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Physics

The Helical Solutions of the Euler-Lagrange Equations for the Free Energy Model F =:~*k* +: ²:² +:¥

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ABSTRACT. The helical solutions of the Euler-Lagrange equations for the free energy model as F =:~*k* +: ²:² +:¥ are obtained. The numerical range of the free energy for A-, B-, and Z-DNA are calculated. *© 2017 Bull. Georg. Natl. Acad. Sci.*

Key words: Euler-Lagrange equations, helical solutions, DNA forms

Recently, the elastic theories have been widely used for studying the DNA structures. Many models have been suggested to study the biopolymer chains such as the worm-like chain (WLC) model [1] and the worm-like rod chain (WLRC) model [2]. The WLC model describes a chain by an elastic continuous curve under a small external force with a single elastic constant as bending modulus. This model has been successfully applied to long biomolecules such as DNA. Goldstein et al.[1] analysed a WLC model with the free energy function as $\mathrm{F} = \left(k - \mu_0\right)^2$, where F_0 and μ_0 are constants. The WLRC model is appropriate to describe the biopolymer structures under a moderate force.

The total free energy $\mathrm{F}_{\mathrm{total}}$ of a biopolymer chain may be considered as a function defined on the smooth curve $\mathrm{x}(s)$ in 3-dimensional space as

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

where *s* is the arclength of the curve and F is the free energy function. We shall use a natural parametrization of curve $\mathrm{x}(s)$ 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 summation over repeated index convention is used. The curvature and torsion are defined by [3]

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

where $\det_G$ is the Gramm determinant [4].

The Euler-Lagrange equations follow by variation of the total free energy, i.e. $\delta F_{total}=0$, and it can be written as follows

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

The Euler-Lagrange equations take the form [5]

$$F_k''+\left(k^2-\tau^2\right)F_k+2\tau\left(\frac{F_\tau'}{k}\right)'+\tau'\frac{F_\tau'}{k}+2k\tau F_\tau-kF=0, \tag{5}$$

$$2\left(\tau F_k\right)'-\left(\frac{F_\tau'}{k}\right)''+\tau^2\frac{F_\tau'}{k}-\left(kF_\tau\right)'-\tau' F_k=0, \tag{6}$$

where the over head prime stand for differentiation with respect to the natural parameter s, $F_k=\frac{\partial F}{\partial k}$ and $F_\tau=\frac{\partial F}{\partial \tau}$. These equations are highly nonlinear and complicated and so, it is very difficult to solve them.

Most of the calculations will be done by using the Maple 18 [6].

Exact Solutions of the Euler-Lagrange Equations

In 3-dimensional flat space, a smooth curve has two local invariants, curvature $k=k(s)$ and torsion $\tau=\tau(s)$. The curvature and torsion encode all geometric information of a curve in space. Hence, the free energy of a biopolymer chain is considered as a function of its curvature and torsion. Let us now discuss the free energy function as follows

$$F=\alpha k+\beta\tau^2+\gamma, \tag{7}$$

where α, β, γ are unknown constants. If we substitute this relation into Euler-Lagrange equations, then we obtain

$$2\tau\left(\frac{\tau'}{k}\right)'+\frac{\left(\tau'\right)^2}{k}+\left(\frac{3}{2}k-\alpha\right)\tau^2-\gamma k=0, \tag{8}$$

$$\left(\frac{\tau'}{k}\right)''-\frac{\tau^2\tau'}{k}+\left(k\tau\right)'-\alpha\tau'=0, \tag{9}$$

for simplicity, we have set $\beta=\frac{1}{2}$. It is obvious that the solution of these equations could not be found easily.

Helices are characterized by the constancy of the quantity $\mu=\frac{\tau}{k}$. A curve is called a helix if and only if $\mu=$ constant. Next, the helical solutions of the equations (8) and (9) are investigated. In this case, we have

$$2\left(\frac{k'}{k}\right)' + \left(\frac{k'}{k}\right)^2 + \frac{3}{2}k^2 - \sim k - \frac{\yen}{\mu^2} = 0, \tag{10}$$

$$\left(\frac{k'}{k}\right)'' - \left[\left(\mu^2 - 2\right)k + \sim\right]k' = 0. \tag{11}$$

By differentiating the equation (10) with respect to *s*, becomes

$$2\left(\frac{k'}{k}\right)'' + 2\frac{k'}{k}\left(\frac{k'}{k}\right)' + \left(3k - \sim\right)k' = 0. \tag{12}$$

By eliminating the variable $\left(\frac{k'}{k}\right)''$ from the equations (11) and (12), yields

$$2\frac{k'}{k}\left(\frac{k'}{k}\right)' + \left[\left(2\mu^2 - 1\right)k + \sim\right]k' = 0. \tag{13}$$

By comparing the last relation with the equation (10), one can deduce

$$\left(\frac{k'}{k}\right)^2 + \left(2\mu^2 + \frac{1}{2}\right)k^2 - 2\sim k - \frac{\yen}{\mu^2} = 0. \tag{14}$$

It can be shown that the exact solution of this differential equation is of the form

$$k = \frac{16\yen\, e^{\frac{\sqrt{\yen}}{\mu}s}}{e^{2\frac{\sqrt{\yen}}{\mu}s} - 16\sim\mu^2 e^{\frac{\sqrt{\yen}}{\mu}s} + 64\left(\sim^2 + 2\yen\right)\mu^4 + 32\yen\mu^2}. \tag{15}$$

In fact by choosing $= \frac{1}{2}$, we could have solved the Euler-Lagrange equations for our model. If we choose $\yen = \frac{\sim^2}{2\mu^2}$, then we have

$$\mathrm{F} = \frac{\mu^2}{2}\left(k + \frac{\sim}{\mu^2}\right)^2, \tag{16}$$

which agrees with the WLC model. In the next section, the numerical range of the free energy for A-, B-, and Z-DNA will be calculated.

Calculation of the Free Energy for DNA Forms

DNA exists in many possible conformations that include A-DNA, B-DNA and Z-DNA forms, although, only B-DNA and Z-DNA have been directly observed in the functional organisms [7]. A-DNA is a right-handed double helix with major and minor grooves fairly similar to B-DNA form, but with a shorter more compact helical structure [8]. Figure 1, shows the shapes of standard A-, B-, and Z-DNA.

B-DNA, the classic structure first described by Watson and Crick [10] is an antiparallel right-handed typical form of double helix DNA in which the chains twist up and to the right around the front of the axis of the helix. Z-DNA is one of the many possible double helical structures of DNA. It is a left-handed double helical structure with a zig-zag pattern [8-11]. The helical parameters of DNA forms are presented in Table.

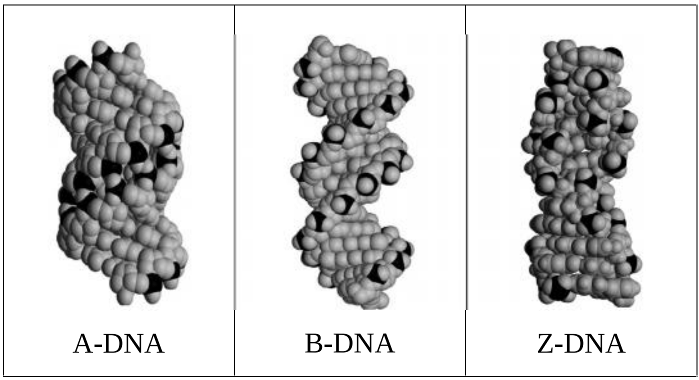

Fig. 1. Space representation of A-, B-, and Z-DNA.[9]

Table. The geometry properties of A-, B-, and Z-DNA[9]

Characteristic	A-DNA	B-DNA	Z-DNA
Helix sense	right-handed	right-handed	left-handed
Pitch (nm)	2.82	3.32	4.46
Radius (nm)	1.15	1	0.90

We now need to calculate the minimum value of the free energy function. To do this, we must have $\frac{\partial \mathrm{F}}{\partial s} = 0.$ Then it follows that

$$\sim = \frac{£\sqrt{2}\mu^2}{s}\mathrm{LambertW}\left(\frac{£\sqrt{2}s}{16\mu^4 + 8\mu^2}\right), \tag{17}$$

here $£ = \pm 1$ and Lambert W function is defined by [12]

$$\mathrm{LambertW(x)e}^{\mathrm{LambertW(x)}} = \mathrm{x}, \tag{18}$$

where x is an arbitrary variable. Also, the Lambert W function has series expansion as

$$\mathrm{LambertW(x)} = \sum_{n=1}^{\infty} \frac{(-n)^{n-1}}{n!}\mathrm{x}^n. \tag{19}$$

Next, there are three cases which must be discussed separately:

Case (1) : A-DNA

Using Table, the geometrical invariants are $k_0 = 0.7546$ and $^2{}_0 = 0.2945$. Thus, we have $\mu = 0.3902$. Using these data and equation (17), after some calculation, becomes

$$\mathrm{F}(s) = \frac{0.2431u^6 + \left(0.1523e^{3u}s^2 + 0.3650£ue^{2u}s + 0.6036u^2e^u + 0.4612£u^3\right)u^2e^us^2}{\left(e^{2u}s^3 + 0.5249£ue^us^2 + 1.2635u^2s\right)^2}, \tag{20}$$

where $u = \mathrm{LambertW}(0.8896£s)$.

By plotting F in terms of s for the case $£ = +1$ (see Figure 2), we find that

$$0 < \mathrm{F}_{\text{A-DNA}} < 1.25, \tag{21}$$

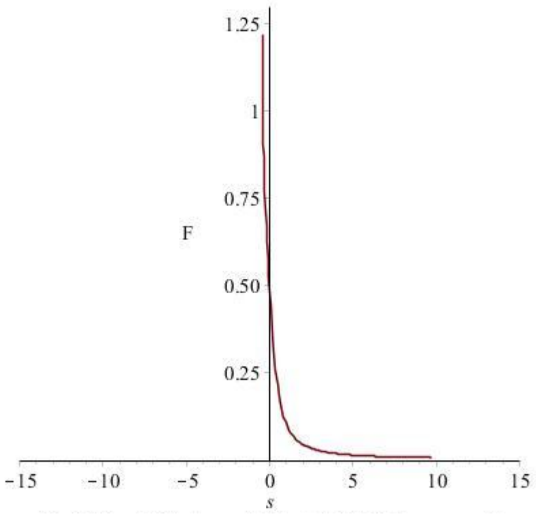

Fig. 2. Graph F in terms of *s* for A-DNA in the case ε=+1

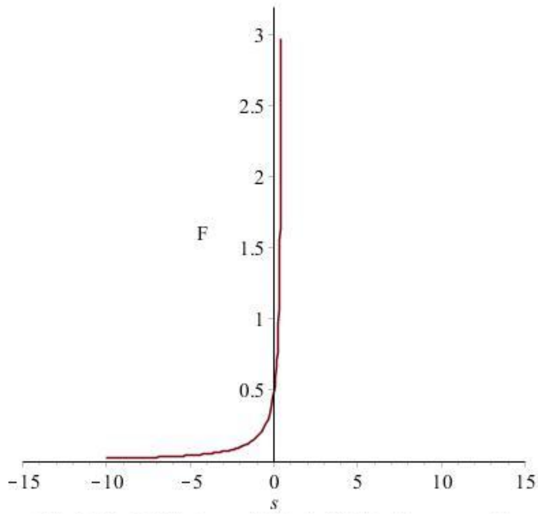

Fig. 3. Graph F in terms of *s* for A-DNA in the case ε= –1

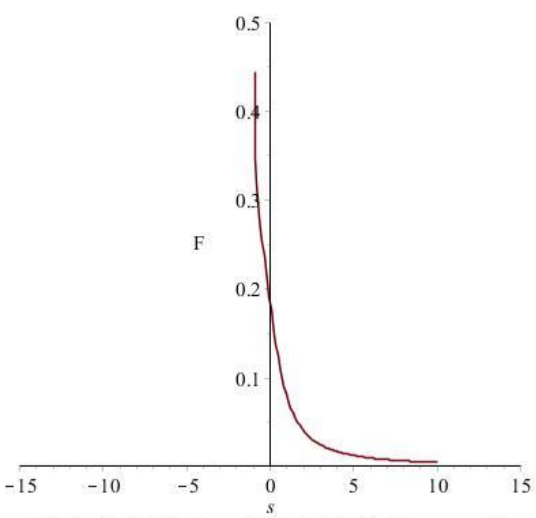

Fig. 4. Graph F in terms of *s* for B-DNA in the case ε=+1

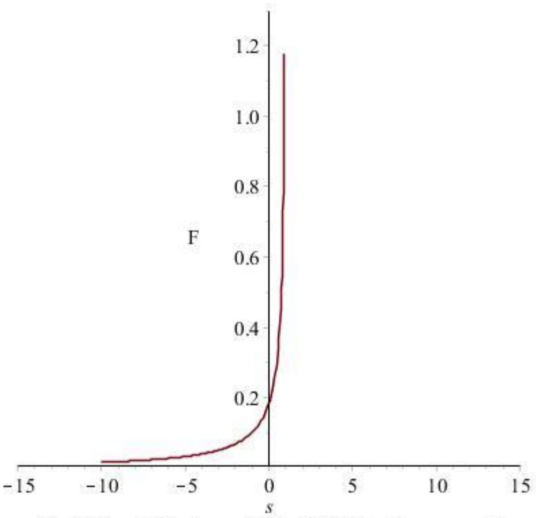

Fig. 5. Graph F in terms of *s* for B-DNA in the case ε= –1

and for the case $\varepsilon = -1$ (see Figure 3), we have

$$0 < \mathrm{F}_{\text{A-DNA}} < 3, \tag{22}$$

we recall that the unit of the free energy is kcal/mol.

Case (2) : B-DNA

In this case, the geometrical invariants are $k_0 = 0.7817$ and $\tau_0 = 0.4130$. So, we have $\mu = 0.5283$. Similarly as in previous case, the following solution is obtained

$$\mathrm{F}(s) = \frac{10.2324y^6 + \left(0.2791e^{3y}s^2 + 0.7787\varepsilon\, ye^{2y}s + 3.9233y^2e^y + 4.7152\varepsilon\, y^3\right)y^2e^ys^2}{\left(e^{2y}s^3 + 1.7630\varepsilon\, ye^ys^2 + 6.0545y^2s\right)^2}, \tag{23}$$

where $y = \mathrm{LambertW}(0.4064\varepsilon\, s)$.

By plotting F in terms of *s* for the case $\varepsilon = +1$ (see Figure 4), we can conclude

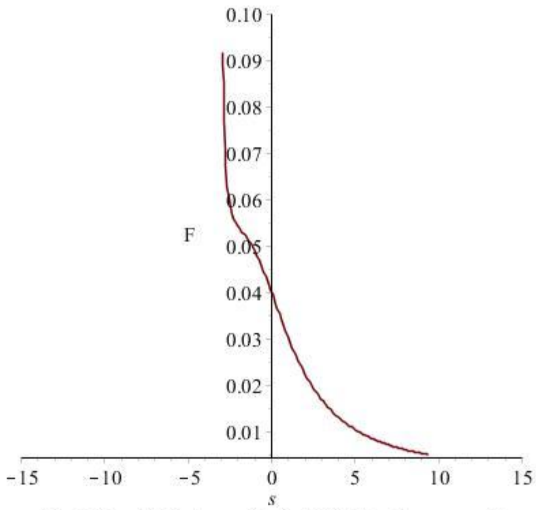

Fig. 6. Graph F in terms of *s* for Z-DNA in the case ε=+1

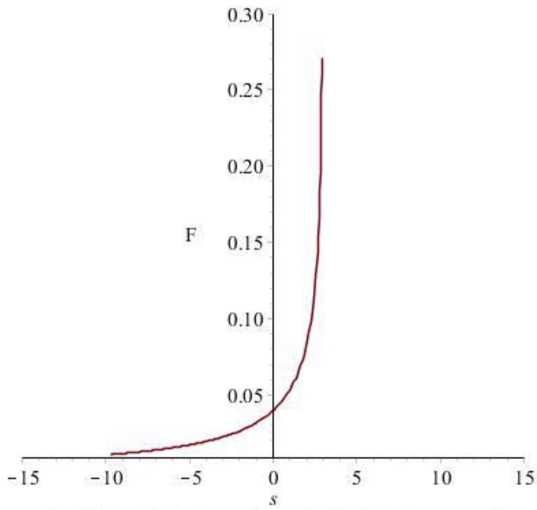

Fig. 7. Graph F in terms of *s* for Z-DNA in the case ε= −1

$$0 < \mathrm{F}_{\text{B-DNA}} < 0.45, \tag{24}$$

and for the case $\varepsilon = -1$ (see Figure 5), we obtain

$$0 < \mathrm{F}_{\text{B-DNA}} < 1.2\ . \tag{25}$$

Case (3) : Z-DNA

In this case, the principal curvatures are $k_0 = 0.6850$ and $\tau_0 = 0.5402$. Hence, $\mu = 0.7886$. After some tedious calculations, the following result is obtained

$$\mathrm{F}(s) = \frac{2414.8666m^6 + \left(0.6219e^{3m}s^2 + 2.1338\varepsilon m e^{2m}s + 79.3373m^2e^m + 132.9674\varepsilon m^3\right)m^2e^m s^2}{\left(e^{2m}s^3 + 8.7516\varepsilon m e^m s^2 + 62.3135m^2 s\right)^2}, \tag{26}$$

where $m = \mathrm{LambertW}(0.1266\varepsilon s)$.

By plotting F in terms of *s* for the case $\varepsilon = +1$ (see Figure 6), one obtains

$$0 < \mathrm{F}_{\text{Z-DNA}} < 0.095, \tag{27}$$

and for the case $\varepsilon = -1$ (see Figure 7), we see that

$$0 < \mathrm{F}_{\text{Z-DNA}} < 0.27\ . \tag{28}$$

Conclusion

The Euler-Lagrange equations are nonlinear and complicated, so it is difficult to solve them. We have solved exactly these equations for a linear model of free energy as a WLC model. Also, we have determined the free energy function in terms of the parameter *s* for DNA forms with the help of Maple software.

ფიზიკა

ეილერ-ლაგრანჟის განტოლებების სპირალური ამოხსნები F =:~*k* +: ^{2}:^{2} +:¥ მოდელში

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(წარმოდგენილია აკადემიის წევრის ა. ხელაშვილის მიერ)

ნაპოვნია ეილერ-ლაგრანჟის განტოლებების ამოხსნა F =:~*k* +: ^{2}:^{2} +:¥ თავისუფალი ენერგიის მოდელში. დადგენილია თავისუფალი ენერგიის რიცხვითი მნიშვნელობების არე A-, B- და Z-DNA-თვის.

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