Physics

Helical Solutions of the Free Energy Model F=Ak^2+Bτ^2

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ABSTRACT. In this paper, we are going to use a geometrical approach for studying the biopolymer structures. The exact solutions of the general equilibrium shape equations for the free energy model F=Ak^2+Bτ^2 (k and τ are the principal curvatures and $A, B \in \mathbb{Z}$) are investigated by using the Feoli's formalism [A. Feoli et al., Nucl. Phys. B 705 (2005) 577]. Using the properties of the principal curvatures, we show that the particular solutions of this model can be matched with the family of protein structures. © *2015 Bull. Georg. Natl. Acad. Sci.*

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1. Introduction

In recent years, the elastic theories have been widely used for studying the biopolymer structures. Theoretical and experimental studies of the elastic properties of biomolecules are important research areas in physics. By using the modern experimental techniques such as magnetic optical microscopy [1], micromanipulation [2-4] and fluorescence microscopy [5], we are now able to study the elastic properties of biomolecules directly. Many models have been suggested to describe the biopolymer chains. For instance, the worm-like chain (WLC) model [6], the worm-like rod chain (WLRC) model [7-9] and Helfrich model [10] are appropriate to describe the biopolymer structures. The WLC model describes a chain by an elastic continuous curve under a small external force with a single elastic constant as the bending modulus. This model has been successfully applied to long biomolecules such as DNA and RNA. The WLRC model is appropriate to describe the biopolymer structures under a moderate force. Helfrich [10] studied the elastic theory of the helical fibers. In Helfrich energy model, the free energy is of the form $F = \gamma_1 k^2 + \gamma_2 k^2 \tau + \gamma_3 k^4 + \gamma_4 \left(k'^2 + k^2 \tau^2 \right) + \gamma_5$, where γ_i are the elastic constants. The importance of the computation of the free energy for the biomolecules has been recognized by many authors in recent years. The free energy of a biopolymer chain is generally considered as a function of its curvature and torsion. The free energy defined in such a way is analogous to the action in quantum field theory [11].

For the study of the biomolecules, we need to study the general equilibrium shape equations [12]. The shape equations play a crucial role in understanding the properties of the biomolecules. The elastic rods

theory has been studied for over two centuries. Many famous authors such as Hooke, Bernoulli, Euler, Lagrange, Poisson, Navier, Stokes and Kirchhoff have studied the various aspects of this theory. In 1859 Kirchhoff provided the general equilibrium shape equations of thin elastic rod, and he found that these equations are mathematically identical to those used to describe the dynamics of the spinning tops [13]. The Kirchhoff method has been generally used to describe the conformations of the biopolymer structures [14-17]. By variation of the free energy of a biopolymer chain, its general equilibrium shape equations are obtained [12-18].

This paper is organized as follows: In section 2, we give a brief review of the general equilibrium shape equations. In section 3, the exact solutions of these equations for the free energy model $F=Ak^2+B\tau^2$ are investigated. In section 4, we apply the results obtained by Feoli et al. for our model. In the last section, we discuss our results.

2. The General Equilibrium Shape Equations

In this section, we intend to give a short review of the general equilibrium shape equations. Taking into account the 1-dimensional nature of many biopolymer chains, the total free energy F_{total} can be defined on the smooth curve $x(s)$ in 3-space as follows

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

where s is arclength 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 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. We now use a natural parametrization of curve $x(s)$ in Euclidean 3-space: $x^i(s)$, $i = 1, 2, 3$. In this parametrization, we have

$$\frac{dx_i}{ds}\frac{dx_i}{ds} = 1,\tag{2}$$

where summation over repeated indices is always understood and in flat spacetime, we have $x^i = x_i$. The curvature and torsion are defined by [19-21]

$$k = \sqrt{\frac{d^2x_i}{ds^2}\frac{d^2x_i}{ds^2}},\tag{3}$$

and

$$\tau = \frac{1}{k^2}\sqrt{\det_G\left(\frac{dx_i}{ds}, \frac{d^2x_i}{ds^2}, \frac{d^3x_i}{ds^3}\right)},\tag{4}$$

in which $\det_G(\mathbf{a}, \mathbf{b}, \mathbf{c})$ is Gramm determinant for vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ [22].

The 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

$$\int \frac{\partial F}{\partial k}\delta k ds + \int \frac{\partial F}{\partial \tau}\delta \tau ds + \int \frac{\partial F}{\partial k'}\delta k' ds + \int \frac{\partial F}{\partial \tau'}\delta \tau' ds + \int F\delta ds = 0.\tag{5}$$

Zhang et al [12]. obtained the shape equations in the case $F = F(k, \tau, k')$. They calculated the variations δk, $\delta \tau$, $\delta k'$ and $F\delta ds$ by using the differential geometry methods as

$$\begin{cases} \delta k = k'\varepsilon_1 + \left(k^2 - \tau^2\right)\varepsilon_2 + \varepsilon_2'' - \tau'\varepsilon_3 - 2\tau\varepsilon_3', \\[4pt] k^2\delta\tau = k^2\tau'\varepsilon_1 + \left(k\tau'' - k'\tau' + 2k^3\tau\right)\varepsilon_2 - \left(2k'\tau - 3k\tau_2'\right)\varepsilon_2' + 2k\tau\varepsilon_2'' \\[4pt] \qquad + \left(k^3k' - 2k\tau\tau'\right)\varepsilon_3 + \left(k^3 - k\tau^2\right)\varepsilon_3' - k'\varepsilon_3'' - k\varepsilon_3''', \\[4pt] \delta k' = \left(k'' - k'\right)\varepsilon_1 + k'\varepsilon_1' + \left(3kk' - 2\tau\tau'\right)\varepsilon_2 + \left(k^2 - \tau^2\right)\varepsilon_2' + \varepsilon_2''' \\[4pt] \qquad - \tau''\varepsilon_3 - 3\tau'\varepsilon_3' - 2\tau\varepsilon_3'', \\[4pt] F\delta ds = -\left(k'\dfrac{\partial F}{\partial k} + \tau'\dfrac{\partial F}{\partial \tau}\right)\varepsilon_1 ds - kF\varepsilon_2 ds, \end{cases} \qquad (6)$$

where $\varepsilon_i(s)$ are the variations of the space form of the biopolymer chain, $\delta x(s) = \varepsilon_i(s)e_i(s)$ with the orthonormal Frenet basis $\{e_i\}$ [20-21]. By substituting these quantities into equation (5), they obtained the two shape equations which are referred to the general equilibrium shape equations. But, Thamwattana et al [23-24]. showed that the second and third equations in equations (6) are incorrect, and this therefore leads to the mistakes in the general equilibrium shape equations presented by Zhang et al. The correct version of these equations has been derived by them as follows

$$\frac{d^3}{ds^3}\left(\frac{\partial F}{\partial k'}\right) - \frac{d^2}{ds^2}\left(\frac{\partial F}{\partial k} + \frac{2\tau}{k}\frac{\partial F}{\partial \tau}\right) - \frac{d}{ds}\left\{\left(\frac{2k'\tau}{k^2} - \frac{3\tau'}{k}\right)\frac{\partial F}{\partial \tau} - \left(k^2 - \tau^2\right)\frac{\partial F}{\partial k'}\right\}$$
$$- \left(k^2 - \tau^2\right)\frac{\partial F}{\partial k} - \left(2k\tau - \frac{k'\tau'}{k^2} + \frac{\tau''}{k}\right)\frac{\partial F}{\partial \tau} - \left(3kk' - 2\tau\tau'\right)\frac{\partial F}{\partial k'} + kF = 0, \qquad (7)$$

and

$$\frac{d^3}{ds^3}\left(\frac{1}{k}\frac{\partial F}{\partial \tau}\right) + \frac{d^2}{ds^2}\left(\frac{k'}{k^2}\frac{\partial F}{\partial \tau} + 2\tau\frac{\partial F}{\partial k'}\right) - \frac{d}{ds}\left\{2\tau\frac{\partial F}{\partial k} - \left(k - \frac{\tau^2}{k}\right)\frac{\partial F}{\partial \tau} + 3\tau'\frac{\partial F}{\partial k'}\right\}$$
$$+ \tau'\frac{\partial F}{\partial k} - \left(\frac{k'\tau^2}{k^2} - \frac{2\tau\tau'}{k}\right)\frac{\partial F}{\partial \tau} + \tau''\frac{\partial F}{\partial k'} = 0. \qquad (8)$$

Furthermore, Thamwattana et al [24]. obtained the shape equations in the general case $F = F\left(k,\tau,k',\tau'\right)$ as follows

$$\frac{d^2}{ds^2}\left[\frac{\partial F}{\partial k} - \frac{d}{ds}\left(\frac{\partial F}{\partial k'}\right)\right] + \frac{2\tau}{k}\frac{d^2}{ds^2}\left[\frac{\partial F}{\partial \tau} - \frac{d}{ds}\left(\frac{\partial F}{\partial \tau'}\right)\right] - \left(\frac{2k'\tau}{k^2} - \frac{\tau'}{k}\right)\frac{d}{ds}\left[\frac{\partial F}{\partial \tau} - \frac{d}{ds}\left(\frac{\partial F}{\partial \tau'}\right)\right]$$
$$+ \left(k^2 - \tau^2\right)\left[\frac{\partial F}{\partial k} - \frac{d}{ds}\left(\frac{\partial F}{\partial k'}\right)\right] + 2k\tau\left[\frac{\partial F}{\partial \tau} - \frac{d}{ds}\left(\frac{\partial F}{\partial \tau'}\right)\right] + k\left[k'\frac{\partial F}{\partial k'} + \tau'\frac{\partial F}{\partial \tau'} - F\right] = 0, \qquad (9)$$

and

$$-\frac{d^3}{ds^3}\left[\frac{\partial F}{\partial \tau} - \frac{d}{ds}\left(\frac{\partial F}{\partial \tau'}\right)\right] + \frac{2k'}{k}\frac{d^2}{ds^2}\left[\frac{\partial F}{\partial \tau} - \frac{d}{ds}\left(\frac{\partial F}{\partial \tau'}\right)\right]$$
$$+ 2k\tau\frac{d}{ds}\left[\frac{\partial F}{\partial k} - \frac{d}{ds}\left(\frac{\partial F}{\partial k'}\right)\right] + \left(\frac{k''}{k} - 2\left(\frac{k'}{k}\right)^2 - k^2 + \tau^2\right)\frac{d}{ds}\left[\frac{\partial F}{\partial \tau} - \frac{d}{ds}\left(\frac{\partial F}{\partial \tau'}\right)\right]$$
$$+ k\tau'\left[\frac{\partial F}{\partial k} - \frac{d}{ds}\left(\frac{\partial F}{\partial k'}\right)\right] - kk'\left[\frac{\partial F}{\partial \tau} - \frac{d}{ds}\left(\frac{\partial F}{\partial \tau'}\right)\right] = 0. \qquad (10)$$
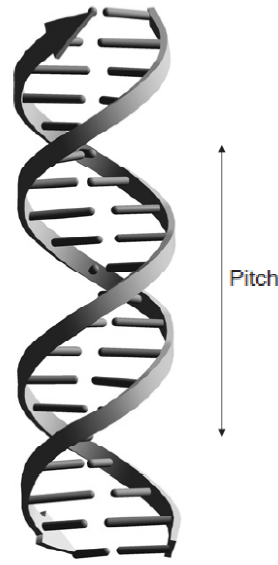
Fig. 1. Schematic representation of DNA

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

3. Exact Solutions of the General Equilibrium Shape Equations

As is well known, the curvature and torsion, i.e. the principal curvatures, encode the all geometric information of a curve in 3-space. Hence, 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 a simple power model as follows

$$F = Ak^2 + B\tau^2, \tag{11}$$

where A and B are arbitrary constants. Firstly, after a rather tedious calculation, the equations (7) and (8) are respectively changed to

$$2Ak^2 k'' + 4Bk\tau\tau'' + 2Bk(\tau')^2 - 4Bk'\tau\tau' + Ak^5 + (3B - 2A)k^3\tau^2 = 0, \tag{12}$$

and

$$Bk^2\tau''' - Bkk''\tau' - 2Bkk'\tau'' + 2B(k')^2\tau' + (B - 2A)k^3 k'\tau$$
$$+ (B - A)k^4\tau' - Bk^2\tau^2\tau' = 0. \tag{13}$$

Unfortunately, the calculations show that we can not solve exactly the above differential equations or any combination of these equations. Since the general equilibrium shape equations are highly nonlinear and complicated, it is very difficult to solve them without any assumption. Next, our calculations show that the following simple expressions

$$k = \frac{c_0}{s}, \quad \tau = \frac{c_1}{s}, \tag{14}$$

and

$$k = c_2 e^{ms}, \quad \tau = c_3 e^{ms}, \tag{15}$$

are the particular solutions of the equations (12) and (13), while m and c_i are constants. Below, for completeness our analysis, we would like to discuss the some physical properties of the last solutions:
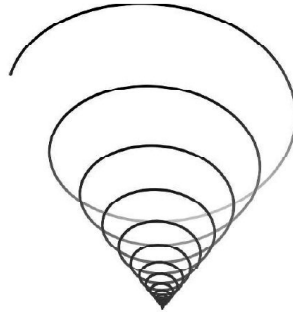
Fig. 2. Conical helix

3.1 Study of the First Solution

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

$$x(t) = \rho \cos t, \quad y(t) = \rho \sin t, \quad z(t) = \omega t, \tag{16}$$

where the constants ρ and ω, 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 chain is a biopolymer of subunits called nucleotides [25-26].

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 [27]. The existence of conical helix protein structures in the form of ribbed end caps of gas vesicle proteins in aquatic bacteria is reported [28-30].

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

$$x(t) = \alpha t \cos(\beta \log t), \quad y(t) = \alpha t \sin(\beta \log t), \quad z(t) = \gamma t, \tag{17}$$

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

$$r(t) = \alpha t, \quad \varphi(t) = \beta \log t, \quad z(t) = \gamma t. \tag{18}$$

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

$$k = \frac{k_0}{s}, \quad \tau = \frac{\tau_0}{s}, \tag{19}$$

where the constants k_0 and τ_0 are defined by

$$k_0 = \frac{\alpha \beta \sqrt{1 + \beta^2}}{\sqrt{\alpha^2(1 + \beta^2) + \gamma^2}}, \tag{20}$$

$$\tau_0 = \frac{\beta \gamma}{\sqrt{\alpha^2(1 + \beta^2) + \gamma^2}}. \tag{21}$$

Also, the parameter t in equation (17) is related to the arclength s by the relation $t = \dfrac{s}{\sqrt{\alpha^2(1 + \beta^2) + \gamma^2}}$.

Consequently, if we substitute the solution (14) into equations (12) and (13), then we obtain respectively

$$Ac_0^4 + 4Ac_0^2 + 6Bc_1^2 + (3B - 2A)c_0^2 c_1^2 = 0, \tag{22}$$

$$(3A - 2B)c_0^2 + Bc_1^2 - 2B = 0. \tag{23}$$

By solving these equations, the following solutions are obtained

$$c_0 = \frac{\sqrt{B}}{\sqrt{A-B}}, \quad c_1 = -\frac{A}{A-B}, \tag{24}$$

and

$$c_0 = \frac{\sqrt{2B}}{\sqrt{A-B}}, \quad c_1 = \frac{2B-4A}{A-B}, \tag{25}$$

in which $A, B > 0$ and $B \neq A, 2A$. Therefore, the solution (14) can describe a family of conical helices with the following two parametric equations

$$\begin{cases} x(t) = t\cos\left(\dfrac{\sqrt{A^2 + AB - B^2}}{A-B}\log t\right), \\[2mm] y(t) = t\sin\left(\dfrac{\sqrt{A^2 + AB - B^2}}{A-B}\log t\right), \\[2mm] z(t) = -\dfrac{A\sqrt{2A^2 - AB}}{(A-B)\sqrt{AB - B^2}}\,t, \end{cases} \tag{26}$$

with the free energy function as follows

$$F = \frac{F_0}{s^2}, \tag{27}$$

where $F_0 = \dfrac{2A^2B - AB^2}{(A-B)^2}$, and also

$$\begin{cases} x(t) = t\cos\left(\dfrac{\sqrt{16A^2 - 14AB + 2B^2}}{A-B}\log t\right), \\[2mm] y(t) = t\sin\left(\dfrac{\sqrt{16A^2 - 14AB + 2B^2}}{A-B}\log t\right), \\[2mm] z(t) = -\dfrac{(2A-B)\sqrt{34A^2 - 32AB + 6B^2}}{(A-B)\sqrt{AB - B^2}}\,t, \end{cases} \tag{28}$$

with the free energy function as follows

$$F = \frac{f_0}{s^2}, \tag{29}$$

in which $f_0 = \dfrac{18A^2B - 18AB^2 + 4B^3}{(A-B)^2}$. Further, for the relations (26-28), we must have

$$B \neq \frac{3}{2}A, \quad \frac{1\pm\sqrt{5}}{2}A, \quad \frac{7\pm\sqrt{17}}{2}A, \quad \frac{8\pm\sqrt{13}}{3}A, \quad 3A. \tag{30}$$

Next, for later use in section 4, we need to rewrite the free energy as $F = F(k)$, which depending only on curvature. Hence, from the relations (14), (24) and (25), becomes

$$F = \xi k^2, \tag{31}$$

where $\xi = \dfrac{2A^2 - AB}{A-B}$ and $\dfrac{9A^2 - 9AB + 2B^2}{A-B}$.

3.2 Study of the Second Solution

If we substitute the solution (15) into equations (12) and (13), then we obtain respectively

$$2m^2\left(Ac_2^2 + Bc_3^2\right) + c_2^2\left[Ac_2^2 + \left(3B - 2A\right)c_3^2\right]e^{2ms} = 0, \tag{32}$$

$$\left(3A - 2B\right)c_2^2 + Bc_3^2 = 0. \tag{33}$$

It is obvious that, we must have $Ac_2^2 + \left(3B - 2A\right)c_3^2 = 0$. From the last consequence, we obtain $A = B$ and $c_3 = \pm ic_2$ while $i = \sqrt{-1}$. On the other hand, we know that the principal curvatures are the real geometric parameters. Thus, no physical conclusion can be drawn from the solution (15).

4. Study of the Feoli's Formalism

For complete our analysis, we need to determine the unknown constants A and B. For do this, we apply the Feoli's formalism [31-32], which is formulated for the free energy function as $F = F(k)$ which depends only on curvature, such as model (31). This formalism has been shown to naturally arise from the Euler-Lagrange equations written in terms of an arbitrary parameter. Hence, we use an arbitrary parametrization of the curve $x(\sigma)$ with arbitrary parameter σ. In this parametric representation, the equations (2) and (3) are respectively changed to

$$\frac{d}{ds} = \frac{1}{\sqrt{\dot{x}^2}}\frac{d}{d\sigma}, \tag{34}$$

and

$$k = \sqrt{\frac{\dot{x}^2\ddot{x}^2 - (\dot{x}\ddot{x})^2}{(\dot{x}^2)^3}}, \tag{35}$$

where $\dot{x}^2 = \dot{x}_i\dot{x}_i$ while the dot over x denotes the differentiation with respect to the parameter σ. In this parametric representation, the total free energy function (1) takes the following form

$$F_{\text{total}} = \int \sqrt{\dot{x}^2}\,F(k)d\sigma. \tag{36}$$

The function (36) is invariant under the translations of the curve coordinates by a constant vector, i.e. $x_i \to x_i + u_i$ where $u_i = \text{constant}$ [31-32]. By using the Noether theorem [11], we know that the invariance of the total free energy function under these translations entails the conservation of the momentum vector under the motion along curve $x(\sigma)$. The components of the momentum vector are defined by

$$P^i = \frac{d}{d\sigma}\left(\frac{\partial(\sqrt{\dot{x}^2}F)}{\partial\ddot{x}_i}\right) - \frac{\partial(\sqrt{\dot{x}^2}F)}{\partial\dot{x}_i}. \tag{37}$$

The Euler-Lagrange equations generated by the relation (37) are written as follows

$$\frac{d}{d\sigma}P^i = 0, \quad i = 1, 2, 3. \tag{38}$$

Now, with the help of the following useful formulas [31-32]
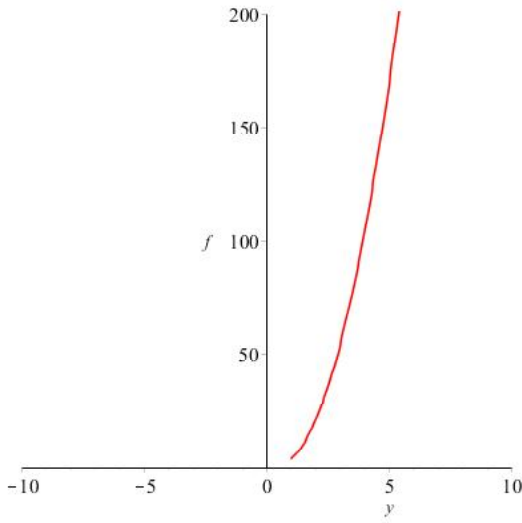
Fig. 3. Graph *f* in terms of *y*
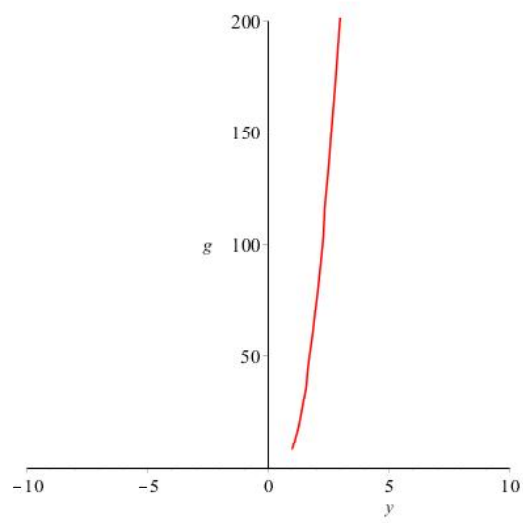
Fig. 4. Graph *g* in terms of *y*

$$k\frac{\partial k}{\partial \ddot{\mathrm{x}}_i} = \frac{[3(\dot{\mathrm{x}}\ddot{\mathrm{x}})^2 - 2\dot{\mathrm{x}}^2\ddot{\mathrm{x}}^2]\ddot{\mathrm{x}}_i - \dot{\mathrm{x}}^2(\ddot{\mathrm{x}}\ddot{\mathrm{x}})\ddot{\mathrm{x}}_i}{(\dot{\mathrm{x}}^2)^4},$$

$$k\frac{\partial k}{\partial \ddot{\mathrm{x}}_i} = \frac{1}{\dot{\mathrm{x}}^2}\frac{d^2\mathrm{x}_i}{ds^2}, \tag{39}$$

$$\frac{d^2\mathrm{x}_i}{ds^2} = \frac{\dot{\mathrm{x}}^2\ddot{\mathrm{x}}_i - (\dot{\mathrm{x}}\ddot{\mathrm{x}})\dot{\mathrm{x}}_i}{(\dot{\mathrm{x}}^2)^2},$$

the momentum vector takes the following form

$$\mathrm{P}^i = \frac{1}{k}\frac{\partial \mathrm{F}}{\partial k}\frac{d^3\mathrm{x}_i}{ds^3} + \frac{k'}{k}\left(\frac{\partial^2 \mathrm{F}}{\partial k^2} - \frac{1}{k}\frac{\partial \mathrm{F}}{\partial k}\right)\frac{d^2\mathrm{x}_i}{ds^2} + \left(2k\frac{\partial \mathrm{F}}{\partial k} - \mathrm{F}\right)\frac{d\mathrm{x}_i}{ds}. \tag{40}$$

Further, from the equations (2-4), the following identities are obtained

$$\frac{d\mathrm{x}_i}{ds}\frac{d^2\mathrm{x}_i}{ds^2} = 0,$$

$$\frac{d\mathrm{x}_i}{ds}\frac{d^3\mathrm{x}_i}{ds^3} = -k^2,$$

$$\frac{d^2\mathrm{x}_i}{ds^2}\frac{d^3\mathrm{x}_i}{ds^3} = kk', \tag{41}$$

$$\frac{d^3\mathrm{x}_i}{ds^3}\frac{d^3\mathrm{x}_i}{ds^3} = (k')^2 + k^4 + k^2\tau^2.$$

By squaring the equation (40) and using the equations (41), yields

$$\mathrm{P}^2 = \left(k'\frac{\partial^2 \mathrm{F}}{\partial k^2}\right)^2 + \left(k^2 + \tau^2\right)\left(\frac{\partial \mathrm{F}}{\partial k}\right)^2 - 2k\mathrm{F}\frac{\partial \mathrm{F}}{\partial k} + \mathrm{F}^2, \tag{42}$$

where $\frac{\partial^2 \mathrm{F}}{\partial k^2} \neq 0$ and $\mathrm{P}^2 = \mathrm{P}^i\mathrm{P}_i$. Moreover, by differentiating the equation (42) with respect to σ and using this fact that

$$P^2 = \text{constant}, \tag{43}$$

the following relation is obtained

$$\left\{ (k')^2 \frac{\partial^3 F}{\partial k^3} + k'' \frac{\partial^2 F}{\partial k^2} + (k^2 + \tau^2) \frac{\partial F}{\partial k} - kF \right\} \frac{\partial^2 F}{\partial k^2} + \frac{\tau\tau'}{k'} \left(\frac{\partial F}{\partial k} \right)^2 = 0. \tag{44}$$

Next, with the help of the relations (14) and (31), the equation (44) is reduced to

$$c_0^3 - 2c_0^2 - 4c_1^2 - 4 = 0. \tag{45}$$

Finally, by considering the relations (24) and (25), the last equation is changed to the following expressions

$$f = 8y^2 - 6y - \sqrt{y-1} + 2 = 0, \tag{46}$$

$$g = 34y^2 - 34y - \sqrt{2y-2} + 8 = 0, \tag{47}$$

where $y = A/B$. In Figures 3 and 4, respectively, we have plotted the functions f and g with respect to parameter y. By analysing these Figures, we find that the existence of the real solutions for the polynomials (46) and (47) are impossible. Consequently, the coefficients A and B can not be determined explicity. But, our presented method seems to be a useful way for determining the unknown parameters of a general free energy model.

Conclusion

The aim of this paper is to extend the results of the Feoli's formalism for the biopolymer structures. We have showed that the family of conical helices are the particular solutions of the shape equations for our model. Actually, we could have proved that this model can be a acceptable physical model for studying the protein structures. It also has been shown that with the help of Feoli's formalism, we can obtain an extra relation among the unknown parameters of the considered model.

ფიზიკა

თავისუფალი ენერგიის $\mathbf{F=A}k^2\mathbf{+B}\tau^2$ მოდელის სპირალური ამოხსნები

მ. იავარი

კაშანის განყოფილება, ისლამური აზადის უნივერსიტეტი, კაშანი, ირანი

ამ ნაშრომში ბიოპოლიმერების სტრუქტურის შესასწავლად ვიყენებთ გეომეტრიულ მიდგომას. ზოგადი წონასწორობის ფორმის ზუსტი ამოხსნები თავისუფალი ენერგიის $\mathbf{F=A}k^2\mathbf{+B}\tau^2$ (k და τ არიან მთავარი სიმრუდეები, ხოლო $\mathbf{A, B} \in \mathbb{Z}$) მოდელში შესწავლილია ფეოლის ფორმალიზმის გამოყენებით [**A. Feoli et al., Nucl. Phys. B705 (2005) 577**]. მთავარი სიმრუდეების თვისებების გამოყენებით ვაჩვენებთ, რომ აღნიშნული მოდელის კერძო ამოხსნები შეიძლება დაკავშირდეს პროტეინების ოჯახის სტრუქტურებთან.

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