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Physics

Study of the Sadowsky Model for the Biopolymer Structures

Morteza Yavari

Department of Physics, Islamic Azad University, Kashan Branch, Kashan, Iran

(Presented by Academy Member Anzor Khelashvili)

ABSTRACT: The exact solutions of the equilibrium shape equations for the Sadowsky model are investigated. Also, we show that the helical solutions of this model can be matched with a family of the biopolymer structures. *© 2014 Bull. Georg. Natl. Acad. Sci.*

Key words: *equilibrium shape equations, Sadowsky model, biopolymer structures.*

Introduction

For the study of the biomolecules, we need to study the equilibrium shape equations. The shape equations play an important role in understanding the properties of the biomolecules.[1,2] Hence, we present a short review of the equilibrium shape equations.

Taking into account the 1-dimensional nature of many biopolymer chains, the total free energy Ftotal can be defined on the smooth curve x(*s*) in 3-space as follows

$$F_{total} = \oint F[x(s)]ds, \tag{1}$$

where *s* is arc-length of the biopolymer chain and F is the free energy function where depends on x(*s*), which describes the shape of the biopolymer chain. In flat 3-space, a smooth curve have two local invariants, i.e. the curvature $k = k(s)$ and the torsion $\tau = \tau(s)$. Therefore, the free energy has the general form $F = F(k, \tau, k', \tau')$ dependent on the curvature, torsion and their derivatives, while the over head prime stand for differentiation with respect to *s*. The curvature and torsion are defined by[3,4]

$$k = \sqrt{\frac{d^2 x_i}{ds^2}\frac{d^2 x_i}{ds^2}} \tag{2}$$

and

$$\tau = \frac{1}{k^2}\sqrt{\det_G\left(\frac{dx_i}{ds}, \frac{d^2 x_i}{ds^2}, \frac{d^3 x_i}{ds^3}\right)}, \tag{3}$$

in which $\det_G$ is the Gramm determinant.

The equilibrium shape equations of the biopolymer chain follow by variation the total free energy, i.e. $\delta F_{total}=0$, and it can be written as

$$\oint \frac{\partial F}{\partial k}\delta k ds+\oint \frac{\partial F}{\partial \tau}\delta \tau ds+\oint \frac{\partial F}{\partial k}\delta k' ds+\oint \frac{\partial F}{\partial \tau}\delta \tau' ds+\oint F\delta ds=0. \tag{4}$$

Thamwattana et al. [6] obtained the shape equations in the general case $F=F\ (k,t,k',\tau')$ as follows

$$\frac{d^2}{ds^2}\left[\frac{\partial F}{\partial k}-\frac{d}{ds}\left(\frac{\partial F}{\partial k'}\right)\right]+\frac{2\tau}{k}\frac{d^2}{ds^2}\left[\frac{\partial F}{\partial \tau}-\frac{d}{ds}\left(\frac{\partial F}{\partial \tau'}\right)\right]-\left(\frac{2k'\tau}{k^2}-\frac{\tau'}{k}\right)\frac{d}{ds}\left[\frac{\partial F}{\partial \tau}-\frac{d}{ds}\left(\frac{\partial F}{\partial \tau'}\right)\right]$$

$$+\left(k^2-\tau^2\right)\left[\frac{\partial F}{\partial k}-\frac{d}{ds}\left(\frac{\partial F}{\partial k'}\right)\right]+2k\tau\left[\frac{\partial F}{\partial \tau}-\frac{d}{ds}\left(\frac{\partial F}{\partial \tau'}\right)\right]+k\left[k'\frac{\partial F}{\partial k'}+\tau'\frac{\partial F}{\partial \tau'}-F\right]=0, \tag{5}$$

and

$$\begin{aligned}&-\frac{d^3}{ds^3}\left[\frac{\partial F}{\partial \tau}-\frac{d}{ds}\left(\frac{\partial F}{\tau'}\right)\right]+\frac{2k'}{k}\frac{d^2}{ds^2}\left[\frac{\partial F}{\partial \tau}-\frac{d}{ds}\left(\frac{\partial F}{\partial \tau'}\right)\right]\\&+2k\tau\frac{d}{ds}\left[\frac{\partial F}{\partial k}-\frac{d}{ds}\left(\frac{\partial F}{\partial k'}\right)\right]+\left(\frac{k''}{k}-2\left(\frac{k'}{k}\right)^2-k^2+\tau^2\right)\frac{d}{ds}\left[\frac{\partial F}{\partial \tau}-\frac{d}{ds}\left(\frac{\partial F}{\partial \tau'}\right)\right]\\&+k\tau'\left[\frac{\partial F}{\partial k}-\frac{d}{ds}\left(\frac{\partial F}{\partial k'}\right)\right]-kk'\left[\frac{\partial F}{\partial \tau}-\frac{d}{ds}\left(\frac{\partial F}{\partial \tau'}\right)\right]=0.\end{aligned} \tag{6}$$

These equations provide a uniform description for the equilibrium shapes of the biopolymer chains.

Exact solutions of the equilibrium shape equations for the Sadowsky model

As is well known, the shape of a biopolymer chain is usually characterized by its curvature and torsion. Let us now discuss the free energy of the biopolymer chain by the Sadowsky model as follows[7]

$$F=k^2\left(1+\frac{\tau^2}{k^2}\right)^2. \tag{7}$$

This model introduced by Sadowsky in 1930. Firstly, after some calculations, the equations (5) and (6) are respectively changed to

$$\begin{aligned}&2k^5k''-10kk''\tau^4+40(k')^2\tau^4-8k^3k'\tau\tau'-80kk'\tau^3\tau'+8k^4\tau\tau''+16k^2\tau^3\tau''\\&+4k^4\left(\tau'\right)^2+36k^2\tau^2\left(\tau'\right)^2+k^8+4k^6\tau^2+5k^4\tau^4+2k^2\tau^6=0,\end{aligned} \tag{8}$$

and

$$\begin{aligned}&4k^2k'''\tau^3-48kk'k''\tau^3+42k^2k''\tau^2\tau'+2k^4k''\tau'\\&+80\left(k'\right)^3\tau^3-4k^3\left(k'\right)^2\tau'-168k\left(k'\right)^2\tau^2\tau'\\&+2k^4k'\tau^3+2k^2k'\tau^5+48k^2k'\tau^2\tau''+4k^4k'\tau''\\&-2k^5\tau'''-6k^3\tau^2\tau'''-36k^3\tau\tau'\tau''-12k^3\left(\tau'\right)^3\\&+96k^2k'\tau\left(\tau'\right)^2-k^7\tau'-4k^5\tau^2\tau'-3k^3\tau^4\tau'=0.\end{aligned} \tag{9}$$

Unfortunately, the calculations show that we can not solve exactly the above differential equations or any combination of these equations. Since the equilibrium shape equations are highly nonlinear and complicated, it is very difficult to solve them without any assumption. Hence, we now assume that $\omega = \frac{\tau}{k}$ is a constant. If we substitute this condition into equations (8) and (9), then we obtain the following equations

$$2(1+3\omega^2)kk'' - 2\omega^2(k')^2 + (1+3\omega^2+2\omega^4)k^4 = 0, \tag{10}$$

and

$$k^2k''' - 3kk'k'' + 2(k')^3 + \frac{1+2\omega^2+\omega^4}{2(1+\omega^2)}k^4k' = 0. \tag{11}$$

By substituting the term k'' from the equation (10) into equation (11), we get

$$4(1+3\omega^2+3\omega^4+\omega^6)(k')^2 - (1+4\omega^2+6\omega^4+4\omega^6+\omega^8)k^4 = 0. \tag{12}$$

Next, we solve the equation (12) and the result is

$$k = \pm\frac{2}{\sqrt{1+\omega^2}}\frac{1}{s+c}, \tag{13}$$

where c is a constant. Finally, we have

$$\tau = \pm\frac{2\omega}{\sqrt{1+\omega^2}}\frac{1}{s+c}. \tag{14}$$

Below, we discuss some physical properties of the last solutions:

Study of the conical helix structures

As is well known, the parametric equations of a circular helix are described by

$$x(t) = \rho\cos t,\ \ y(t) = \rho\sin t,\ \ z(t) = \mu t, \tag{15}$$

where the constants ρ and μ, gives rise to the constant curvature and torsion. For example, DNA is a double helix and has two strands running in opposite directions (displayed in Fig. 1). Each component of a chain is a biopolymer of subunits called nucleotides.[8,9]

There are many different forms of helices, including the elliptical, spherical and conical and these structures play an important role in the study of the protein folding.[10] The existence of conical helix protein

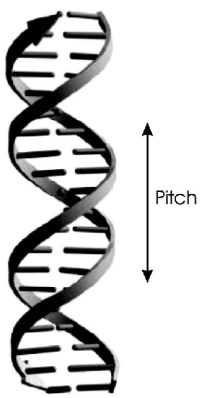

Fig. 1. Schematic representation of DNA

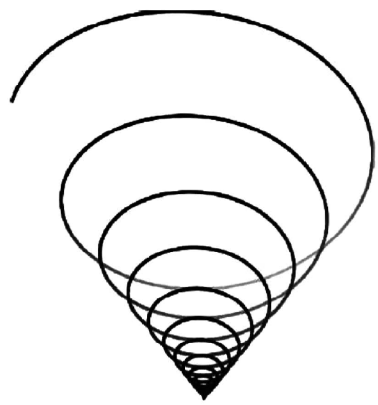

Fig. 2. Conical helix

structures in the form of ribbed end caps of gas vesicle proteins in aquatic bacteria is reported [11-13].

We now consider a particular conical helix given by the following parametric equations

$$x(t) = \alpha t\cos(\beta\log t),\ \ y(t) = \alpha t\sin(\beta\log t),\ \ z(t) = \gamma t, \tag{16}$$

in which α , β and γ are constants. Also, in cylindrical polar coordinate system (r ,φ, z), this curve (displayed in Fig. 2) is represented as

$$r(t) = \alpha t,\ \ \varphi(t) = \beta\log t,\ \ z(t) = \gamma t. \tag{17}$$

The curvature and torsion of a conical helix are obtained as follows

$$k = \frac{k_0}{s},\ \ \tau = \frac{\tau_0}{s}, \tag{18}$$

where the constants k_0 and τ_0 are defined by

$$k_0 = \frac{\alpha\beta\sqrt{1+\beta^2}}{\sqrt{\alpha^2(1+\beta^2)+\gamma^2}}, \tag{19}$$

$$\tau_0 = \frac{\beta\gamma}{\sqrt{\alpha^2(1+\beta^2)+\gamma^2}}. \tag{20}$$

The parameter t in equation (16) is related to the arclength s by the relation $t = \dfrac{s}{\sqrt{\alpha^2(1+\beta^2)+\gamma^2}}$.

If we take $c = 0$ into equations (13) and (14), then we obtain

$$k = \pm\frac{2}{s\sqrt{1+\omega^2}}, \tag{21}$$

$$\tau = \pm\frac{2\omega}{s\sqrt{1+\omega^2}}. \tag{22}$$

Therefore, these solutions can describe a family of conical helices with the following parametric equations

$$\begin{cases} x(t) = t\cos(2\log t), \\ y(t) = t\sin(2\log t), \\ z(t) = \omega\sqrt{5}t, \end{cases} \tag{23}$$

with the free energy function as follows

$$\mathrm{F} = \frac{\mathrm{F}_0}{s^2}, \tag{24}$$

in which $\mathrm{F}_0 = 4(1+\omega^2)$.

Conclusion

In this paper, we show that the family of conical helices are the solutions of the equilibrium shape equations for the Sadowsky model. In fact, we could have proved that this model can be an acceptable physical model for studying the biopolymer structures.

ფიზიკა

რელატივისტური საცდელი ნაწილაკის კლასიკური მოძრაობა ცილინდრულად სიმეტრიულ სტატიკურ მეტრიკაში

მ. იავარი

ასადის ისლამური უნივერსიტეტი, ქაშანის განყოფილება, ქაშანი, ირანი

(წარმოდგენილია აკადემიის წევრის ა.ხელაშვილის მიერ)

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