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Physics

Study of DNA Structures for the Free Energy Model $F = \sqrt{Ak^2 + B}$

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ABSTRACT. In this paper, we are going to generalize the results of the Feoli's formalism for DNA structures. This formalism is formulated for the free energy $F = F(k)$**, which depends on the curvature** k**. Firstly, the general equilibrium shape equations are presented. The exact solutions of these equations for the free energy model** $F = \sqrt{Ak^2 + B}$ **are investigated in Feoli's formalism.** *© 2015 Bull. Georg. Natl. Acad. Sci.*

Key words: *general equilibrium shape equations, Feoli's formalism, DNA structures.*

1. Introduction

In recent years, *in vitro* experiments done on the single DNA molecules show that DNA double helix structures have the nontrivial elastic properties [1, 2]. Thus, the measurements on the single DNA molecules afford a useful laboratory for the studies of a single biopolymer chain. The topological properties of the biopolymer chains play an important role in replication and transcription processes [1]. Theoretical analysis about the configurations of DNA molecules often are based on the elastic rod theory. The biopolymer chains are described by using the free energy models [3]. From the conformation and dynamical characteristics of helical structures, we are able to determine the exact form of the free energy function. Generally, the free energy of a biopolymer chain is considered to be as a function of its curvature and torsion.

For the study of DNA molecules, it is necessary to study the general equilibrium shape equations of the biopolymer chains [3]. It plays a crucial role in understanding the properties of the biomolecules. By calculating the variation of the free energy function of a biopolymer chain, its general equilibrium shape equations are obtained [3, 4].

Most of the calculations be carried out with the Maple software [5].

2. The General Equilibrium Shape Equations

Taking into account the 1-dimensional nature of many biopolymer chains, the total free energy F_{total} may be considered as a function defined on the smooth curve $x(s)$ in 3-dimensional space

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

where s is the arclength of the biopolymer chain and F is the free energy function which depends on x(s), which describes the spatial shape of the biopolymer chain. In 3-dimensional flat space, a smooth curve has two local invariants, curvature $k = k(s)$ and torsion $\tau = \tau(s)$. So, the free energy function has the general form $\mathrm{F} = \mathrm{F}\left(k, \tau, k'\right)$, where the overhead prime stands for differentiation with respect to the natural parameter s. We shall use a natural parametrization of curve x(s) in 3-dimensional Euclidean space: $\mathrm{x}^i(s)$, $i = 1, 2, 3$. In this parametrization, we have:

$$\frac{d\mathrm{x}_i}{ds}\frac{d\mathrm{x}_i}{ds} = 1, \tag{2}$$

where the summation over the repeated indices is assumed in the corresponding range. The curvature is defined by

$$k = \sqrt{\frac{d^2\mathrm{x}_i}{ds^2}\frac{d^2\mathrm{x}_i}{ds^2}}. \tag{3}$$

The torsion is defined in the following way [6-8]:

$$\tau = \frac{1}{k^2}\sqrt{\det_{\mathrm{G}}\left(\frac{d\mathrm{x}_i}{ds}, \frac{d^2\mathrm{x}_i}{ds^2}, \frac{d^3\mathrm{x}_i}{ds^3}\right)}, \tag{4}$$

here $\det_{\mathrm{G}}(\mathbf{a}, \mathbf{b}, \mathbf{c})$ is the Gramm determinant for vectors **a**, **b** and **c** [9]. By taking the variation from the total free energy, i.e. $\delta \mathrm{F}_{\text{total}} = 0$, one can derive the shape equations of the biopolymer chain and it can be written as follows:

$$\oint \mathrm{F}_1 \delta k ds + \oint \mathrm{F}_2 \delta\tau ds + \oint \mathrm{F}_3 \delta k' ds + \oint \mathrm{F}\delta ds = 0, \tag{5}$$

where $\mathrm{F}_1 = \frac{\partial \mathrm{F}}{\partial k}$, $\mathrm{F}_2 = \frac{\partial \mathrm{F}}{\partial \tau}$ and $\mathrm{F}_3 = \frac{\partial \mathrm{F}}{\partial k'}$. Zhang et al. [3] calculated the variations δk, $\delta\tau$, $\delta k'$ and $\mathrm{F}\delta ds$ by using the differential geometry methods as follows:

$$\begin{cases} \delta k = k'\varepsilon_1 + \left(k^2 - \tau^2\right)\varepsilon_2 + \varepsilon_2'' - \tau'\varepsilon_3 - 2\tau\varepsilon_3', \\ k^2\delta\tau = k^2\tau'\varepsilon_1 + \left(k\tau'' - k'\tau' + 2k^3\tau\right)\varepsilon_2 - \left(2k'\tau - 3k\tau_2'\right)\varepsilon_2' + 2k\tau\varepsilon_2'' \\ \qquad + \left(k^3k' - 2k\tau\tau'\right)\varepsilon_3 + \left(k^3 - k\tau^2\right)\varepsilon_3' - k'\varepsilon_3'' - k\varepsilon_3''', \\ \delta k' = \left(k'' - k'\right)\varepsilon_1 + k'\varepsilon_1' + \left(3kk' - 2\tau\tau'\right)\varepsilon_2 + \left(k^2 - \tau^2\right)\varepsilon_2' + \varepsilon_2''' \\ \qquad - \tau''\varepsilon_3 - 3\tau'\varepsilon_3' - 2\tau\varepsilon_3'', \\ \mathrm{F}\delta ds = -\left(k'\mathrm{F}_1 + \tau'\mathrm{F}_2\right)\varepsilon_1 ds - k\mathrm{F}\varepsilon_2 ds, \end{cases} \tag{6}$$

in which $\varepsilon_i(s)$ are the variations of the space form of the biopolymer chain, $\delta\mathrm{x}(s) = \varepsilon_i(s)\mathrm{e}_i(s)$ with the orthonormal Frenet basis $\{\mathrm{e}_i\}$ [7, 8]. Then, by substituting these quantities into equation (5), they obtained the two shape equations, which refer to the general equilibrium shape equations. Thamwattana et al. [10, 11] show 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. Also, the correct version of these equations was derived by them as follows:

$$\begin{aligned}&\frac{d^3}{ds^3}\mathrm{F}_3-\frac{d^2}{ds^2}\left(\mathrm{F}_1+\frac{2\tau}{k}\mathrm{F}_2\right)-\frac{d}{ds}\left\{\left(\frac{2k'\tau}{k^2}-\frac{3\tau'}{k}\right)\mathrm{F}_2-\left(k^2-\tau^2\right)\mathrm{F}_3\right\}\\&-\left(k^2-\tau^2\right)\mathrm{F}_1-\left(2k\tau-\frac{k'\tau'}{k^2}+\frac{\tau''}{k}\right)\mathrm{F}_2-\left(3kk'-2\tau\tau'\right)\mathrm{F}_3+k\mathrm{F}=0,\end{aligned}\tag{7}$$

$$\begin{aligned}&\frac{d^3}{ds^3}\left(\frac{1}{k}\mathrm{F}_2\right)+\frac{d^2}{ds^2}\left(\frac{k'}{k^2}\mathrm{F}_2+2\tau\mathrm{F}_3\right)-\frac{d}{ds}\left\{2\tau\mathrm{F}_1-\left(k-\frac{\tau^2}{k}\right)\mathrm{F}_2+3\tau'\mathrm{F}_3\right\}\\&+\tau'\mathrm{F}_1-\left(\frac{k'\tau^2}{k^2}-\frac{2\tau\tau'}{k}\right)\mathrm{F}_2+\tau''\mathrm{F}_3=0.\end{aligned}\tag{8}$$

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

3. Exact Solutions of the Shape Equations for a Radical Model of Free Energy

As is well known, the curvature and torsion, i.e. the principal curvatures, encode the all geometric information of a curve in 3-dimensional space. Hence, the shape of a biopolymer chain is usually characterized by its curvature and torsion. Usually, the contribution of torsion is often neglected in the free energy. Let us now discuss the free energy of the biopolymer chain by a radical function of curvature as follows:

$$\mathrm{F}=\sqrt{\mathrm{A}k^2+\mathrm{B}},\tag{9}$$

where A and B are unknown constants in which B denotes a constraint. If we substitute this relation into second shape equations (8), after integration, we lead to

$$\mathrm{A}^2k^2\tau-(\mathrm{A}k^2+\mathrm{B})\mathrm{C}=0,\tag{10}$$

in which $\mathrm{C}\ (\neq 0)$ is an unknown constant of integration. Furthermore, from the first shape equations (7), we can conclude

$$\begin{aligned}&k''\frac{d}{dk}\left(\frac{\mathrm{A}k}{\sqrt{\mathrm{A}k^2+\mathrm{B}}}\right)+\left(k'\right)^2\frac{d^2}{dk^2}\left(\frac{\mathrm{A}k}{\sqrt{\mathrm{A}k^2+\mathrm{B}}}\right)\\&+(k^2-\tau^2)\left(\frac{\mathrm{A}k}{\sqrt{\mathrm{A}k^2+\mathrm{B}}}\right)-k\sqrt{\mathrm{A}k^2+\mathrm{B}}=0.\end{aligned}\tag{11}$$

At this stage, we restrict our analysis to the study of DNA. Deoxyribonucleic acid, or DNA, is a macromolecule found in all living cells. 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 [12, 13].

To continue our analysis, we are going to rewrite the equations (10) and (11) for a double helix structure. For

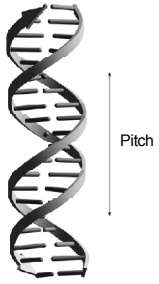

Fig. 1. Schematic representation of DNA double helix.

doing this, we use from the parametric equation of a double helix which is described by

$$\mathbf{r}(s) = \left(r_0 \cos(\omega s), r_0 \sin(\omega s), h\omega s\right), \tag{12}$$

where the coiled pitch of helix is $2\pi h$, r_0 is the radius of helix and $\omega = \dfrac{1}{\sqrt{r_0^2 + h^2}}$. It is shown that the curvature and torsion of a helix are given by $k_0 = r_0\omega^2$ and $\tau_0 = h\omega^2$. The subscript 0 in k_0 and τ_0 refer respectively to the constant curvature and torsion. Finally, by applying these results into equation (11), yields

$$\mathrm{A}\tau_0^2 + \mathrm{B} = 0. \tag{13}$$

4. Study of DNA Structures in Feoli's Formalism

In previous section, it was shown that there are only two equations, i.e. (10) and (13), containing three unknowns. Hence, we need to more relations among the variables. For doing this, we apply below the Feoli's formalism [14, 15], which is formulated for the free energy $\mathrm{F} = \mathrm{F}(k)$, which depending on the curvature *k*, for the suggested model (9). In this formalism, we shall use an arbitrary parametrization of the curve $\mathrm{x}(\sigma)$ with arbitrary parameter σ . In this parametric representation, the relations (2) and (3) are respectively changed to

$$\frac{d}{ds} = \frac{1}{\sqrt{\dot{\mathrm{x}}^2}}\frac{d}{d\sigma}, \tag{14}$$

$$k = \sqrt{\frac{\dot{\mathrm{x}}^2\ddot{\mathrm{x}}^2 - (\dot{\mathrm{x}}\ddot{\mathrm{x}})^2}{(\dot{\mathrm{x}}^2)^3}}, \tag{15}$$

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

$$\mathrm{F}_{\mathrm{total}} = \oint \sqrt{\dot{\mathrm{x}}^2}\,\mathrm{F}(k)\,d\sigma. \tag{16}$$

It is shown that the total free energy function (16) is invariant under the translations of the curve coordinates by a constant vector, i.e. $\mathrm{x}_i \to \mathrm{x}_i + \mathrm{u}_i$ where $\mathrm{u}_i = \text{constant}$ [14, 15]. Next, by using the Noether theorem [16], we know that the invariance of total free energy function under these translations entails the conservation of the momentum vector under the motion along the curve $\mathrm{x}(\sigma)$. The components of momentum vector are defined by

$$\mathrm{P}^i = \frac{d}{d\sigma}\left(\frac{\partial(\sqrt{\dot{\mathrm{x}}^2}\mathrm{F})}{\partial\ddot{\mathrm{x}}_i}\right) - \frac{\partial(\sqrt{\dot{\mathrm{x}}^2}\mathrm{F})}{\partial\dot{\mathrm{x}}_i}. \tag{17}$$

The Euler-Lagrange equations generated by (17) are written in terms of the momentum vector as follows:

$$\frac{d}{d\sigma}\mathrm{P}^i = 0,\ i = 1,2,3. \tag{18}$$

Next, with the help of the following useful formulas [14, 15]

$$k\frac{\partial k}{\partial \dot{\mathrm{x}}_i}=\frac{[3(\dot{\mathrm{x}}\ddot{\mathrm{x}})^2-2\dot{\mathrm{x}}^2\ddot{\mathrm{x}}^2]\dot{\mathrm{x}}_i-\dot{\mathrm{x}}^2(\dot{\mathrm{x}}\ddot{\mathrm{x}})\ddot{\mathrm{x}}_i}{(\dot{\mathrm{x}}^2)^4},$$
$$k\frac{\partial k}{\partial \ddot{\mathrm{x}}_i}=\frac{1}{\dot{\mathrm{x}}^2}\frac{d^2\mathrm{x}_i}{ds^2},\quad \frac{d^2\mathrm{x}_i}{ds^2}=\frac{\dot{\mathrm{x}}^2\ddot{\mathrm{x}}_i-(\dot{\mathrm{x}}\ddot{\mathrm{x}})\dot{\mathrm{x}}_i}{(\dot{\mathrm{x}}^2)^2}, \tag{19}$$

the momentum vector takes the following form

$$\mathrm{P}^i=\frac{1}{k}\frac{\partial \mathrm{F}}{\partial k}\frac{d^3\mathrm{x}_i}{ds^3}+\frac{k'}{k}\left(\frac{\partial^2\mathrm{F}}{\partial k^2}-\frac{1}{k}\frac{\partial \mathrm{F}}{\partial k}\right)\frac{d^2\mathrm{x}_i}{ds^2}+\left(2k\frac{\partial \mathrm{F}}{\partial k}-\mathrm{F}\right)\frac{d\mathrm{x}_i}{ds}. \tag{20}$$

From the equations (2) and (3), the following consequences can be concluded

$$\frac{d\mathrm{x}_i}{ds}\frac{d^2\mathrm{x}_i}{ds^2}=0,\quad \frac{d\mathrm{x}_i}{ds}\frac{d^3\mathrm{x}_i}{ds^3}=-k^2,\quad \frac{d^2\mathrm{x}_i}{ds^2}\frac{d^3\mathrm{x}_i}{ds^3}=kk'. \tag{21}$$

From these relations together with the equation (4), after some calculations, we can get:

$$\frac{d^3\mathrm{x}_i}{ds^3}\frac{d^3\mathrm{x}_i}{ds^3}=(k')^2+k^4+k^2\tau^2. \tag{22}$$

Next, we square the right and left hand sides of the equation (20) and with using the equations (21) and (22), we lead to

$$\mathrm{P}^2=\left(k'\frac{\partial^2\mathrm{F}}{\partial k^2}\right)^2+(k^2+\tau^2)\left(\frac{\partial \mathrm{F}}{\partial k}\right)^2-2k\mathrm{F}\frac{\partial \mathrm{F}}{\partial k}+\mathrm{F}^2, \tag{23}$$

where $\frac{\partial^2\mathrm{F}}{\partial k^2}\neq 0$ and $\mathrm{P}^2=\mathrm{P}^i\mathrm{P}_i$.

5. Calculation of the Pauli-Lubanski Pseudoscalar

In a flat spacetime, the Pauli-Lubanski pseudoscalar is defined by [14, 15]

$$\mathrm{W}=\frac{1}{2}\mathrm{M}_{ij}\mathrm{M}^{ij}\mathrm{P}^2-\left(\mathrm{M}_{ij}\mathrm{P}^j\right)^2, \tag{24}$$

where P^i is momentum vector and M_{ij} is momentum tensor with the following form:

$$\mathrm{M}_{ij}=\sum_{a=1}^{2}\left(q_{ai}p_{aj}-q_{aj}p_{ai}\right),\quad i<j, \tag{25}$$

in which the canonical variables q_{ai} and p_{ai} are defined as follows:

$$q_{1i}=\mathrm{x}_i,\ q_{2i}=\dot{\mathrm{x}}_i,\ p_{1i}=\mathrm{P}^i=-\frac{\partial(\sqrt{\dot{\mathrm{x}}^2}\mathrm{F})}{\partial \dot{\mathrm{x}}_i}-\frac{dp_{2i}}{d\sigma},\ p_{2i}=-\frac{\partial(\sqrt{\dot{\mathrm{x}}^2}\mathrm{F})}{\partial \ddot{\mathrm{x}}_i}. \tag{26}$$

From these equations, after some calculations, one obtains:

$$\mathrm{W}=\tau^2\left(\frac{\partial \mathrm{F}}{\partial k}\right)^4. \tag{27}$$

On the other hand, in a flat spacetime, it can be shown that the relation between the invariants W and P^2 is given by [14, 15]

$$W = S^2 P^2, \tag{28}$$

in which S is a parameter of system. Next, from the equations (27) and (28), yields:

$$\tau^2 \left(\frac{\partial F}{\partial k} \right)^4 - S^2 P^2 = 0. \tag{29}$$

In the next step, combining this result with the equation (23), yields

$$2\left(k' \frac{d}{dk} \left(\frac{Ak}{\sqrt{Ak^2 + B}} \right) \right)^2 + \frac{A^2 k^2 \left(k^2 + \tau^2 \right)}{Ak^2 + B} - Ak^2 + B - \frac{C^2}{S^2} = 0. \tag{30}$$

If we rewrite the above equation for the double helix structures with the parametric equation (12), then we lead to

$$A^2 \left(k_0^2 + \tau_0^2 \right) k_0^2 - A\left(Ak_0^2 + B \right) k_0^2 + \left(B - \frac{C^2}{S^2} \right) \left(Ak_0^2 + B \right) = 0. \tag{31}$$

We now solve the three equations (10), (13) and (31) in terms of S, then the following solutions are obtained:

$$A = \frac{k_0^4 - \tau_0^4}{k_0^4} S^2, \quad B = \frac{\tau_0^4 - k_0^4}{k_0^4} \tau_0^2 S^2, \quad C = \frac{k_0^4 + \tau_0^4}{k_0^4} \tau_0 S^2. \tag{32}$$

By substituting the equations (32) into equation (9), we conclude:

$$F = \frac{k_0^2 - \tau_0^2}{k_0^2} \sqrt{k_0^2 + \tau_0^2}\ S. \tag{33}$$

Consequently, with applying the Feoli's formalism, the considered free energy model, which contains three unknown constants A, B and C, is reduced to the simple equation (33) with only one parameter S.

6. Conclusion

In this work, we have solved the shape equations for a radical model of free energy with the help of Feoli's formalism. Applying this formalism, we show that the unknown parameters of our model are reduced.

ფიზიკა

დნმ-ის სტრუქტურის შესწავლა თავისუფალი ენერგიის მოდელში, $F = \sqrt{Ak^2 + B}$

მ. იავარი

აზადის ისლამური უნივერსიტეტი, ფიზიკის დეპარტამენტი, ქაშანის განყოფილება, ქაშანი, ირანი

(წარმოდგენილია აკადემიის წევრის ა. ხელაშვილის მიერ)

ნაშრომში ვაზოგადებთ ა. ფეოლის ფორმალიზმის შედეგებს დნმ-ის სტრუქტურისათვის. პირველად წარმოდგენილია პროფილის წონასწორული განტოლებები. ა. ფეოლის ფორმალიზმში შესწავლილია ამ განტოლებების ზუსტი ამოხსნები $F = \sqrt{Ak^2 + B}$ თავისუფალი ენერგიის მოდელში.

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