b_j(\mathrm{grad}\ g_j)_p$ for some nonzero a_i, b_j.

For a critical point $p \in M(n)$ of $h|M(n)$, we define a matrix $H_p = P(H(h)_p - \sum_{i=3}^{n-1} a_i H(f_i)_p - \sum_{i=2}^{n-2} b_i H(g_i)_p)P$, where $P : (\mathbf{R}^3)^{n-3} \to T_p(M(n))$ is the orthogonal projection and $H(f)_p$ denotes the Hessian matrix $\left(\frac{\partial^2 f}{\partial x_i \partial x_j}(p)\right)_{i,j}$ of f at p. Due to [4], a critical point p is non-degenerate if and only if rank $H_p = n-3$, and for a non-degenerate critical point, its index is equal to the number of negative eigenvalues of H_p.

It is convenient to decompose the Hessian matrices of f_k, g_j and h into 3×3 blocks. We can easily check the following:

$$H(f_3)_p = \left(\begin{array}{c|c} I & O \\ \hline O & O \end{array}\right), H(f_4)_p = \left(\begin{array}{c|c} I & -I \\ \hline -I & I \end{array}\right),$$

$$H(g_2)_p = \left(\begin{array}{c|c} O & O \\ \hline O & O \end{array}\right), H(g_3)_p = \left(\begin{array}{c|c} 2I & -I \\ \hline -I & O \end{array}\right),$$

$$H(h)_p = \left(\begin{array}{c|c} O & O \\ \hline O & 2I \end{array}\right),$$

where I denotes 3×3 unit matrix and O denotes 3×3 zero matrix.

The tangent space $T_p(M(5))$ of $M(5)$ at p is equal to the orthogonal complement $\{\mathrm{Span}\,\langle(\mathrm{grad}\ f_i)_p,(\mathrm{grad}\ g_j)_p\rangle\}^{\perp}$ of $\mathrm{Span}\,\langle(\mathrm{grad}\ f_i)_p,(\mathrm{grad}\ g_j)_p\rangle$, where $\mathrm{Span}\,\langle(\mathrm{grad}\ f_i)_p,(\mathrm{grad}\ g_j)_p\rangle$ denotes the linear subspace of $(\mathbf{R}^3)^{n-3}$ spanned by $(\mathrm{grad}\ f_i)_p$, $(\mathrm{grad}\ g_j)_p$. We put $W=\mathrm{Span}\,\langle\boldsymbol{\beta}_1,\dots,\boldsymbol{\beta}_5\rangle^{\perp}$. We have that $T_p(M(5))\supseteq W\oplus W$. Because $\mathrm{Span}\,\langle\boldsymbol{\beta}_1,\dots,\boldsymbol{\beta}_5\rangle$ is xy-space, we have that $\dim(W\oplus W)=2$. Because the gradient vectors $(\mathrm{grad}\ f_3)_p$, $(\mathrm{grad}\ f_4)_p$, $(\mathrm{grad}\ g_2)_p$, $(\mathrm{grad}\ g_3)_p$ are linearly independent, we see that $\dim T_p(M(5))=2$. So, we obtain the decomposition $T_p(M(5))=W\oplus W\subset(\mathbf{R}^3)^2$.

Let $A=\begin{pmatrix}0&0&0\\0&0&0\\0&0&1\end{pmatrix}$ be the matrix of the orthogonal projection from $\mathbf{R}^3$ to $W\subset\mathbf{R}^3$ the orthogonal complement. Then, we have the matrix of the orthogonal projection P relative to the standard basis as the following:

$$P=\begin{pmatrix}A&O\\O&A\end{pmatrix}.$$

Thus we have the following form of matrix H_p relative to the standard basis:

$$H_p=\left(\begin{array}{c|c}-(a_3+a_4+2b_3)A&(a_4+b_3)A\\\hline(a_4+b_3)A&(2-a_4)A\end{array}\right).$$

Since A has the above form, by basic matrix operations we can obtain the following matrices with the same rank and the same number of negative eigenvalues as H_p:

$$\begin{pmatrix}-(a_3+a_4+2b_3)&a_4+b_3\\a_4+b_3&2-a_4\end{pmatrix}.$$

We can calculate the rank and the number of negative eigenvalues concretely by substituting the calculated values of a_i,b_j, and we obtain the result of Theorem 1.1. $\square$

Proof of Theorem 1.2. We prove Theorem 1.2 by the similar argument in the proof Theorem 1.1. It is convenient to decompose gradient vectors of f_i, g_j and h into 1×3 blocks. We have the following forms:

$$\begin{aligned}(\mathrm{grad}\ f_3)_p&=(\boldsymbol{\beta}_3,\mathbf{0},\mathbf{0}),\\(\mathrm{grad}\ f_4)_p&=(-\boldsymbol{\beta}_4,\boldsymbol{\beta}_4,\mathbf{0}),\\(\mathrm{grad}\ f_5)_p&=(\mathbf{0},-\boldsymbol{\beta}_5,\boldsymbol{\beta}_5),\\(\mathrm{grad}\ g_2)_p&=(-\boldsymbol{\beta}_2,\mathbf{0},\mathbf{0}),\\(\mathrm{grad}\ g_3)_p&=(\boldsymbol{\beta}_3-\boldsymbol{\beta}_4,-\boldsymbol{\beta}_3,\mathbf{0}),\\(\mathrm{grad}\ g_4)_p&=(\boldsymbol{\beta}_5,\boldsymbol{\beta}_4-\boldsymbol{\beta}_5,-\boldsymbol{\beta}_4),\\(\mathrm{grad}\ h)_p&=(\mathbf{0},\mathbf{0},-2\boldsymbol{\beta}_6),\end{aligned}$$

where $\boldsymbol{\beta}_k$ denotes bond vectors of the closed chain corresponding to $p \in M(6)$, $\mathbf{0} = (0,0,0)$.

We assume that $p \in M(6)$ is a critical point of $h|M(6)$. Then, $(\text{grad } h)_p = \sum_{i=3}^{5} a_i (\text{grad } f_i)_p + \sum_{j=2}^{4} b_j (\text{grad } g_j)_p$ for some nonzero a_i, b_j. The first 1×3 blocks of gradient vectors implies the equation $(-b_2)\boldsymbol{\beta}_2 + (a_3+b_3)\boldsymbol{\beta}_3 + (-a_4-b_3)\boldsymbol{\beta}_4 + b_4\boldsymbol{\beta}_5 = 0$. The second 1×3 blocks of gradient vectors implies the equation $(-b_3)\boldsymbol{\beta}_3 + (a_4 + b_4)\boldsymbol{\beta}_4 + (-a_5 - b_4)\boldsymbol{\beta}_5 = 0$. The third 1×3 blocks of gradient vectors implies the equation $-b_4\boldsymbol{\beta}_4 + a_5\boldsymbol{\beta}_5 = -2\boldsymbol{\beta}_6$. Hence, we have the following three cases (a), (b) and (c) for the configuration corresponding to the critical point $p \in M(6)$ of $h|M(6)$:

(a) $\boldsymbol{\beta}_1, \boldsymbol{\beta}_2, \ldots, \boldsymbol{\beta}_6$ are in one plane,

(b) $\boldsymbol{\beta}_4, \ldots, \boldsymbol{\beta}_6$ are in one plane and $b_3 = 0$, $a_4 = a_5 = -b_4$,

(c) $\boldsymbol{\beta}_3, \boldsymbol{\beta}_4, \ldots, \boldsymbol{\beta}_6$ are in one plane and $b_2 = 0$.

In the case (b), we have the relation $\boldsymbol{\beta}_6 = \frac{b_4}{2}(\boldsymbol{\beta}_4 + \boldsymbol{\beta}_5)$, and we see that $\boldsymbol{\beta}_4 + \boldsymbol{\beta}_5$, $\boldsymbol{\beta}_2$ and $\boldsymbol{\beta}_3$ are in one plane from the relation of the first 1×3 blocks. With some computations, we obtain that there exsits no such a chain.

Note that we have the relation $3\boldsymbol{\beta}_k - 2\boldsymbol{\beta}_{k+1} + 3\boldsymbol{\beta}_{k+2} = 0$ for a planar local configuration $c(k)$ (Fig. 1) and $\boldsymbol{\beta}_k = \boldsymbol{\beta}_{k+2}$ for a planar local configuration $z(k)$ (Fig. 2).

If a chain has a local configuration $c(3)$ in the case (c), we get the relation $a_5 = 0$ from the relation of the first and second 1×3 blocks. So, we have the relation $\boldsymbol{\beta}_6 = \frac{b_4}{2}\boldsymbol{\beta}_4$. With some computations, we obtain that the chains have non-planar configurations as in Fig. 3 and its mirror image with respect to xy-plane with squared chain length $\frac{49+20\sqrt{6}}{9}$.

If a chain has a local configuration $z(3)$ in the case (c), we get the relation $a_5 = -2b_4$ from the relation of the first and second 1×3 blocks. So, we have the relation $\boldsymbol{\beta}_6 = b_4(\frac{1}{2}\boldsymbol{\beta}_4 + \boldsymbol{\beta}_5)$. With some computations, we obtain that there exists no such a chain.

Now, we check up all the planar configurations of chains.

If a chain has a planar configuration with $c(1)$, $c(2)$,$c(3)$ (Theorem 1.2 (1)), we have the relation $\boldsymbol{\beta}_6 = -\frac{2}{27}\boldsymbol{\beta}_4 + \frac{3}{27}\boldsymbol{\beta}_5$. Then, a squared chain length is $\frac{1}{81}$ and we see that $b_4 = -\frac{4}{27}$ and $a_5 = -\frac{6}{27}$.

If a chain has a planar configuration with $c(1)$, $c(2)$, $z(3)$ (Theorem 1.2 (2)), we have the relation $\boldsymbol{\beta}_6 = \frac{2}{3}\boldsymbol{\beta}_4 - \frac{19}{9}\boldsymbol{\beta}_5$. Then, a squared chain length is $\frac{107}{27}$ and we see that $b_4 = \frac{4}{3}$ and $a_5 = \frac{38}{9}$.

If a chain has a planar configuration with $z(1)$, $c(2)$, $c(3)$ (Theorem 1.2 (2)), we have the relation $\boldsymbol{\beta}_6 = -\frac{16}{9}\boldsymbol{\beta}_4 + \frac{5}{3}\boldsymbol{\beta}_5$. Then, a squared chain length is $\frac{107}{27}$ and we see that $b_4 = -\frac{32}{9}$ and $a_5 = -\frac{10}{3}$.

If a chain has a planar configuration with $c(1)$, $z(2)$, $z(3)$ (Theorem 1.2 (3)), we have the relation $\boldsymbol{\beta}_6 = -\frac{8}{3}\boldsymbol{\beta}_4 - \boldsymbol{\beta}_5$. Then, a squared chain length is $\frac{89}{3}$ and we see that $b_4 = -\frac{16}{3}$ and $a_5 = 2$.

If a chain has a planar configuration with $c(1)$, $z(2)$, $c(3)$ (Theorem 1.2 (3)), we have the relation $\boldsymbol{\beta}_6 = -\frac{8}{3}\boldsymbol{\beta}_4 - \boldsymbol{\beta}_5$. Then, a squared chain length is $\frac{89}{3}$ and we see that $b_4 = -\frac{16}{3}$ and $a_5 = 2$.

If a chain has a planar configuration with $z(1)$, $z(2)$, $c(3)$ (Theorem 1.2 (4)), we have the relation $\boldsymbol{\beta}_6 = -\frac{10}{3}\boldsymbol{\beta}_4 + \frac{5}{3}\boldsymbol{\beta}_5$. Then, a squared chain length is $\frac{275}{27}$ and we see that $b_4 = -\frac{20}{3}$ and $a_5 = -\frac{10}{3}$.

If a chain has a planar configuration with $z(1)$, $c(2)$, $z(3)$ (Theorem 1.2 (5)), we have the relation $\boldsymbol{\beta}_6 = -\frac{11}{3}\boldsymbol{\beta}_5$. Then, a squared chain length is $\frac{121}{9}$ and we see that $b_4 = 0$ and $a_5 = \frac{22}{3}$.

If a chain has a planar configuration with $z(1)$, $z(2)$, $z(3)$ (Theorem 1.2 (6)), we have the relation $\boldsymbol{\beta}_6 = -2\boldsymbol{\beta}_4 - 3\boldsymbol{\beta}_5$. Then, a squared chain length is 17 and we see that $b_4 = -4$ and $a_5 = 6$.

When a chain has a planar configuration, we can calculate all a_i, b_i concretely from the relations of the first and second 1×3 blocks. Then, we can see that $(\text{grad } h)_p = \sum_{i=3}^{5} a_i (\text{grad } f_i)_p + \sum_{j=2}^{4} b_j (\text{grad } g_j)_p$ for some nonzero a_i, b_j.

It is convenient to decompose the Hessian matrices of f_i, g_j and h into 3×3 blocks. We can easily check the following:

$$H(f_3)_p = \left(\begin{array}{c|c|c} I & O & O \\ \hline O & O & O \\ \hline O & O & O \end{array}\right), H(f_4)_p = \left(\begin{array}{c|c|c} I & -I & O \\ \hline -I & I & O \\ \hline O & O & O \end{array}\right),$$

$$H(f_5)_p = \left(\begin{array}{c|c|c} O & O & O \\ \hline O & I & -I \\ \hline O & -I & I \end{array}\right), H(g_2)_p = \left(\begin{array}{c|c|c} O & O & O \\ \hline O & O & O \\ \hline O & O & O \end{array}\right),$$

$$H(g_3)_p = \left(\begin{array}{c|c|c} 2I & -I & O \\ \hline -I & O & O \\ \hline O & O & O \end{array}\right), H(g_4)_p = \left(\begin{array}{c|c|c} O & -I & I \\ \hline -I & 2I & -I \\ \hline I & -I & O \end{array}\right),$$

$$H(h)_p = \left(\begin{array}{c|c|c} O & O & O \\ \hline O & O & O \\ \hline O & O & 2I \end{array}\right).$$

The tangent space $T_p(M(6))$ of $M(6)$ at p is equal to the orthogonal complement $\{\text{Span } \langle (\text{grad } f_i)_p, (\text{grad } g_j)_p \rangle\}^{\perp}$ of Span $\langle (\text{grad } f_i)_p, (\text{grad } g_j)_p \rangle$. We put $W = \text{Span } \langle \boldsymbol{\beta}_1, \ldots, \boldsymbol{\beta}_6 \rangle^{\perp}$. We have $T_p(M(6)) \supseteq W \oplus W \oplus W$. Because Span $\langle \boldsymbol{\beta}_1, \ldots, \boldsymbol{\beta}_6 \rangle$ is xy-space, we have that $\dim(W \oplus W \oplus W) = 3$. Because the gradient vectors $(\text{grad } f_3)_p, \ldots, (\text{grad } f_5)_p, (\text{grad } g_2)_p, \ldots, (\text{grad } g_4)_p$ are linearly independent, we see that $\dim T_p(M(6)) = 3$. So, we obtain the decomposition $T_p(M(6)) = W \oplus W \oplus W \subset (\mathbf{R}^3)^3$. Let $A = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ be the matrix of the orthogonal projection from $\mathbf{R}^3$ to $W \subset \mathbf{R}^3$ the orthogonal complement. Then, we have the matrix of the orthogonal projection P relative to the standard basis as the following:

$$P = \begin{pmatrix} A & O & O \\ O & A & O \\ O & O & A \end{pmatrix}.$$

Thus we have the following form of matrix H_p relative to the standard basis:

$$H_p = \left(\begin{array}{c|c|c} -(a_3 + a_4 + 2b_3)A & (a_4 + b_3 + b_4)A & -b_4 A \\ \hline (a_4 + b_3 + b_4)A & -(a_4 + a_5 + 2b_4)A & (a_5 + b_4)A \\ \hline -b_4 A & (a_5 + b_4)A & (2 - a_5)A \end{array}\right).$$

Since A has the above form, by basic matrix operations we can obtain the following matrices with the same rank and the same number of negative eigenvalues as H_p:

$$\begin{pmatrix} -(a_3 + a_4 + 2b_3) & a_4 + b_3 + b_4 & -b_4 \\ a_4 + b_3 + b_4 & -(a_4 + a_5 + 2b_4) & a_5 + b_4 \\ -b_4 & a_5 + b_4 & 2 - a_5 \end{pmatrix}.$$

We can calculate the rank and the number of negative eigenvalues concretely by substituting the calculated values of a_k, b_k, and we obtain the result of Theorem 1.2. $\square$

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