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Infinitesimal bending of DNA helices

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Abstract: The mathematics of DNA molecules is often studied as a double helix model. This paper focuses on the modelling of infinitesimal bending of DNA helices. The paper checks the flexibility of DNA molecule, i.e. the flexibility of double helix in infinitesimal bending theory. Actually, first, we find infinitesimal bending field of an arbitrary curve on the helicoid, that leaves bent curves on the helicoid, and show that helix bending on the helicoid is not possible. Finally, we deal with the infinitesimal bending of helicoid, using PDEs. Visualization of infinitesimal bending was done in Mathematica.

Key words: DNA, double helix, helicoid, infinitesimal bending

1. Introduction

There are many fields in global differential geometry and one of them is the infinitesimal deformation theory. Infinitesimal bending is a special part of the infinitesimal deformation theory. A concept of infinitesimal bending of surfaces and curves is very interesting in mathematics and is applied in mechanics, physics, biology, medicine, architecture, etc. For instance, papers [16] and [17] present the applications of infinitesimal bending in biology, article [18] presents its application in architecture. During the infinitesimal bending of curves are obtained the ruled surfaces [5]. More about infinitesimal deformation theory can be found in [1, 4, 7, 8, 10, 11, 13, 14].

Following the presentation of the DNA structure as a double helix [21], many works dealt with analysis of its structure and flexibility [2, 6, 9, 19, 20]. The intrinsic rigidity of the DNA double helix is usually modeled in terms of the resistance to distortion of vertical base stacking interactions [9] and theoretical analysis shows that sharp bends or kinks have to facilitate strong bending of the double helix [20], but bending interval is very short (in nanometer). In this article, we will examine the influence of infinitesimal bending on the DNA molecule.

We will begin the study by observing surfaces with Helix, that is, we are going to observe if infinitesimal bending of Helix which leaves bent curves on that surface is allowed. Paper [10] has already proven that curves on the cylinder, which are not in $z = const.$ plane, have only rigid motion, i.e. translation along the $z-$ axis. Helix is the curve on the cylinder, but it is not in $z = const$ plane, so only rigid motion is possible. On the other hand, helix is the $v-$ parameter curve on the helicoid, so we are going to study infinitesimal bending of curves on the helicoid and infinitesimal bending of helicoid.

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2. Preliminaries

We will give the necessary theory for studying the infinitesimal bending of surfaces and curves, according to Efimov [4] and Velimirović [13, 14]. Since we will deal with surfaces and curves in the vector form, we will denote the vector product with "$\times$" and the scalar product with "$\cdot$".

Definition 2.1 *Let a regular surface $\mathcal{S}$ of the class C^k $(k \geq 3)$ be given in the vector form with*

$$\mathcal{S} : \mathbf{r} = \mathbf{r}(u, v), \quad (u, v) \in D \subset \mathbb{R}^2, \tag{2.1}$$

that is included in the family of surfaces

$$\mathcal{S}_\epsilon : \mathbf{r}_\epsilon = \mathbf{r}(u, v, \epsilon) = \mathbf{r}(u, v) + \epsilon \mathbf{z}(u, v), \tag{2.2}$$

where $\epsilon \in (-1, 1)$, $\mathcal{S} = \mathcal{S}_0$, and $\mathbf{z} \in C^k$ $(k \geq 3)$. The surfaces $\mathcal{S}_\epsilon$ are infinitesimal bending of the first order of the surface $\mathcal{S}$ if

$$ds_\epsilon^2 - ds^2 = o(\epsilon). \tag{2.3}$$

The field $\mathbf{z}(u, v)$ is infinitesimal bending field of the infinitesimal bending of the surface $\mathcal{S}$.

Definition 2.2 *If a bending field $\mathbf{z}(u, v)$ can be written in a form*

$$\mathbf{z} = \mathbf{a} \times \mathbf{r} + \mathbf{b}, \tag{2.4}$$

where $\mathbf{a}, \mathbf{b} = const.$ then it is a trivial bending field.

Based on the definition 2.1, it can be shown that the following theorem holds.

Theorem 2.3 *[4] Necessary and sufficient condition for $\mathbf{z}(u, v)$ to be an infinitesimal bending field of the surface (2.1) is*

$$d\mathbf{r} \cdot d\mathbf{z} = 0. \tag{2.5}$$

Definition 2.4 *The fields $\mathbf{y}(u, v)$ and $\mathbf{s}(u, v)$ determined from the equations*

$$d\mathbf{z} = \mathbf{y} \times d\mathbf{r} \tag{2.6}$$

and

$$\mathbf{s} = \mathbf{z} - \mathbf{y} \times \mathbf{r} \tag{2.7}$$

are rotational and translational field of the surface $\mathcal{S}$ under infinitesimal bending generated by $\mathbf{z}(u, v)$, respectively.

Theorem 2.5 *[4] The derivatives $\mathbf{y}_u$, $\mathbf{y}_v$ of the rotation field $\mathbf{y}(u, v)$ are given with the equations*

$$\mathbf{y}_u = \alpha \mathbf{r}_u + \beta \mathbf{r}_v, \quad \mathbf{y}_v = \gamma \mathbf{r}_u - \alpha \mathbf{r}_v \tag{2.8}$$

where the functions $\alpha(u, v)$, $\beta(u, v)$, $\gamma(u, v)$ are determined by solving the system of partial differential equations

$$\begin{cases} \alpha_v - \gamma_u = \Gamma_{11}^1 \gamma - 2\Gamma_{12}^1 \alpha - \Gamma_{22}^1 \beta \\ \alpha_u - \beta_v = \Gamma_{11}^2 \gamma - 2\Gamma_{12}^2 \alpha - \Gamma_{22}^2 \beta \\ b_{11}\gamma - 2b_{12}\alpha - b_{22}\beta = 0. \end{cases} \tag{2.9}$$

where Γ^i_{jk} *are Christoffel's symbols of the surface (2.1) and* b_{ij} *are the coefficients of the second fundamental form.*

The equation

$$d\mathbf{y} = \mathbf{y}_u du + \mathbf{y}_v dv = (\alpha \mathbf{r}_u + \beta \mathbf{r}_v)du + (\gamma \mathbf{r}_u - \alpha \mathbf{r}_v)dv \tag{2.10}$$

is the total differential of the vector function $\mathbf{y}(u,v)$ and by integrating it we determine the rotational field $\mathbf{y}(u,v)$ for a unilaterally connected surface $\mathcal{S}$. After determining the field $\mathbf{y}(u,v)$, the infinitesimal bending field $\mathbf{z}(u,v)$ can be determined by the integration of Equation (2.6).

Now, we will give the necessary definition and theorems for the infinitesimal bending of curves.

Definition 2.6 *Let us consider a continuous regular curve* $C \subset \mathbb{R}^3$

$$C : \mathbf{r} = \mathbf{r}(t), \ \ t \in I \subseteq \mathbb{R}, \tag{2.11}$$

that is included in a family of the curves

$$C_\epsilon : \mathbf{r}_\epsilon = \mathbf{r}(t) + \epsilon \mathbf{z}(t), \ \ t \in I, \ \epsilon \in (-1, 1), \tag{2.12}$$

where t *is a real parameter and we get* $C = C_0$ *for* $\epsilon = 0$. *Family of curves* C_ϵ *is infinitesimal bending of the curve* C *if*

$$ds_\epsilon^2 - ds^2 = o(\epsilon), \tag{2.13}$$

where $\mathbf{z} = \mathbf{z}(t)$, $\mathbf{z} \in C^1$, *is the infinitesimal bending field of the curve* C.

Theorem 2.7 *[4] The necessary and sufficient condition for* $\mathbf{z}(t)$ *to be an infinitesimal bending field of the curve* C *(2.11) is*

$$d\mathbf{r} \cdot d\mathbf{z} = 0. \tag{2.14}$$

Let $\mathbf{n}(t)$ and $\mathbf{b}(t)$ denote unit principal normal and binormal vector fields of the curve C, respectively, then the following theorem holds.

Theorem 2.8 *[13] Infinitesimal bending field for the curve* C *(2.11) is*

$$\mathbf{z}(t) = \int \left(p(t)\mathbf{n}(t) + q(t)\mathbf{b}(t)\right) dt, \tag{2.15}$$

where $p(t)$ *and* $q(t)$ *are arbitrary integrable functions.*

An interesting problem of the infinitesimal bending of a curve is presented in [13]. Namely, the paper determines the infinitesimal bending field of a plane curve which stays in the plane after bending. Later, this research was continued for curves on different surfaces in [10, 15]. This has motivated us to study the infinitesimal bending of curves on the Helicoid.

3. Infinitesimal bending of curves on the helicoid

This section is devoted to investigating and presenting the infinitesimal bending of curves on the helicoid. The helicoid is a very interesting surface, it is the only ruled minimal surface other than the plane [3]. The helicoid is the only nonrotary surface which can glide along itself [12]. Firstly, we find an infinitesimal bending field of a curve on the helicoid, that leaves the bent curves on the helicoid.

Theorem 3.1 *Let the Helicoid be*

$$\mathcal{S} : \mathbf{r}(u, v) = (u \cos v, u \sin v, cv),\ u \in (u_1, u_2), v \in (-\pi, \pi), c = const. \tag{3.1}$$

Let $C : \mathbf{r} : (t_1, t_2) \to \mathbb{R}^3$ *be a regular continuous curve on the helicoid* $\mathcal{S}$*. Then the vector field* $\mathbf{z}(t)$ *determined from the equation*

$$\mathbf{z}(t) = \bar{C} e^{-\int \frac{\dot{v}(t)(u(t)\sin v(t))^{\cdot}}{\dot{u}(t)\cos v(t)} dt}(1, \tan v(t), 0), \quad \dot{u}(t)\cos v(t) \neq 0, \tag{3.2}$$

where $\bar{C} = const$*, is the infinitesimal bending field which includes the given curve in the family of the curves* $C_\epsilon : \mathbf{r}_\epsilon = \mathbf{r}(t) + \epsilon \mathbf{z}(t)$*,* $\epsilon \in (-1, 1)$*, on the helicoid* $\mathcal{S}$*.*

Proof The equation of the helicoid in cartesian coordinates is $\mathcal{S} : \frac{y}{x} = \tan \frac{z}{c}$. The equation of the curve C on the helicoid (3.1) will be

$$C : \mathbf{r}(t) = \mathbf{r}(u(t), v(t)) = (u(t)\cos v(t), u(t)\sin v(t), cv(t)),\ t \in (t_1, t_2). \tag{3.3}$$

From here, the equation of the curves C_ϵ will be

$$\begin{aligned} C_\epsilon : \mathbf{r}_\epsilon(t) &= \mathbf{r}(t) + \epsilon \mathbf{z}(t) = \\ &= (u(t)\cos v(t) + \epsilon z_1(t), u(t)\sin v(t) + \epsilon z_2(t), cv(t) + \epsilon z_3(t)), \end{aligned} \tag{3.4}$$

where $\mathbf{z}(t) = (z_1(t), z_2(t), z_3(t))$ and $z_i(t), i = 1, 2, 3$ are real continuous functions. Considering that all the curves of the family C_ϵ are on the helicoid (3.1), it must be valid

$$\frac{u(t)\sin v(t) + \epsilon z_2(t)}{u(t)\cos v(t) + \epsilon z_1(t)} = \tan \frac{cv(t) + \epsilon z_3(t)}{c}, \tag{3.5}$$

wherefrom, after recombination we have

$$\begin{aligned} &\epsilon \left(z_2(t) \left(1 - \tan v(t) \tan \frac{\epsilon z_3(t)}{c} \right) - z_1(t) \left(\tan v(t) + \tan \frac{\epsilon z_3(t)}{c} \right) \right) \\ &- \frac{u(t)}{\cos v(t)} \tan \frac{\epsilon z_3(t)}{c} = 0 \end{aligned} \tag{3.6}$$

for $\epsilon \in (-1, 1)$. If we put $z_3(t) = 0$, we obtain

$$z_2(t) = z_1(t) \tan v(t).$$

Thus we have

$$\mathbf{z}(t) = (z_1(t), z_1(t) \tan v(t), 0). \tag{3.7}$$

Let "$\cdot$" denote derivative by parameter t. For (3.3) and (3.7) $\dot{\mathbf{r}} \cdot \dot{\mathbf{z}} = 0$ must apply and we obtain

$$(\dot{u}(t) \cos v(t))\dot{z_1} + (\dot{v}(t)(u(t) \sin v(t))^{\cdot})z_1 = 0. \tag{3.8}$$

Solving the differential equation (3.8) by z_1, we obtain

$$\mathbf{z}(t) = \bar{C} e^{-\int \frac{\dot{v}(t)(u(t) \sin v(t))^{\cdot}}{\dot{u}(t) \cos v(t)} dt} (1, \tan v(t), 0), \quad \dot{u}(t) \cos v(t) \neq 0, \tag{3.9}$$

where $\bar{C}$ is arbitrary constant. □

Consequently, (3.2) is the infinitesimal bending field of the curve (3.3) which leaves that curve after bending on the helicoid $\mathcal{S}$. To illustrate the previous theorem we give the following example.

Example 1. Let the curve

$$C_1 : \mathbf{r}(t) = (t \cos t, t \sin t, t), \ t \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right),$$

be given on the helicoid (3.1), for $c = 1$. If we take $\bar{C} = 1$, according to (3.2), the infinitesimal bending field of C_1 will be

$$\mathbf{z}(t) = (e^{-t^2/2} \cos t, e^{-t^2/2} \sin t, 0).$$

Therefrom,

$$C_{1\epsilon} : \mathbf{r}_\epsilon = (t \cos t + \epsilon e^{-t^2/2} \cos t, t \sin t + \epsilon e^{-t^2/2} \sin t, t).$$

In Figure 1 the curve C_1 (red) and corresponding bent curves $C_{1\epsilon}$ (blue for positive ϵ, black for negative ϵ) for $\epsilon = \pm 0.25, \ \pm 0.5, \ \pm 0.75, \ \pm 0.95$ are shown.

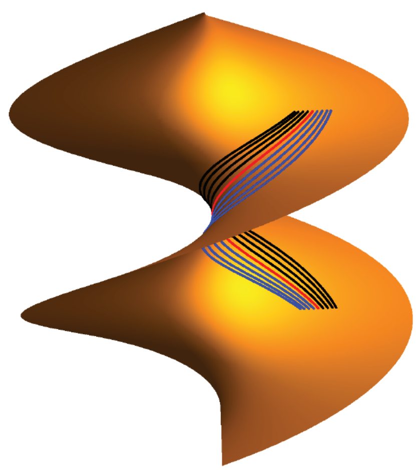

Figure 1. Infinitesimal bending of the curve C_1 on the helicoid.

◁

From the condition $\dot{u}(t) \cos v(t) \neq 0$ for equation (3.2), $u \neq const.$ must apply, i.e. the $v-$ parameter curves on the helicoid cannot bend in field $\mathbf{z}(t)$ that is given with equation (3.2). Also, the $u-$ parameter curves on the helicoid cannot bend, as in that case, infinitesimal bending field is constant. Helix is a $v-$ parameter curve on the helicoid, therefore, based on previous, we have the direct corollary.

Corollary 3.2 *The infinitesimal bending of helix in the field (3.2) is impossible.*

Hence, the infinitesimal bending of DNA helices in the field (3.2) is not possible. The following theorem shows that there is no bending field of helix on the helicoid.

Theorem 3.3 *Let the helix be*

$$C : \mathbf{r}(t) = (\cos t, \sin t, ct), \quad t \in (-\pi, \pi)\,, \tag{3.10}$$

on the Helicoid (3.1). There is no nontrivial bending field $\mathbf{z}(t)$ *that leaves the bent curves*

$$C_\epsilon : \mathbf{r}_\epsilon(t) = \mathbf{r}(t) + \epsilon \mathbf{z}(t), \ \epsilon \in (-1, 1), \tag{3.11}$$

on the Helicoid (3.1).

In the following example, we will examine arbitrary infinitesimal bending of double helix.

Example 2. As an illustration of a DNA molecule we will observe two helices

$$C_2 : \mathbf{r}(t) = (\cos t, \sin t, t), \quad C_3 : \mathbf{r}(t) = (\cos t, \sin t, t+2).$$

Normal and binormal of C_2 and C_3 are

$$\mathbf{n}(t) = (-\cos t, -\sin t, 0), \quad \mathbf{b}(t) = \left(\frac{\sin t}{\sqrt{2}}, -\frac{\cos t}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right).$$

For $p = 1$ and $q = \sqrt{2}$, based on (2.15) we get the infinitesimal bending field of helices C_2 and C_3:

$$\mathbf{z}(t) = (-\cos t - \sin t, \cos t - \sin t, t).$$

In Figure 2 the double helix, C_2 and C_3, and corresponding bent curves $C_{2\epsilon}$ and $C_{3\epsilon}$ for $\epsilon = \pm 0.1$, ± 0.15, ± 0.25 are shown.

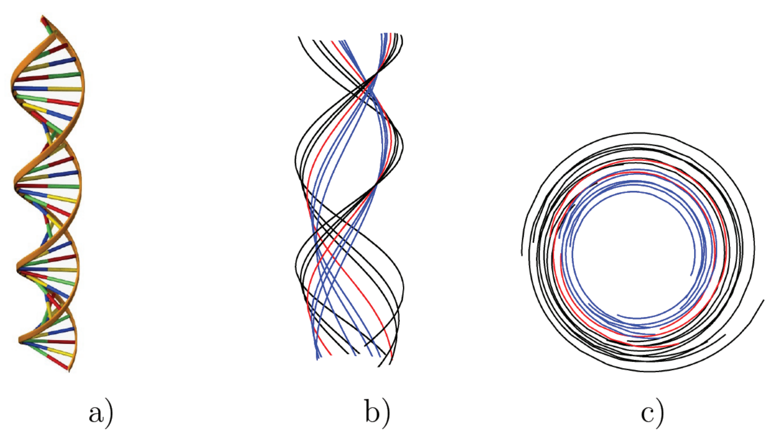

Figure 2. DNA and infinitesimal bending of the double helix.

◁

4. Infinitesimal bending of helicoid

Below we will see the influence of infinitesimal bending on the helicoid.

After determining the Christoffel symbols of the helicoid, as well as the coefficients of the second fundamental form and applying them in the system (2.9), we obtain a system of partial differential equations

$$\begin{cases} \alpha_v - \gamma_u = -u\beta \\ \alpha_u - \beta_v = -\frac{2u}{c^2+u^2}\alpha \\ \frac{2c}{\sqrt{c^2+u^2}}\alpha = 0. \end{cases} \tag{4.1}$$

From the third and the second equation of this system, we get $\alpha = 0$ and $\beta = f(u)$. Now, from the first equation of system (4.1) we get

$$\gamma = \int u f(u) du + g(v), \tag{4.2}$$

where $f(u)$ is an arbitrary integrable function and $g(v)$ is an arbitrary function. For example, if we take $f(u) = \frac{1}{u}$, $u \neq 0$ and $g(v) = 0$, after determining β, γ and applying in (2.10), we have

$$d\mathbf{y} = \mathbf{y}_u du + \mathbf{y}_v dv = \frac{1}{u}\mathbf{r}_v du + u\mathbf{r}_u dv, \tag{4.3}$$

and, after integration

$$\mathbf{y} = (y_1, y_2, y_3) = (0, 0, c\ln|u|). \tag{4.4}$$

Consequently, based on (2.6) and (4.4),

$$d\mathbf{z} = \mathbf{y} \times d\mathbf{r} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ 0 & 0 & c\ln|u| \\ \cos v du - u \sin v dv & \sin v du + u\cos v dv & c du \end{vmatrix},$$

after integration, we get the field of infinitesimal bending of the helicoid. Then, the bending field $\mathbf{z}(u,v)$ given with the equation

$$\mathbf{z}(u,v) = \left(cu(1 - 2\ln|u|)\sin v + \bar{C}_1, cu(2\ln|u| - 1)\cos v + \bar{C}_2, \bar{C}_3\right), \tag{4.5}$$

$u \in (-a,a)\backslash\{0\}$ and $\mathbf{z}(u,v) = (\bar{C}_1, \bar{C}_2, \bar{C}_3)$, when $u = 0$, where $\bar{C}_i$, $i = 1,2,3$, are arbitrary constant. It means that the straight line $u = 0$ is not deforming. The field of translation is determined with the equation

$$\mathbf{s}(u,v) = \left(cu(1 - \ln|u|)\sin v + \bar{C}_1, cu(\ln|u| - 1)\cos v + \bar{C}_2, \bar{C}_3\right), \tag{4.6}$$

$u \in (-a,a)\backslash\{0\}$ and $\mathbf{s}(u,v) = (\bar{C}_1, \bar{C}_2, \bar{C}_3)$, when $u = 0$.

Figure 3 shows helicoid and its infinitesimal deformations under infinitesimal bending in field (4.5).

5. Conclusion

Using different methods, many authors showed that the DNA molecule is flexible in very short fragments. Here, by the theory of infinitesimal bending, we showed that the helix bending on helicoid is impossible and that arbitrary infinitesimal bending of DNA helices leads to damaging the DNA molecule structure.

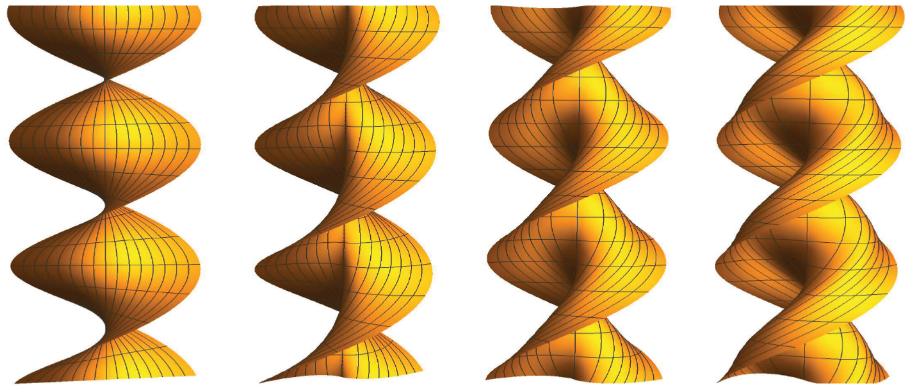

Figure 3. Helicoid and infinitesimal deformations for $\epsilon = 0.25, 0.5, 0.75$ and $\bar{C}_1 = 1$, $\bar{C}_2 = 2$, $\bar{C}_3 = 2$.

From Figure 2c we can see that two helices approach for positive ϵ, while for the negative ϵ they move further off. Also, for positive ϵ bent curves tend to have the shape of a straight line, while for the negative ϵ they tend to have the shape of a circle (we get circle for $\epsilon = -1$). Consequently, during infinitesimal bending relations between two helices can be broken, i.e. the structure of the DNA molecule can be damaged.

From Figure 3 it can be clearly seen that determined bending field $\mathbf{z}(u, v)$ spreads the interior of the helicoid and the $u-$ parameter curves deform into curves. This can cause breaking relations between the two helices, i.e. relations in the structure of the DNA molecule can break.

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