Comment on “Modulating DNA configuration by interfacial traction: an elastic rod model to characterize DNA folding and unfolding”

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Abstract In this comment, we point out that the tractions induced by interfacial energy, which are referred to as the tractions on the central axis curve of the DNA elastic rod presented by Huang (J. Biol. Phys. **37**(1), 79–90, 2011), are incorrect. The correct tractions are provided in this literature. Further, with the use of the correct tractions, we present new numerical results, which for the values given by Zaixing Huang do not give rise to the physical behavior observed for DNA by the author.

Keywords DNA configuration · Interfacial traction · DNA folding and unfolding · Comment

1 Introduction

The mechanical deformation of DNA is important in many biological processes, such as genome packaging, DNA replication, and transcription. Kirchhoff's theory of elastic rods [4, 8, 9, 11] can be easily applied to many systems with great success, leading to a simple and elegant way for developing some insight into possible behaviors of rods. This approach is used to research DNA configuration and successfully explain many phenomena, which are observed in experiments [6].

It is well-known that DNA is always in an intracellular solution. The interaction of the DNA chain with the intracellular solution is a very important determinant of the DNA configuration [1]. Recently, Huang used an elastic rod model to characterize DNA folding and unfolding subjected to a rod-solution interfacial traction. However, in that work, the calculations of the interfacial energy tractions are incorrect. Thus, the aim of this paper is to correct this error and show the DNA configurations under revised tractions.

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Fig. 1 **a** A fragment of a DNA elastic rod with radius r_0 , and the length of central line ds . C and C' are the cross-sections on the two ends. **b** The left cross-section of the rod. When the cross-section moves along the central line from the left end to the right end, Q changes to Q'

The layout of this paper is as follows. Firstly, in the next section, the tractions induced by DNA-solution interaction are corrected. In Section 3, equilibrium configuration equations of DNA are proposed and Section 4 numerically simulates the DNA configuration under revised tractions. Finally, some conclusions are drawn.

2 Interfacial tension acting at an elastic rod

In order to characterize DNA folding and unfolding, Huang used a thin elastic rod, which was subjected to interfacial interactions to investigate the equilibrium configuration of DNA in solution. Here we point out that the tractions induced by the interfacial energy are incorrect, and state the correct version of the tractions.

As a coarse-grained description, a DNA can be approximately regarded as a thin flexible and inextensible circular rod or string [9, 12, 13]. The classical theory of elasticity describes the geometry of an elastic rod in terms of its center line $\mathbf{R} = \mathbf{R}(s) = (x(s), y(s), z(s))$, a three-dimensional curve parameterized by its arclength s and a frame of three unit vectors α, β, γ associated with each cross-section of the rod, where $\alpha = \dot{\mathbf{R}}$ is the tangent vector ($\dot{\mathbf{R}}$ denotes the derivative of $\mathbf{R}$ with respect to s), $\beta = \dot{\alpha}$ is the main normal vector and $\gamma = \alpha \times \beta$ is the binormal vector. Between those unit vectors, these are the Frenet formulae: $d\alpha/ds = \kappa\beta$, $d\beta/ds = -\kappa\alpha + \tau\gamma$ and $d\gamma/ds = -\tau\beta$, where κ and τ are the curvature and torsion of the central line $\mathbf{R}$, respectively [12]. In local orthonormal basis P -xyz, the x - and y - axes are the two principal inertial axes of the cross-section through the point P . The angle between the principal normal α and the x -axis (or the binormal β and y -axis) is called the twisting angle, denoted by χ .

As shown in Fig. 1, point Q is fixed on the cross-section ring (on the left end of the rod) and the angle between PQ and β is θ . When the cross-section ring moves along the central line from the left end to the right end, Q changes to Q' (note that the cross-section ring can turn around the central axis). In this process, the angular displacement of point P in the local coordinates (x, y, z) is $d\theta$ and the change of χ is $d\chi$. The shape of the rod surface can be

obtained by this way: the central point of a ring with the radius r_0 moves along a line R and keeps the ring upright to the tangent of R . It means the ring is in the normal plane of the central line R . When Y is the shape of the rod surface:

$$Y = R + r = R + r_0 \cos \theta \beta + r_0 \sin \theta \gamma, \quad (1)$$

where the parameter $0 \leq \theta < 2\pi$. Defining (μ, ν) to be the local coordinates on Y , where μ is along the tangent of the central line of R and ν is upright to R , there are $d\mu = ds$ and $d\nu = r_0 d\theta$. Making use of Frenet formulae, we obtain the first fundamental quantity of the surface:

$$\begin{aligned} E &= Y_\mu \cdot Y_\mu = (1 - r_0 \kappa \cos \theta)^2 + r_0^2 \tau^2, \\ F &= Y_\mu \cdot Y_\nu = r_0 \tau, \\ G &= Y_\nu \cdot Y_\nu = 1. \end{aligned} \quad (2)$$

where $Y_\mu = \frac{\partial Y}{\partial \mu}$. The second fundamental quantity of the surface is:

$$\begin{aligned} L &= Y_{\mu,\mu} \cdot n = -\kappa \cos \theta (1 - r_0 \kappa \cos \theta) r_0 \tau^2, \\ M &= Y_{\mu,\nu} \cdot n = \tau, \\ N &= Y_{\nu,\nu} \cdot n = 1/r_0. \end{aligned} \quad (3)$$

where n is the main normal vector of the rod surface:

$$n = \frac{Y_\mu \times Y_\nu}{|Y_\mu \times Y_\nu|} = -r/r_0 \quad (4)$$

Consequently we can easily obtain the mean curvature of the surface at the point Q :

$$\Lambda = \frac{LG - 2MF + NE}{2(EG - F^2)} = \frac{1 - 2r_0 \kappa \cos \theta}{2r_0(1 - r_0 \kappa \cos \theta)}. \quad (5)$$

Following ref. [4], the interactions of the DNA chain with the solution surrounding the rod can be characterized by interfacial pressure between the solution and the rod. According to the Young-Laplace formula [7], the interfacial traction at point Q reads:

$$p = \sigma(\kappa_1 + \kappa_2) = 2\sigma\Lambda = \sigma \frac{1 - 2r_0 \kappa \cos \theta}{r_0(1 - r_0 \kappa \cos \theta)} \quad (6)$$

where p is the normal traction on the interfacial surface and κ_1, κ_2 are two principal curvatures of the surface at point Q . And σ is the interfacial energy factor, which is a positive constant and represents a composite effect of hydrophilic and hydrophobic patches along the DNA surface and relates to the solution environment. In coordinates P -xyz, (6) can be decomposed into:

$$\begin{aligned} p_1 &= -\sigma \frac{1 - 2r_0 \kappa \cos \theta}{r_0(1 - r_0 \kappa \cos \theta)} \cos(\theta - \chi), \\ p_2 &= -\sigma \frac{1 - 2r_0 \kappa \cos \theta}{r_0(1 - r_0 \kappa \cos \theta)} \sin(\theta - \chi), \\ p_3 &= 0. \end{aligned} \quad (7)$$

Fig. 2 The tractions f_1 and f_{1h} with $\sigma = 5.0 \times 10^{-4}$ nN/nm, $\chi = 0$, $r_0 = 1$ nm

By integrating the above equations along the perimeter of the cross-section of the rod, the correct tractions on the central axis curve $\mathbf{R}$ can be obtained:

$$f_1 = \int_0^{2\pi} -\sigma r_0 \frac{1 - 2r_0\kappa \cos \theta}{r_0(1 - r_0\kappa \cos \theta)} \cos(\theta - \chi) d\theta = -\frac{2\pi\sigma \cos \chi}{r_0\kappa} \left(1 - \frac{1}{\sqrt{1 - r_0^2\kappa^2}} \right),$$

$$f_2 = \int_0^{2\pi} -\sigma r_0 \frac{1 - 2r_0\kappa \cos \theta}{r_0(1 - r_0\kappa \cos \theta)} \sin(\theta - \chi) d\theta = \frac{2\pi\sigma \sin \chi}{r_0\kappa} \left(1 - \frac{1}{\sqrt{1 - r_0^2\kappa^2}} \right),$$

$$f_3 = 0. \quad (8)$$

In the following, we compare the above f_1 and $f_{1h} = \frac{2\pi\sigma}{r_0\kappa} \cos \chi$ in ref. [4]. Figure 2 shows the figures of f_1 and f_{1h} with respect to κ at the condition $\sigma = 5.0 \times 10^{-4}$ nN/nm, $\chi = 0$, $r_0 = 1$ nm. It is easy to find that the difference between f_1 and f_{1h} is substantial. Because of the different interfacial tractions, the DNA segment may undergo a different reconfiguration. One can find that the interfacial f_1 increases with the increase of the curvature κ . Especially, when the curvature $\kappa = 0$,

$$f_1(0) = \lim_{\kappa \rightarrow 0} -\frac{2\pi\sigma \cos \chi}{r_0\kappa} \left(1 - \frac{1}{\sqrt{1 - r_0^2\kappa^2}} \right) = 0. \quad (9)$$

This is to say that, for a straight that rod, the interfacial traction is zero, which is canceled out around the rod. However, $\kappa = 0$ is the singularity of $f_{1h} = \frac{2\pi\sigma}{r_0\kappa} \cos \chi$, which means the curvature cannot be zero, which is inconsistent with reality.

Fig. 3 **a** DNA configuration under revised traction. **b** DNA configuration under incorrect traction in ref. [4] with $\sigma = 5.0 \times 10^{-4} \text{ nN/nm}$, $E = 0.16 \text{ nN/nm}^2$

3 Kirchhoff's equations

For the simplified 2D model, which is referred to in ref. [4], the equilibrium configuration equations of the simplified model, which follows $\tau = 0$ and $\chi = 0$, should be modified to:

$$\begin{aligned} \frac{dF_1}{ds} + (\kappa_0 + \kappa) F_3 - \frac{2\pi\sigma}{r_0(\kappa + \kappa_0)} \left(1 - \frac{1}{\sqrt{1 - r_0^2(\kappa + \kappa_0)^2}} \right) &= 0, \\ \frac{dF_3}{ds} - (\kappa_0 + \kappa) F_1 &= 0, \\ B \frac{d\kappa}{ds} + F_1 &= 0, \\ \frac{dx}{ds} &= \cos \theta, \\ \frac{dy}{ds} &= \sin \theta, \\ \frac{d\theta}{ds} &= \kappa + \kappa_0. \end{aligned} \quad (10)$$

where $F_i (i = 1, 3)$ is the stress resultant acting at the center of the cross-section and κ_0 denotes the curvature of the original configuration of the rod. x, y are the horizontal and vertical coordinates of the central axis curve $\mathbf{R}$ in the plane, respectively. The bending stiffness is $B = \pi E r_0^4 / 4$, and E is Young's modulus.

4 Numerical results

In this section, we use the values of ref. [4] to numerically solve the above equilibrium configuration equations. The aim is to show the configuration under the correct interfacial tractions. In ref. [4], $r_0 = 1 \text{ nm}$, the initial condition is $F_1(0) = F_3(0) = 0$, $\kappa(0) = 0$, $x(0) = y(0) = 0$ and $\theta(0) = 0$.

Fig. 4 **a** DNA configuration under revised traction. **b** DNA configuration under incorrect traction in ref. [4] with $\sigma = 5.0 \times 10^{-6} \text{ nN/nm}$, $E = 1.6 \text{ nN/nm}^2$

Firstly, consider the interfacial energy factor $\sigma = 5.0 \times 10^{-4} \text{ nN/nm}$, and Young's modulus $E = 0.16 \text{ nN/nm}^2$. Using the classical Runge-Kutta algorithm, we calculate the configuration corresponding to the original configuration in Fig. 3 of ref. [4]. From the result that is shown in Fig. 3, one can see that the DNA segment does not coil into a “toroid” as shown in Fig. 3b spontaneously [5]. However, the shape of the DNA segment changes and the area occupied by the DNA segment decreases comparing with the original configuration.

Figures 4a and 5a show the DNA configuration under revised traction with $\sigma = 5.0 \times 10^{-6} \text{ nN/nm}$, $E = 1.6 \text{ nN/nm}^2$ and $\sigma = 5.0 \times 10^{-8} \text{ nN/nm}$, $E = 16 \text{ nN/nm}^2$, respectively. Clearly, the reconfiguration of the DNA is significantly different with respect to Figs. 4b and 5b. This shows that the interfacial traction has a significant influence on the conformation of the DNA and correct traction is important for the DNA configuration

Fig. 5 **a** DNA configuration under revised traction. **b** DNA configuration under incorrect traction in ref. [4] with $\sigma = 5.0 \times 10^{-8} \text{ nN/nm}$, $E = 16 \text{ nN/nm}^2$

Fig. 6 DNA configuration with initial curvature 0.1nm^{-1} , $\sigma = 4.5 \times 10^{-2}\text{nN/nm}$ and $E = 1.6\text{nN/nm}^2$

research. From Figs. 3a–5a, one can also observe that the DNA segment has experienced different degrees of deformation under different interfacial tension σ and Young’s modulus E , which are on behalf of different solution environments qualitatively and consistent with ref. [4].

To one’s surprise, the DNA segment coils into a toroid with the interfacial traction increasing, which is shown in Fig. 6. This further illustrates that the equilibrium configuration of DNA can be determined by competition between the interfacial energy and elastic strain energy.

5 Conclusions

In this paper, the incorrect interfacial tractions are corrected and numerical simulations of DNA configuration are done by using the values of ref. [4]. Numerical results show that the DNA segment does not coil into a ‘toroid’ and undergoes a different configuration compared with the ones in ref. [4]. However, a toroid can appear when the interfacial traction is great.

Finally, it should be noted that, this is only a coarse-grained model characterizing interaction potentials between DNA segments and solution, and the deformations of elastic under applied end forces [2, 3, 10] should be considered in future models.

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