Infinitesimal bending of knots and energy change

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Abstract

We discuss infinitesimal bending of curves and knots in $\mathbb{R}^3$. A brief overview of the results on the infinitesimal bending of curves is outlined. Change of the Willmore energy, as well as of the Möbius energy under infinitesimal bending of knots is considered. Our visualization tool devoted to visual representation of infinitesimal bending of knots is presented.

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1 Introduction

This paper is devoted to studying the shape descriptors of knots during infinitesimal bending. The problem of infinitesimal bending of knots is a special part of the theory of deformation. Bending theory considers bending of
manifolds, isometrical deformations as well as infinitesimal bending. It requires use of differential geometry, mechanics, physics and has applications in modern computer graphics. Infinitesimal bending is "almost" an isometric deformation, or it is an isometric deformation in a precise approximation. Arc length is stationary under infinitesimal bending with a given precision. The infinitesimal bending caught the attention of many of the brightest minds in the history of mathematics, including A. D. Alexandrov [1], W. Blaschke [2], A. Cauchy [3], S. Cohn-Vossen [5], R. Connelly [6], N. V. Efimov [8], V. T. Fomenko [9], A. V. Pogorelov [18], I. N. Vekua [21], I. Ivanova-Karatopraklieva and I. Kh. Sabitov [11].

The physical properties of knotted and linked configurations in space have long been of interest to mathematicians. More recently, these properties have become significant to biologists, physicists, and engineers among others. Their depth of importance and breadth of application are now widely appreciated and steady progress continues to be made each year.

There are a few major fields in applied knot theory: physical knot theory, knot theory in the life sciences, computational knot theory, and geometric knot theory.

Physical knot theory is the study of mathematical models of knotting phenomena, often motivated by considerations from biology, chemistry, and physics (Kauffman 1991 [13]. Physical knot theory is used to study how geometric and topological characteristics of filamentary structures, such as magnetic flux tubes, vortex filaments, polymers, DNA’s, influence their physical properties and functions. It has applications in various fields of science, including topological fluid dynamics, structural complexity analysis and DNA biology (Kauffman 1991 [13], Ricca 1998, [20]).

Traditional knot theory models a knot as a simple closed loop in three-dimensional space. Such a knot has no thickness or physical properties such as tension or friction. Physical knot theory incorporates more realistic models. The traditional model is also studied but with an eye toward properties of specific embeddings ("conformations") of the circle. Such properties include ropelength and various knot energies (O’Hara 2003 [17]).

The most abstract connection between knots and science is the phenomenon we might call "patterns of analysis", where purely mathematical definitions and relationships in abstract knot theory are echoed by definitions and relationships in physics. This is a connection developed by L. Kauffman [13, 14] and others such as V. Jones [12], V. Turaev and N. Reshetikin [19], E. Witten [28].

Topologically ambient isotopic knots are by definition considered equivalent. It is therefore possible to think of a knot as a curve with small but positive thickness which allows us to present it as a tube. But in geometrical sense we could observe small deformations of knots as a family of different curves.

Infinitesimal bending of a manifold, and particularly of a surface or a curve in Euclidean 3-space, is a type of deformation characterized by the rigidity of the arc length with a given precision. In this case one observes changes of other magnitudes, and then we say that they are rigid or flexible. For example, the
coefficients of the first quadratic form are rigid and of the second one are flexible in the infinitesimal bending of a surface. The theory of infinitesimal bending is in close connection with thin elastic shell theory and leads to major mechanical applications. Infinitesimal bending of curves and surfaces is studied, for instance, in (A. D. Aleksandrov 1936) [1], (N. V. Efimov 1948) [8], M. Najdanović [13, 16], I. Vekua [21], Velimirović et al [22–26]. Infinitesimal bending in generalized Riemannian space was studied at Velimirović et al [27].

The paper is organized as follows: in Section 2, preliminary results and notation regarding infinitesimal bending of curves are presented. In Section 3, knot Willmore energy change under infinitesimal bending is studied and the corresponding variation is determined. In Section 4, the change of the Möbius energy under infinitesimal bending of knots is considered. In Section 5, our visualization tool devoted to visual representation of infinitesimal bending of knots is presented. The trefoil knot under infinitesimal bending is visualized.
2 Infinitesimal bending of curves-preliminaries

Let us consider a continuous biregular curve

\[ C : \mathbf{r} = \mathbf{r}(u), \quad u \in I \subseteq \mathcal{R} \]  

(2.1)

included in a family of the curves

\[ C_\epsilon : \tilde{\mathbf{r}}(u, \epsilon) = \mathbf{r}(u) + \epsilon \mathbf{z}(u), \quad u \in I, \quad \epsilon \geq 0, \quad \epsilon \to 0, \]  

(2.2)

where \( u \) is a real parameter and we get \( C \) for \( \epsilon = 0 \) (\( C = C_0 \)).

**Definition 2.1** [8] A family of curves \( C_\epsilon \) is an infinitesimal bending of a curve \( C \) if

\[ ds^2_\epsilon - ds^2 = o(\epsilon), \]  

(2.3)

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

**Theorem 2.1** [8] A necessary and sufficient condition that \( \mathbf{z}(u) \) is the infinitesimal bending field of a curve \( C \) is to be

\[ \dot{\mathbf{r}} \cdot \dot{\mathbf{z}} = 0, \]  

(2.4)

where \( \cdot \) stands for the scalar product in \( \mathcal{R}^3 \).

**Proof 2.1** According to the definition of the infinitesimal bending of a curve \( C \) the following holds

\[ ds^2_\epsilon - ds^2 = d\mathbf{r}^2_\epsilon - d\mathbf{r}^2 = d\mathbf{r}^2 + 2\epsilon \mathbf{d}\mathbf{r} \cdot d\mathbf{z} + \epsilon^2 d\mathbf{z}^2 - d\mathbf{r}^2 = 2\epsilon \mathbf{d}\mathbf{r} \cdot d\mathbf{z} + \epsilon^2 d\mathbf{z}^2 = o(\epsilon) \]

\[ \iff \mathbf{d}\mathbf{r} \cdot d\mathbf{z} = 0. \]

**Theorem 2.2** [15] Under infinitesimal bending of the curves each line element undertakes a non-negative addition, which is the infinitesimal value of order at least 2 (in \( \epsilon \)), i.e.

\[ ds_\epsilon - ds = o(\epsilon) \geq 0. \]  

(2.5)

**Proof 2.2** As

\[ d\mathbf{r} = \dot{\mathbf{r}}(u)du, \quad d\mathbf{z} = \dot{\mathbf{z}}(u)du, \]

according to [24], for infinitesimal bending field of a curve \( C \) we have

\[ \dot{\mathbf{r}}(u) \cdot \dot{\mathbf{z}}(u) = 0, \]  

(2.6)

where dot denotes derivative with respect to \( u \). Based on that we have

\[ ds_\epsilon = \| \dot{\mathbf{r}}(u) \| du = \| \dot{\mathbf{r}}(u) + \epsilon \dot{\mathbf{z}}(u) \| du = (\| \dot{\mathbf{r}}(u) \|^2 + \epsilon^2 \| \dot{\mathbf{z}}(u) \|^2)^{\frac{1}{2}} du \]

\[ = \| \dot{\mathbf{r}}(u) \| \left(1 + \epsilon^2 \frac{\| \dot{\mathbf{z}}(u) \|^2}{\| \dot{\mathbf{r}}(u) \|^2} \right)^{\frac{1}{2}} du = ds \left(1 + \epsilon^2 \frac{\| \dot{\mathbf{z}}(u) \|^2}{\| \dot{\mathbf{r}}(u) \|^2} \right)^{\frac{1}{2}} \]  

(2.7)
After using of Maclaurin formula we get
\[ ds_\varepsilon = ds \left( 1 + \varepsilon^2 \frac{\|\dot{z}(u)\|^2}{2 \|\dot{r}(u)\|^2} - \varepsilon^4 \frac{\|\ddot{z}(u)\|^4}{8 \|\dot{r}(u)\|^4} + \ldots \right) \]
i.e.
\[ ds_\varepsilon - ds = \varepsilon^2 \frac{\|\dot{z}(u)\|^2}{2 \|\dot{r}(u)\|^2} ds - \ldots, \]
which leads to \((2.5)\).

The next theorem is related to determination of the infinitesimal bending field of a curve \(C\).

**Theorem 2.3** \([22]\) The infinitesimal bending field for the curve \(C\) \((2.1)\) reads
\[ z(u) = \int [p(u)n_1(u) + q(u)n_2(u)] du, \quad (2.8) \]
where \(p(u)\) and \(q(u)\) are arbitrary integrable functions, and vectors \(n_1(u)\) and \(n_2(u)\) are respectively unit principal normal and binormal vector fields of a curve \(C\).

**Proof 2.3** According to \((2.9)\) we have
\[ \dot{r} \cdot \dot{z} = 0, \quad \text{i.e.} \quad \dot{r} \perp \dot{z}. \quad (2.9) \]
Based on that we conclude that \(\dot{z}\) lies in the normal plane of the curve \(C\), i.e.
\[ \dot{z}(u) = p(u)n_1(u) + q(u)n_2(u), \quad (2.10) \]
where \(p(u)\) and \(q(u)\) are arbitrary integrable functions. Integrating \((2.10)\) we obtain \((2.3)\).

As
\[ n_1 = \frac{(\dot{r} \cdot \dot{r}) \dot{r} - (\dot{r} \cdot \ddot{r}) \dot{r}}{\|\dot{r}\| \|\dot{r} \times \ddot{r}\|}, \quad n_2 = \frac{\dot{r} \times \ddot{r}}{\|\dot{r} \times \ddot{r}\|}, \quad (2.11) \]
in infinitesimal bending field can be written in the form
\[ z(u) = \int [p(u)\dot{r} + q(u)\dot{r} \times \ddot{r}] du \]
where \(p(u)\) and \(q(u)\) are arbitrary integrable functions, or in the form
\[ z(u) = \int [P_1(u)\dot{r} + P_2(u)\dot{r} + Q(u)\dot{r} \times \ddot{r}] du \quad (2.12) \]
where \(P_i(u), \ i = 1, 2, \) and \(Q(u)\) are arbitrary integrable functions, too.

Under an infinitesimal bending, geometric magnitudes of the curve are changed which is described with variations of these geometric magnitudes.
Definition 2.2 Let $A = A(u)$ be a magnitude which characterizes a geometric property on the curve $C$ and $A_e = A_e(u)$ the corresponding magnitude on the curve $C_e$ being infinitesimal bending of the curve $C$, and set

$$\Delta A = A_e - A = \epsilon \delta A + \epsilon^2 \delta^2 A + \ldots + \epsilon^n \delta^n A + \ldots$$  \hfill (2.13)

The coefficients $\delta A, \delta^2 A, \ldots, \delta^n A, \ldots$ are the first, the second, ..., the $n$-th variation of the geometric magnitude $A$, respectively under the infinitesimal bending $C_e$ of the curve $C$.

Let us mark some properties of the variations according to [16]:

I. For the variations of the product of geometric magnitudes it is effective the equation

$$\delta^n AB = \sum_{i=0}^{n} \delta^i A \delta^{n-i} B, \quad n \geq 0, \quad (\delta^0 A \overset{def}{=} A).$$  \hfill (2.14)

According to Def. (2.2), the variations of geometric magnitudes $A$ and $B$, as well as of the product $AB$ are:

$$\Delta A = A_e - A = \epsilon \delta A + \epsilon^2 \delta^2 A + \ldots + \epsilon^n \delta^n A + \ldots$$  \hfill (2.15)

$$\Delta B = B_e - B = \epsilon \delta B + \epsilon^2 \delta^2 B + \ldots + \epsilon^n \delta^n B + \ldots$$  \hfill (2.16)

$$\Delta AB = A_e B_e - AB = \epsilon \delta (AB) + \epsilon^2 \delta^2 (AB) + \ldots + \epsilon^n \delta^n (AB) + \ldots$$  \hfill (2.17)

respectively. On the other hand, the following equality is satisfied:

$$\Delta AB = A_e B_e - AB = A_e (B_e - B) + (A_e - A) B$$  \hfill (2.18)

Substituting (2.15) and (2.16) into equation (2.18) we obtain

$$\Delta AB = \epsilon (A \delta B + B \delta A) + \epsilon^2 (A \delta^2 B + \delta A \delta B + B \delta^2 A) + \ldots + \epsilon^n \sum_{i=0}^{n} \delta^i A \delta^{n-i} B + \ldots$$  \hfill (2.19)

As the left sides of the last equation and of the equation (2.17) are equal, the equation (2.14) is a valid one.

II. An arbitrary order variation of a derivative is the derivative of the variation, i. e.

$$\delta^n \left( \frac{dA}{du} \right) = \frac{d(\delta^n A)}{du}, \quad n \geq 0.$$  \hfill (2.20)

For

$$\frac{dA}{du} = B,$$  \hfill (2.21)

using (2.13) we obtain the equation

$$\Delta \frac{dA}{du} = \Delta B = \epsilon \delta B + \epsilon^2 \delta^2 B + \ldots + \epsilon^n \delta^n B + \ldots = \epsilon \delta \frac{dA}{du} + \epsilon^2 \delta^2 \frac{dA}{du} + \ldots + \epsilon^n \delta^n \frac{dA}{du} + \ldots$$  \hfill (2.22)
By comparing the equations (2.22) and (2.23), we confirm validity of the equation (2.20). The same case is for the differential, i.e.

\[ \delta^n(dA) = d(\delta^nA), \quad n \geq 0. \]

In the case when we consider only the first variations we can represent the magnitude \( A \) as

\[ A_\epsilon = A + \epsilon \delta A, \]

by neglecting the \( \epsilon^n \)-terms, \( n \geq 2 \).

The first variation is of course given by

\[ \delta A = \frac{d}{d\epsilon} A_\epsilon(u)|_{\epsilon=0}, \]

i.e.

\[ \delta A = \lim_{\epsilon \to 0} \frac{\Delta A}{\epsilon} = \lim_{\epsilon \to 0} \frac{A_\epsilon(u) - A(u)}{\epsilon}. \]

According to (2.5) we have

\[ \Delta (ds) = 0 \cdot \epsilon + \epsilon^2 \delta^2(ds) + \ldots = \delta(ds)\epsilon + \delta^2(ds)\epsilon^2 + \ldots \]

thus

\[ \delta(ds) = 0. \]

Therefore, under infinitesimal bending of a curve, the first variation of the line element \( ds \) is equal to zero.

A curve parameterized by the arc length under infinitesimal bending. Let us consider a curve

\[ C : r = r(s) = r[u(s)], \quad s \in J = [0, L], \]

parameterized by the arc length \( s \). The unit tangent to the curve is given by \( t = r' \), where prime denotes a derivative with respect to arc length \( s \). Clearly, \( t' \) is orthogonal to \( t \), but \( t'' \) is not. The classical Frenet equations

\[ t' = k n_1, \]
\[ n'_1 = -k t + \tau n_2, \]
\[ n'_2 = -\tau n_1, \]

where

\[ k = \frac{\theta'}{\rho}, \quad \tau = \frac{\kappa}{\rho}, \quad \rho = \sqrt{\kappa^2 + \tau^2}. \]
describe the construction of an orthonormal basis \{t, n_1, n_2\} along a curve, where \(n_1\) and \(n_2\) are respectively unit principal normal and binormal vector fields of the curve. Note that for the Frenet trihedron to be well-defined, we need \(k \neq 0\) throughout. We choose an orientation with \(n_2 = t \times n_1\). \(k\) and \(\tau\) are respectively the curvature and the torsion.

Let us consider an infinitesimal bending of the curve (2.28),

\[
C_\epsilon : \tilde{r}(s, \epsilon) = r(s) + \epsilon z(s).
\] (2.30)

As the vector field \(z\) is defined in the points of the curve (2.28), it can be presented in the form

\[
z = z_t + z_1 n_1 + z_2 n_2,
\] (2.31)

where \(z_t\) is tangential and \(z_1 n_1 + z_2 n_2\) is normal component, \(z, z_1, z_2\) are the functions of \(s\).

**Theorem 2.4** [15] Necessary and sufficient condition for the field \(z\) (2.31) to be infinitesimal bending field of the curve \(C\) (2.28) is

\[
z' - k z_1 = 0,
\] (2.32)

where \(k\) is the curvature of \(C\).

**Proof 2.4** According to (2.4), the necessary and sufficient condition for the field \(z\) to be infinitesimal bending field of the curve \(C\) is

\[
r' \cdot z' = 0,
\] (2.33)

i. e. \(t \cdot z' = 0\). Substituting Eq. (2.31) into the previous equation and using Frenet equations (2.29), we obtain (2.32).

Let us describe the behavior of some geometric magnitudes under infinitesimal bending of a curve according to [15]. As it is \(\delta t = \delta r' = (\delta r)' = z'\), using \(2.31, 2.32\) and Frenet equations we obtain

\[
\delta t = (z'_1 - \tau z_2 + k z) n_1 + (z'_2 + \tau z_1) n_2.
\] (2.34)

Applying commutativity of the variation and the derivative, we have \(\delta t' = (\delta t)'\). Based on (2.34), Frenet equations and \(z' = k z_1\) (due to (2.32)), one obtains

\[
\delta t' = -k(k z + z'_1 - \tau z_2) t + (k' z + z''_1 + (k^2 - \tau^2) z_1 - 2 \tau z'_2 - \tau' z_2) n_1 \\
+ (k \tau z + 2 \tau z'_1 + \tau' z_1 + z''_2 - \tau^2 z_2) n_2.
\] (2.35)

To evaluate \(\delta k\), we take a variation of the first equation in (2.29). We obtain

\[
\delta t' = \delta k n_1 + k \delta n_1.
\]
From (2.37), (2.38) and (2.39) we obtain

$$\delta k = k'z + z'' + (k^2 - \tau^2)z_1 - 2\tau z'z_2 - \tau'z_2.$$  (2.36)

after using (2.35).

Let us take a variation of the Frenet equation for $\mathbf{n}_1'\,$ and dot with $\mathbf{n}_2$. We have

$$\delta \tau = k\mathbf{n}_2 \cdot \delta \mathbf{t} + \mathbf{n}_2 \cdot \delta \mathbf{n}_1'. \quad (2.37)$$

We now rewrite the second term on the right hand side as

$$\mathbf{n}_2 \cdot \delta \mathbf{n}_1' = (\mathbf{n}_2 \cdot \delta \mathbf{n}_1)' - \mathbf{n}_2 \cdot \delta \mathbf{n}_1 = (\mathbf{n}_2 \cdot \delta \mathbf{n}_1)', \quad (2.38)$$

after using the third Frenet equation. As it is $\mathbf{r}'' = k\mathbf{n}_1$, we have $\mathbf{t}' = k\mathbf{n}_1$, i.e. $\mathbf{n}_1' = \frac{1}{k} \mathbf{t}'$. Further, $\delta \mathbf{n}_1 = \delta (\frac{1}{k}) \mathbf{t}' + \frac{1}{k} \delta \mathbf{t}'$

$$\mathbf{n}_2 \cdot \delta \mathbf{n}_1 = \mathbf{n}_2 \cdot \left[ \delta (\frac{1}{k}) k\mathbf{n}_1 + \frac{1}{k} \delta \mathbf{t}' \right] = \frac{1}{k} \mathbf{n}_2 \cdot \delta \mathbf{t}' . \quad (2.39)$$

From (2.37), (2.38) and (2.39) we obtain

$$\delta \tau = k\mathbf{n}_2 \cdot \delta \mathbf{t} + \left( \frac{1}{k} \mathbf{n}_2 \cdot \delta \mathbf{t}' \right)' . \quad (2.40)$$

Substituting (2.34) and (2.35) into (2.40) and using (2.32) we obtain

$$\delta \tau = z\tau' + k(z'_2 + 2\tau z_1) + \left\{ \frac{1}{k} \left[ 2\tau z'_1 + \tau' z_1 + z''_2 - \tau^2 z_2 \right] \right\}' . \quad (2.41)$$

Applying the known roles about the variation, Frenet formulas, the facts that $\mathbf{n}_1 = \frac{\mathbf{t}'}{\kappa}$ and $\mathbf{n}_2 = \mathbf{t} \times \mathbf{n}_1$, we simply get the variations of the normals:

$$\delta \mathbf{n}_1 = -(kz + z'_1 - \tau z_2)\mathbf{t} + \frac{1}{k} (k\tau z + z'' + \tau^2 z_2 + 2\tau z'_1 + \tau' z_1)\mathbf{n}_2 , \quad (2.42)$$

$$\delta \mathbf{n}_2 = -(z'_2 + \tau z_1)\mathbf{t} - \frac{1}{k} (k\tau z + z'' - \tau^2 z_2 + 2\tau z'_1 + \tau' z_1)\mathbf{n}_1 . \quad (2.43)$$

Based on the previous considerations, corresponding geometric magnitudes of deformed curves under infinitesimal bending are:

$$\mathbf{k} = k_e = k + \epsilon [k'z + z'' + (k^2 - \tau^2)z_1 - 2\tau z'_2 - \tau'z_2], \quad (2.44)$$

$$\tau = \tau_e = \tau + \epsilon \left\{ z\tau' + k(z'_2 + 2\tau z_1) + \left[ \frac{1}{k} \left( 2\tau z'_1 + \tau' z_1 + z'' - \tau^2 z_2 \right) \right] \right\}' , \quad (2.45)$$

$$\mathbf{t} = \mathbf{t}_e = \mathbf{t} + \epsilon \left[ (z'_1 - \tau z_2 + kz)\mathbf{n}_1 + (z'_2 + \tau z_1)\mathbf{n}_2 \right] , \quad (2.46)$$

$$\mathbf{n}_1 = \mathbf{n}_1_e = \mathbf{n}_1 + \epsilon \left[ -(kz + z'_1 - \tau z_2)\mathbf{t} + \frac{1}{k} (k\tau z + z'' - \tau^2 z_2 + 2\tau z'_1 + \tau' z_1)\mathbf{n}_2 \right] , \quad (2.47)$$

$$\mathbf{n}_2 = \mathbf{n}_2_e = \mathbf{n}_2 + \epsilon \left[ -(z'_2 + \tau z_1)\mathbf{t} - \frac{1}{k} (k\tau z + z'' - \tau^2 z_2 + 2\tau z'_1 + \tau' z_1)\mathbf{n}_1 \right] , \quad (2.48)$$

after neglecting the terms with $\epsilon^n , \quad n \geq 2$. 

9
3 Knot Willmore energy change under infinitesimal bending

Curvature-based energies play a main role in the description of both physical and non-physical systems (see [3, 7, 10, 25, 26]).

Let us observe the Willmore energy of a knot $K$:

$$W = \frac{1}{2} \int_J k^2 ds.$$  

(3.1)

The Willmore energy of a deformed knot will be

$$W_\epsilon = \frac{1}{2} \int_J k_\epsilon^2 ds_\epsilon = \frac{1}{2} \int_J (k + \epsilon \delta k)^2 [ds + \epsilon \delta (ds)],$$  

(3.2)

i. e.

$$W_\epsilon = W + \epsilon \left[ \int_J k \delta k ds + \frac{1}{2} \int_J k^2 \delta (ds) \right].$$  

(3.3)

As it is $\delta (ds) = 0$, we obtain that

$$\delta W = \int_J k \delta k ds,$$  

(3.4)

Applying (2.36) we get

$$\delta W = \int_J k [k' z' z'' + (k^2 - \tau^2) z_1 - 2 \tau z_2'] ds,$$  

(3.5)

wherefrom we have the next equation

$$\delta W = \int_J ds \left[ (k'' + \frac{1}{2} k^3 - k \tau^2) z_1 + (2 k' \tau + k \tau') z_2 \right]$$

$$+ \int_J ds \left[ \frac{1}{2} k^2 z - k' z_1 + k z'_1 - 2 k \tau z_2 \right]',$$  

(3.6)

after a bit of calculation.

The Willmore energy of a deformed knot under infinitesimal bending is

$$W_\epsilon = W + \epsilon \left\{ \int_J ds \left[ (k'' + \frac{1}{2} k^3 - k \tau^2) z_1 + (2 k' \tau + k \tau') z_2 \right]$$

$$+ \int_J ds \left[ \frac{1}{2} k^2 z - k' z_1 + k z'_1 - 2 k \tau z_2 \right]' \right\}. $$  

(3.7)

In the case of infinitesimal bending of knots we specify the condition $z(0) = z(L)$ for the infinitesimal bending field in order to get a family of closed curves. Also, we suppose that the knot, as well as the infinitesimal bending field are sufficiently smooth. Keeping this in mind we have the following theorem.
Theorem 3.1  Under infinitesimal bending of a knot $K$, variation of its Willmore energy is

$$\delta W = \int J ds \left[ (k'' + \frac{1}{2}k^3 - k\tau^2)z_1 + (2k'^{\tau} + k\tau')z_2 \right], \quad (3.8)$$

where $k$ and $\tau$ are the curvature and the torsion of $K$, respectively.

4  Knot Möbius energy change under infinitesimal bending

In mathematics, the Möbius energy of a knot is a particular knot energy, i.e. a functional on the space of knots. It was discovered by Jun O’Hara, who demonstrated that the energy blows up as the knot’s strands get close to one another. This is a useful property because it prevents self-intersection and ensures the result under gradient descent is of the same knot type.

We will here consider this type of energy under infinitesimal bending of knot.

Let $K$ be a smooth knot in 3-space $\mathbb{R}^3$. We can present $K$ as the image of the standard unit circle $S$ in the plane under a smooth map $r : S \to \mathbb{R}^3$. Then the Möbius energy of a knot is

$$E(K) = \int_S \int_S \left( \frac{1}{\|r(s) - r(t)\|^2} - \frac{1}{l(s,t)^2} \right) \|\dot{r}(s)\| \|\dot{r}(t)\| dsdt,$$

where $l(s,t)$ denotes the minimum distance along the knot $K$ between points $r(s)$ and $r(t)$.

Let us assume the parametrization $r$ be by arc length, then

$$\|\dot{r}(s)\| = \|r'(s)\| = 1. \quad (4.1)$$

So, we have

$$E(K) = \int_S \int_S \left( \frac{1}{\|r(s) - r(t)\|^2} - \frac{1}{l(s,t)^2} \right) dsdt. \quad (4.2)$$

Let us observe infinitesimal bending of $K$:

$$K_\epsilon : r_\epsilon = r(s) + \epsilon z(s).$$

The energy of the deformed knot $K_\epsilon$ will be

$$E(K_\epsilon) = \int_S \int_S \left( \frac{1}{\|r_\epsilon(s) - r_\epsilon(t)\|^2} - \frac{1}{l_\epsilon(s,t)^2} \right) \|\dot{r}_\epsilon'(s)\| \|\dot{r}_\epsilon'(t)\| dsdt,$$

where $l_\epsilon(s,t)$ is the distance long the deformed knot $K_\epsilon$ between the points $r_\epsilon(s)$ and $r_\epsilon(t)$.

Let us consider the following integrals:

$$E_1(K_\epsilon) = \int_S \int_S \frac{1}{\|r_\epsilon(s) - r_\epsilon(t)\|^2} \|\dot{r}_\epsilon'(s)\| \|\dot{r}_\epsilon'(t)\| dsdt, \quad (4.3)$$
Therefore, \( \delta E_2 \) and \( \delta E_2 \). It holds

\[
\|\mathbf{r}'(s)\| = \|\mathbf{r}'(s) + c\mathbf{z}'(s)\| = (\|\mathbf{r}'(s) + c\mathbf{z}'(s)\|^2)^{1/2} = (\|\mathbf{r}'(s)\|^2 + 2c\mathbf{r}'(s) \cdot \mathbf{z}'(s) + c^2\|\mathbf{z}'(s)\|^2)^{1/2}
\]

Using (2.33), (4.1) and Maclaurin formula, we obtain

\[
\|\mathbf{r}'(s)\| = 1 + \frac{1}{2}c^2\|\mathbf{z}'(s)\|^2 - \frac{1}{8}c^4\|\mathbf{z}'(s)\|^4 + \ldots \quad (4.5)
\]

Therefore, \( \delta \|\mathbf{r}'(s)\| = 0 \), i.e. \( \|\mathbf{r}'(s)\| = 1 \) after neglecting the terms with \( c^n, n \geq 2 \). Further,

\[
E_1(K_\epsilon) = \int_S \int_S \frac{1}{\epsilon^2} \|\mathbf{r}_s(s) - \mathbf{r}_t(t)\|^2 \, ds dt
\]

\[
= \int_S \int_S \frac{1}{\epsilon^2} \|\mathbf{r}(s) - \mathbf{r}(t)\|^2 + \epsilon\|\mathbf{z}(s) - \mathbf{z}(t)\|^2 \, ds dt
\]

\[
= \int_S \int_S \frac{1}{\epsilon^2} \|\mathbf{r}(s) - \mathbf{r}(t)\|^2 \left(1 - \frac{2c\mathbf{r}(s) \cdot \mathbf{z}(s) - \mathbf{z}(t)}{\|\mathbf{r}(s) - \mathbf{r}(t)\|^2} + c^2 \ldots \right) \, ds dt
\]

wherefrom we obtain that

\[
\delta E_1(K_\epsilon) = \frac{dE_1(K_\epsilon)}{d\epsilon} \bigg|_{\epsilon = 0} = -2 \int_S \int_S \frac{(\mathbf{r}(s) - \mathbf{r}(t)) \cdot (\mathbf{z}(s) - \mathbf{z}(t))}{\|\mathbf{r}(s) - \mathbf{r}(t)\|^4} \, ds dt \quad (4.6)
\]

On the other hand, we have

\[
l_\epsilon(s, t) = \int_s^t \|\dot{\mathbf{r}}_\epsilon(u)\| \, du = \int_s^t \|\dot{\mathbf{r}}(u) + c\mathbf{z}(u)\| \, du
\]

\[
= l(s, t) + \frac{1}{2}c^2 \int_s^t \|\dot{\mathbf{z}}(u)\|^2 \, du - \frac{1}{8}c^4 \int_s^t \|\dot{\mathbf{z}}(u)\|^4 \, du + \ldots ,
\]

i.e. \( \delta l(s, t) = 0 \) and, using (4.4) and (4.5), we get

\[
\delta E_2(K_\epsilon) = \frac{dE_2(K_\epsilon)}{d\epsilon} \bigg|_{\epsilon = 0} = 0. \quad (4.7)
\]

According to (4.6) and (4.7) we obtain the next theorem.

**Theorem 4.1** Under infinitesimal bending of a knot \( K \), variation of the M"obius energy is

\[
\delta E(K) = \frac{dE(K)}{ds} \bigg|_{\epsilon = 0} = 2 \int_S \int_S \frac{(\mathbf{r}(t) - \mathbf{r}(s)) \cdot (\mathbf{z}(s) - \mathbf{z}(t))}{\|\mathbf{r}(s) - \mathbf{r}(t)\|^4} \, ds dt. \quad (4.8)
\]

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5 Knot infinitesimal bending - examples

Here we will illustrate infinitesimally bending on knots, given by a simple parametric representation. Our aim is to visualize changing in shape and geometrical magnitudes when infinitesimal bending is applied. We start from knot representations as a curve in $\mathbb{R}^3$. Then, according to (2.8) we apply the bending described by $p(u)$ and $q(u)$. The bending field, given by (2.8) is defined by an integral whose sub integral function include arbitrary functions $p(u)$ and $q(u)$. The knot is visualized as polygonal line which connect points on them. At every such point, as well as, every subdivision point for the purpose of numerically integral calculation we should calculate functions: the curve, $p(u)$ and $q(u)$, first and second derivative and normals of the curve. Those calculations are necessary to obtain transformed shape of the curve. Instead of using existing software capable to do symbolic and numeric calculations, we decided to develop our own software tool in Microsoft Visual C++. The tool is aimed for manipulating explicitly defined functions, starting from its usual symbolic definitions as a string. The second step is parsing its symbolic definitions to obtain an internal, tree like, form. For the purpose of efficiency we parse function once, then calculate it many times. There are some important benefits of the tree like form as: combine more functions to obtain a compound function like sub integral function for infinitesimal field, make derivatives. Our tool has not possibility to calculate integral symbolically, instead we are using ability for fast calculation of sub integral function according to $F(x) = \int_{0}^{x} f(x) dx$, with possibility to add a integration constant.

Visualization of the knot and obtaining 3D model is done by using OpenGL. In the figures Figs. 1-4 the knots are represented as a tube around a curve. It looks like a rope, but without examination physical characteristics of the rope.

A trefoil knot, see Figs. 1-2, is given by parametric equations: $x = \sin(u) + 2\cos(2u), y = \cos(y) - 2\cos(2u), z = -\sin(3u)$ and bending field is defined by: $p(u) = \cos(3u)$ and $q(u) = \sin(3u)$.

A figure eight knot is given by the parametric equations: $x = (2 + \cos(2u)) \times \cos(3u), y = (2 + \cos(2u)) \times \sin(3u), z = \sin(4u)$. The basic and infinitesimally bent figure eight knot are given in Figs. 3-4.

The bending fields are defined by: $p(u) = \cos(6u)$ and $q(u) = \sin(6u)$. 

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Figure 3: Figure eight knot: basic and infinitesimally bent with $\epsilon = 1.4$.

Figure 4: Figure eight knot: basic and infinitesimally bent with $\epsilon = 1.4$ together.

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