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Curvature-based interaction potential between an isolated particle and micro/nano space curve

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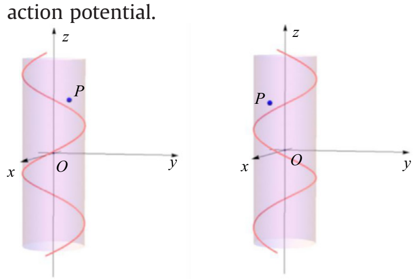
HIGHLIGHTS

- The curvature-based interaction potential between micro/nano-space curve and a particle located outside the curve is derived on the basis of pair potential $u(r) = \varepsilon(\sigma/r)^n$.
- The abnormal driving force induced by the micro/nano-space curve is predicted by curvature-based potential. It is proved that the essential factors constituting the driving force are the curvature, torsion and their gradients.
- The mechanics for micro/nano-curves is proved to be differential-geometry-based instead of Euclid-geometry-based.

GRAPHICAL ABSTRACT

The interaction between space curve with isolated particle outside the curve can be expressed as the function of curvature and torsion, and the sign of torsion has no effects on the curvature-based interaction potential.



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ABSTRACT

Based on the negative exponent pair potential, the interaction potential between micro/nano space curve and an isolated particle outside the curve (called off-curve-particle) is studied. By the parametric variable series expansion method, we verified that the space-curve/particle interaction potential is mainly determined by the curvature and torsional curvature of the curve. Therefore, we infer that the isolated particle will be subjected to the abnormal driving force induced by the space curve, and the essential factors constituting the driving force are the curvature, torsion and their gradients.

1. Introduction

Recently, more and more researchers discovered that if the space is curved in micro/nano scale, the mechanical behavior is curvature dependent, which is different from that in planar space. Therefore, the model in curved space needs to be modified to take the curvature of the space into account [1–5].

The previous papers [6–8], studied the interaction potential between the off-curve-particle and the planar curve or the interaction between an isolated particle or micro/nano curved body, and all finally derived the curvature-based potential of the particle. However, in nature, most of the line-shaped material structures are not planar curve but space curve. For instance, the double helix structure of DNA, the microfilaments in the cells, Amyloid fibers, secondary structure of Coiled coil protein and so on, all consist of twisting curve elements [9–11]. On the other hand, some artificially synthetized organic and inorganic nanowires are also in

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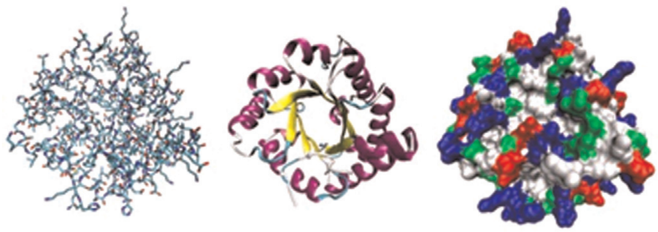

Fig. 1. Three types of different spatial structures of the same protein.

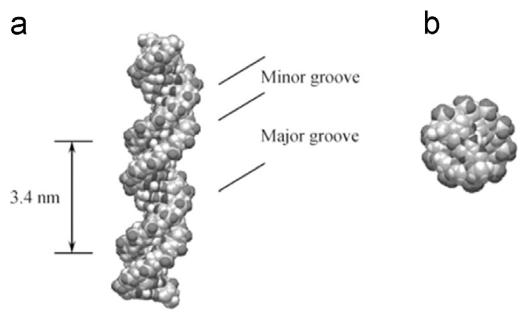

Fig. 2. Molecular structure of the double-strand DNA: (a) side view, (b) top view [9].

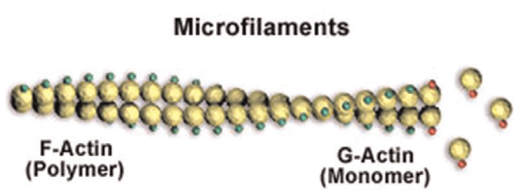

Fig. 3. The sturcture of the microfliament in a cell.

the configurations of double or multiple strands [12,13]. All of them exist in 3D space as space curves. Similar to the previous paper [6], we abstract those curve-shaped material structures as space curves in 3D Euclid Space. This paper will study the interaction between space curve and the off-curve-particle (Figs. 1–3).

This paper contains the following contents: (a) The general formulation of the interaction potential between space curve and the off-curve-particle is deduced. (b) By the small parametric variable series expansion method, the interaction potential between space-curve and off-curve-particle is expressed as the function of curvatures of the curve. (c) The accuracy of the curvature-based potential is verified by numerical experiments.

2. Interaction between space curve and outside particle

In 1903, Mie proposed an interaction pair potential of the form:

$$u(r) = -A/r^n + B/r^m$$

This potential includes a repulsive term B/r^m as well as an attractive term $-A/r^n$. Here, A and B are parameters related with the physical nature of the molecule, and are also adjustable for different systems, and r is the distance between two molecules. Most of the newly developed potential functions are all based on the pair potential Mie proposed [8]. It is noted that the main difference between repulsive and attractive terms is the sign. Besides, the repulsive term and attractive term can be added algebraically to depict various interactions. Therefore, these two terms can be

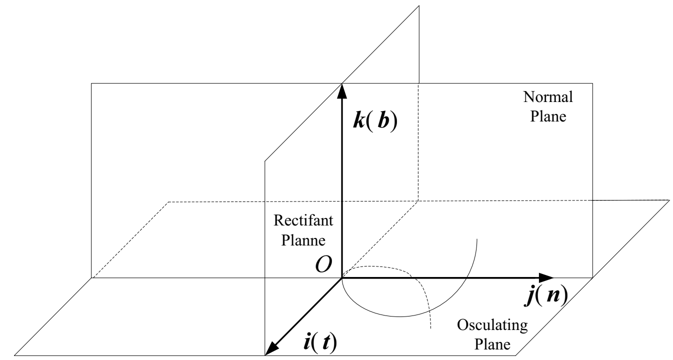

Fig. 4. Frenet frame of the space curve at point O.

written in the unified form as follows:

$$u(r) = \varepsilon\left(\frac{\sigma}{r}\right)^n \tag{1}$$

In Eq. (1), the index n can be taken as different integers, and the value of ε can be either positive or negative. Positive ε is used to describe the repulsive term, and negative ε is used to describe the attractive term.

2.1. Geometrical description for space curve

Suppose that the point O is the nearest point to the off-curve-particle on the curve. We build Frenet frame $\{\boldsymbol{r};\, \boldsymbol{t}, \boldsymbol{n}, \boldsymbol{b}\}(O)$ at point O, and mark it as the standard orthonormal frame $\{\boldsymbol{o};\, \boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k}\}$ in E^3 (Fig. 4). In Fig. 4, $\boldsymbol{t}-\boldsymbol{n}$ is the osculating plane for the curve at point O, $\boldsymbol{n}-\boldsymbol{b}$ is the normal plane and $\boldsymbol{b}-\boldsymbol{t}$ is the rectifying plane.

According to the curve theory in differential geometry [1], components of the radius vector $\boldsymbol{r}(s)$ on the space curve at point O can be expressed approximately as [14]:

$$x(s) = s - \frac{k_g^2 s^3}{6},\ y(s) = \frac{k_g}{2}s^2 + \frac{k_g' s^3}{6},\ z(s) = \frac{k_g \tau_g}{6}s^3 \tag{2}$$

Here, s is the arc-length parameter, k_g is the curvature of the space curve at point O on osculating plane, $k_g' = (dk_g/ds)$ is the derivative of the curvature with respect to arc-length parameter, τ_g is the torsion of the space curve at point O.

To simplify further, we just keep the first term in Eq. (2) and get:

$$x(s) = s,\ y(s) = \frac{k_g}{2}s^2,\ z(s) = \frac{k_g \tau_g}{6}s^3 \tag{3a}$$

This formula is equivalent to:

$$y(x) = \frac{k_g}{2}x^2,\ z(x) = \frac{k_g \tau_g}{6}x^3 \tag{3b}$$

In the neighborhood around point O, we can use the approximated curve shown in Eq. (3) to approach the local shape of the original space curve. It is noted that the approximated curve and the original curve are of same curvature k_g and torsion τ_g at point O.

2.2. Interaction potential between approximated curve and off-curve-particle

The off-curve-particle is supposed to locate in the normal plane, i.e. the yoz plane (Fig. 5), at point P with the coordinate $(0, h_y, h_z)$.