Closed loops of a thin elastic rod and its symmetric shapes with self-contacts

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Abstract

The thin elastic rod is a traditional model for the large-scale structure of long DNA molecules. The solutions for closed equilibria are considered. Particular attention is paid to the shapes with self-contacts. A new class of analytical solutions of the corresponding boundary value problem is presented. Its relation to the known multi-leafed "rose-like" symmetric shapes is discussed.

Key words: Thin elastic rod, Equilibrium, Loop, BVP, DNA.

AMS subject classifications: 73K05, 92E10.

1 Introduction

Since late 70-s, there has been a considerable interest in studying the large-scale conformations of deoxyribonucleic acid (DNA) molecules by using the model of a thin elastic rod [1, 2]. The radius of the double right-handed helix of DNA is about 1 nm and its length may achieve 1000 nm or even more. Approximately 10 base pairs correspond to one turn of the helix in the relaxed state. The specific conformations of DNA can facilitate or hinder various biochemical processes, including replication, transcription, and recombination. The segments as long as 150-200 base pairs are relatively stiff and may be modelled on the basis of Kirchoff's theory of linear elastic rods [3, 4, 5]. The elastic properties of the rod are characterized by three stiffness coefficients: two bending and one torsional. Their effective values for the DNA rod were determined by using the experimental data [2, 6].

2 Model and equations

A thin elastic rod is considered. It is assumed to be inextensible and homogeneous in the sense that its elastic properties are independent of the position on the rod axis. The centerline of the rod is parametrized with the arc length s. The points on the centerline are described by their radius vector $\mathbf{r}(s)$ with respect to an origin O. The tangent vector $\mathbf{t}(s) = \frac{d\mathbf{r}(s)}{ds}$, the normal $\mathbf{n}(s) = \frac{d\mathbf{r}(s)}{ds}/|\frac{d\mathbf{r}(s)}{ds}|$ and the binormal $\mathbf{b} = \mathbf{t} \times \mathbf{n}$ form a natural trihedral $\mathbf{t}, \mathbf{n}, \mathbf{b}$. We define also the principal trihedral $\mathbf{e_1}(s), \mathbf{e_2}(s), \mathbf{e_3}(s), \mathbf{e_1} = \mathbf{t}$ and the unit vectors $\mathbf{e_2}, \mathbf{e_3}$ are along the principal axes of the cross section of the rod.

The vector $\boldsymbol{\omega}$ is the angular velocity of rotation of the trihedral $\mathbf{e_1}, \mathbf{e_2}, \mathbf{e_3}$ as it moves along the centerline with the unit velocity. It may be represented as a sum of three components $\boldsymbol{\omega} = \sum_{i=1}^{3} \omega_i \mathbf{e_i}$, $\omega_1 = \tau + \frac{d\chi}{ds}$ is the torsion of the rod, χ the angle between $\mathbf{n}$ and $\mathbf{e_2}$, $\omega_2 = \kappa \sin\chi, \omega_3 = \kappa\cos\chi$ are the principal curvatures of the rod, κ and τ are the geometrical curvature and the torsion of the centerline, respectively.

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The equilibrium state of the rod is described in the principal reference frame by the equations [3]

$$\frac{d\mathbf{F}}{ds}+\boldsymbol{\omega}\times\mathbf{F}+\mathbf{f}=0\ ,\quad \frac{d\mathbf{M}}{ds}+\boldsymbol{\omega}\times\mathbf{M}+\mathbf{t}\times\mathbf{F}+\mathbf{m}=0. \tag{1}$$

Here $\mathbf{F}(s)$ denotes the resultant of the internal forces acting on the cross section and $\mathbf{M}(s)$ the net moment of these forces. We assume that $\mathbf{F}(\sigma)$ $(\mathbf{M}(\sigma))$ is the force (moment) with which one part of the rod $(s>\sigma)$ acts on the other part. In Eq. (1), $\mathbf{f}(s)$ and $\mathbf{m}(s)$ are the densities of external forces and moments applied to the rod.

The first case we consider is one when no such external forces and moments act, i.e., we put $\mathbf{f}=0, \mathbf{m}=0$. Then the first Eq. (1) implies $\mathbf{F}=\boldsymbol{const}$ in the absolute space. Let $\boldsymbol{\gamma}$ be the unit vector in the direction of $\mathbf{F}$. We may write $\mathbf{F}=P\boldsymbol{\gamma},\ P=\|\mathbf{F}\|\geq 0,\ \|\boldsymbol{\gamma}\|=1,\ \boldsymbol{\gamma}=\sum_{i=1}^{3}\gamma_i\mathbf{e_i}$.

The Hooke constitutive relation completes the equilibrium equations

$$M_i=\sum_{j=1}^{3}B_{ij}(\omega_j-\omega_j^0),\quad \mathbf{M}=\sum_{i=1}^{3}M_i\mathbf{e_i},$$

$\omega_j^0, j=1,2,3$, are the torsion and curvatures of the rod in its relaxed, non-deformed state. We assume that the rod is initially straight (i.e., $\omega_2^0=\omega_3^0=0$) but it may be twisted. The rod is supposed to be symmetric and we put $B_{ij}=0$ for $i\neq j, B_{ii}=B_i, B_2=B_3$.

Under the above assumptions we come after normalization to the equilibrium equations

$$\frac{d\omega_1}{ds}=0,\quad \frac{d\omega_2}{ds}+\omega_3(d-\omega_1)-\frac{p}{2}\gamma_3=0,\quad \frac{d\omega_3}{ds}-\omega_2(d-\omega_1)+\frac{p}{2}\gamma_2=0, \tag{2}$$

where $b=B_1/B_2, p=2P/B_2, d=b(\omega_1-\omega_1^0)$.

Eqs. (2) allow for the first integrals:

$$\omega_1=\omega_1^*=const, \tag{3}$$
$$\gamma_1 d+\omega_2\gamma_2+\omega_3\gamma_3=l=const, \tag{4}$$
$$\omega_2^2+\omega_3^2+p\gamma_1=h=const. \tag{5}$$

Eq. (3) implies immediately that $d=b(\omega_1^*-\omega_1^0)=const$.

We choose an absolute coordinate system $O\xi\eta\zeta$ fixed in space such that the direction of the ζ-axis is opposite to $\boldsymbol{\gamma}$. The three Euler angles ψ,ϕ,θ are chosen to describe rotation of the principal trihedral with respect to the absolute coordinates. Then we have in these coordinates $-\boldsymbol{\gamma}=(\cos\theta,\sin\theta\sin\phi,\sin\theta\cos\phi)^T$ and

$$\omega_1=\frac{d\phi}{ds}+\frac{d\psi}{ds}\cos\theta,\quad \omega_2=\frac{d\psi}{ds}\sin\theta\sin\phi+\frac{d\theta}{ds}\cos\phi,\quad \omega_3=\frac{d\psi}{ds}\sin\theta\cos\phi-\frac{d\theta}{ds}\sin\phi. \tag{6}$$

The integrals Eq. (4) and Eq. (5) take the form

$$\gamma_1 d-(1-\gamma_1^2)\frac{d\psi}{ds}=l, \tag{7}$$

$$(1-\gamma_1^2)\left(\frac{d\psi}{ds}\right)^2+\left(\frac{d\theta}{ds}\right)^2+p\gamma_1=h. \tag{8}$$

After eliminating the derivative $\frac{d\psi}{ds}$ from Eq. (7) and Eq. (8), we obtain

$$\left(\frac{d\gamma_1}{ds}\right)^2=f(\gamma_1),\quad f(\gamma_1)=(h-p\gamma_1)(1-\gamma_1^2)-(l-\gamma_1 d)^2. \tag{9}$$

We are here interested in the case of non-zero end force, when the cubic polynomial $f(\gamma_1)$ may be written as

$$f(\gamma_1)=p(\gamma_1-g_1)(\gamma_1-g_2)(\gamma_1-g_3),\quad -1\leq g_1\leq g_2\leq 1\leq g_3. \tag{10}$$

Since $|\gamma_1|\leq 1$, a real solution of Eq. (9) is possible only in the interval $g_1\leq\gamma_1\leq g_2$.

Eq. (9) may be integrated to find

$$\gamma_1=g_1+(g_2-g_1)\,\mathrm{sn}^2\,\Omega(s-s_0), \tag{11}$$

where $\Omega^2 = p(g_3 - g_1)/4$, sn is the Jacobi elliptic sine of the modulus k, $k^2 = (g_2 - g_1)/(g_3 - g_1)$.

It is convenient to express the shape of the centerline in space in the cylindrical coordinates ρ, α, ζ (see the solution of problem 5 on pp. 87–88 in [4]): $\zeta = \rho\cos\alpha, \eta = \rho\sin\alpha$. The equations for these coordinates are as follows [5]

$$\rho = \frac{2\sqrt{d^2 - l^2 + h - p\gamma_1}}{p}, \tag{12}$$

$$\frac{d\alpha}{ds} = \frac{p(l\gamma_1 - d)}{2(d^2 - l^2 + h - p\gamma_1)}, \tag{13}$$

$$\frac{d\zeta}{ds} = -\gamma_1. \tag{14}$$

The two last equations may be readily integrated to get

$$\alpha - \alpha_0 = -\frac{l}{2}(s - s_0) + \frac{l(d^2 - l^2 + h) - pd}{2\Omega(d^2 - l^2 + h - pg_1)}\Pi(\Omega(s - s_0), n, k), \quad n = \frac{p(g_2 - g_1)}{d^2 - l^2 + h - pg_1}, \tag{15}$$

$$\zeta - \zeta_0 = -g_3(s - s_0) + 2\sqrt{\frac{g_3 - g_1}{p}}\,\mathrm{E}(\Omega(s - s_0), k), \tag{16}$$

where

$$\mathrm{E}(u, k) = \int_0^u \mathrm{dn}^2\, w dw, \quad \Pi(u, n, k) = \int_0^u \frac{dw}{1 - n\,\mathrm{sn}^2\, w}$$

are the incomplete elliptic integrals of the second and third kind, respectively.

It may be shown that Eq. (12) and Eq. (13) take a simpler form in case when the centerline intersects the ζ-axis, i.e., when $\rho(s^*) = 0$ for some s^*. Namely,

$$\rho = \frac{4\Omega k}{p}|\,\mathrm{cn}\,\Omega(s - s_0)|, \tag{17}$$

$$\alpha - \alpha_0 = -\frac{l}{2}(s - s_0) \pm \begin{cases} \pi\lfloor\frac{\Omega(s - s_0) + \mathrm{K}}{2\,\mathrm{K}}\rfloor, & \Omega(s - s_0) \neq \mathrm{K}(2j + 1), \\ \frac{\pi}{2} + \pi j, & \Omega(s - s_0) = \mathrm{K}(2j + 1), \quad j = 0, \pm1, \pm2, \ldots \end{cases}, \tag{18}$$

where $\lfloor x \rfloor$ signifies the greatest integer not greater than x, $\mathrm{K} = \mathrm{K}(k)$ is the complete elliptic integral of the first kind.

This case was specifically considered by Shi and Hearst ([7], Appendix C) though taking the limit was not carried out correctly and, as a result, their expression for the polar angle is different from Eq. (18).

3 Closed shapes

In this paper we deal with closed configurations of a special kind. It is assumed that the rod loop begins and ends in the same point, and this point is the origin of the absolute reference frame that was introduced above. Suppose that the length of the loop is $S = \frac{1}{m_0}$, where m_0 is an integer parameter (this causes no loss of generality, since the proper scaling of parameters may compensate for the fixation of the rod length). The following boundary value problem (BVP) may be formulated then

$$1)\ \ \rho(s_1) = \rho\left(s_1 + \frac{1}{m_0}\right) = 0, \quad 2)\ \ \zeta(s_1) = \zeta\left(s_1 + \frac{1}{m_0}\right). \tag{19}$$

Taking into account the symmetry property of the function $\gamma_1(s)$ with respect to the s_0: $\gamma_1(s_0 - s) = \gamma_1(s_0 + s)$, we put $s_1 = s_0 - \frac{1}{2m_0}$ to satisfy the first equality in Eq. (19,1). Eq. (16) and the last condition of the BVP, Eq. (19,2), with the help of the definition of Ω, imply

$$g_3 = \frac{8m_0\Omega}{p}\,\mathrm{E}\left(\frac{\Omega}{2m_0}, k\right) \quad g_1 = \frac{4\Omega}{p}\left[2m_0\,\mathrm{E}\left(\frac{\Omega}{2m_0}, k\right) - \Omega\right]. \tag{20}$$

Using the expression for the modulus k, we can obtain the equation for the remaining root

$$g_2 = \frac{4\Omega}{p}\left[2m_0\,\mathrm{E}\left(\frac{\Omega}{2m_0}, k\right) - (1 - k^2)\Omega\right]. \tag{21}$$

Our aim now is to obtain the parameters p, l, d and h as functions of the normalized roots $\overline{g}_i = pg_i, i = 1, 2, 3$. To achieve this, we may use the form of the function f in Eq. (9). After some algebra, we come to the expression for p: $p_{1,2}^2 = 2l^2 G_2 - B \pm \sqrt{-f(G_2)}$, where $B = \overline{g}_1\overline{g}_2 + \overline{g}_2\overline{g}_3 + \overline{g}_3\overline{g}_1$ and $G_2 = \overline{g}_1 + (\overline{g}_2 - \overline{g}_1)\,\mathrm{sn}^2\left(\frac{\Omega}{2m_0}\right)$. Clearly, $\overline{g}_1 \le G_2 \le \overline{g}_2$ and $-f(G_2) \le 0$. The only possibility to have the parameter p real is to put $G_2 = \overline{g}_2$, which implies $\Omega = 2\,\mathrm{K}\,m_0$ (we are here interested in the minimal value for Ω). We have for the parameters then

$$p^2 = \overline{g}_1\overline{g}_2 + \overline{g}_2\overline{g}_3 - \overline{g}_3\overline{g}_1, \quad l^2 = \overline{g}_1 + \overline{g}_3, \quad d^2 = \frac{\overline{g}_2^2 l^2}{p^2}, \quad h = \overline{g}_1 + \overline{g}_2 + \overline{g}_3 - d^2. \tag{22}$$

The values $\overline{g}_1, \overline{g}_2, \overline{g}_3$ can be found as functions of m_0 and k from Eqs. (20), (21)

$$\overline{g}_1 = 16m_0^2\,\mathrm{K}(k)[\mathrm{E}(k) - \mathrm{K}(k)], \quad \overline{g}_2 = 16m_0^2\,\mathrm{K}(k)[\mathrm{E}(k) - (1-k^2)\,\mathrm{K}(k)], \quad \overline{g}_3 = 16m_0^2\,\mathrm{K}(k)\,\mathrm{E}(k), \tag{23}$$

where $\mathrm{E}(k)$ denotes the complete elliptic integral of the second kind. Eq. (22), together with Eq. (23), gives us the analytical expressions of the parameters p, l, d, h as functions of k and m_0. The modulus k varies between zero and the maximal value $k_{max} \approx 0.9089$, which is the root of the equation $\mathrm{K}(k) = 2\,\mathrm{E}(k)$. It may be obtained as an equation for the extremal values of the roots g_1 and g_3: $g_1 = -g_3$. Since $g_1 \ge -1$ and $g_3 \ge 1$, the last equation implies both $g_1 = -1$ and $g_3 = 1$. For $k = k_{max}$, we obtain from Eq. (22) $l = 0$ and $d = 0$. The centerline shape is (one half of) the planar figure-8 with self-contact at the origin:

$$\xi = \frac{k}{2\,\mathrm{K}(k)}\,\mathrm{cn}((4s-1)\,\mathrm{K}(k)), \quad \zeta = \frac{1}{2\,\mathrm{K}(k)} Z((4s-1)\,\mathrm{K}(k)), \quad 0 \le s \le \frac{1}{2} \tag{24}$$

(we chose $m_0 = 2$, hence, the length of the whole figure-8 is equal to 1); $Z(u) = \mathrm{E}(u,k) - \mathrm{E}(k)u/\,\mathrm{K}(k)$ is Jacobi's Zeta function.

The figure-8 gives us the simplest example of a smoothly-closed configuration with self-contact in the origin. The shape consists of two identical loops, one of which is turned through the angle π around the ζ-axis with respect to the other. It is known [8] that there exists a countable set of more complex spatial conformations, containing m_0 identical loops which have been turned accordingly around the ζ-axis. These particular symmetric solutions were called roses and their existence was shown in [9] though no closed form expression was obtained for them. Now we compute the values of parameters that allow for assembling the rose-like shapes from the loop solutions. From Eqs. (17), (18), and (16), we can find the shape of the loop of length $1/m_0$

$$\rho = \frac{8m_0 k\,\mathrm{K}(k)}{p}\,\mathrm{cn}((2m_0 s - 1)\,\mathrm{K}(k)), \ \alpha = -\frac{l}{2}\left(s - \frac{1}{2m_0}\right), \ \zeta = \frac{8m_0\,\mathrm{K}(k)}{p} Z((2m_0 s - 1)\,\mathrm{K}(k)), \ 0 \le s \le \frac{1}{m_0}.$$

The rotation angle between the projections of the tangents at the initial and end points of the rod on the $\xi\eta$-plane is

$$\Delta\alpha = \frac{-l}{2m_0}. \tag{25}$$

Now suppose that we have m_0 copies of the loop, each rotated through the angle $(j-1)(\Delta\alpha \pm \pi)$, $j = 1, \ldots, m_0$, around the ζ-axis. The projection of the end tangent vector of the j-th loop then coincides with the projection of the initial tangent of the $(j+1)$-th loop $(j = 1, \ldots, m_0 - 1)$. We may request that the end tangent of the last m_0-th loop coincides with initial tangent of the 1-st loop, i.e., $m_0(\Delta\alpha + \pi\,\mathrm{sign}\,m_1) = 2\pi m_1$, $\quad m_1 = \pm1, \pm2, \ldots$, m_1 is the number of turns which makes the radius vector $\mathbf{r}(s)$ around the ζ-axis as the arc coordinate varies over the whole interval $0 \le s \le 1$ (the points with coordinates $(j-1)/m_0 \le s < j/m_0$ belong to the j-th copy of the loop).

Substituting $\Delta\alpha$ from Eq. (25) into the last equation, we obtain $l = 2\pi(m_0\,\mathrm{sign}\,m_1 - 2m_1)$. Comparing this expression with the second Eq. (22), where the values of the roots from Eq. (23) are substituted, yields an equation for the elliptic modulus

$$\pi\left|1 - 2\frac{|m_1|}{m_0}\right| = 2\sqrt{\mathrm{K}(k)(2\,\mathrm{E}(k) - \mathrm{K}(k))}.$$

The solutions of this equation are given in Tabl. 1 for some values of m_0 and m_1.

For each element loop (leaf), the angle between the tangent at the initial point and the ζ-axis is equal to one between the tangent at the end point and the same axis. This follows from the symmetry of the loop and from Eqs. (14), (11).

Therefore, not only projections of the tangent vectors coincide but also the tangents themselves. This is sufficient in order that such an assembly results in a smoothly closed solution for a rod of length 1, since the rotational symmetry

m_0	2	3	4	5	6
$m_1 = 1$	0.9089085575	0.8909131369	0.8617750161	0.8315214520	0.8024216633
$m_1 = 2$		0.8909131369	0.9089085575	0.9028843308	0.8909131369
m_0	7	8	9	10	11
$m_1 = 1$	0.7751554280	0.7498694109	0.7265052907	0.7049273686	0.6849768529
$m_1 = 2$	0.8767597839	0.8617750161	0.8465855842	0.8315214520	0.8167660048

Table 1: The values of the elliptic modulus k for various m_0-leafed roses.

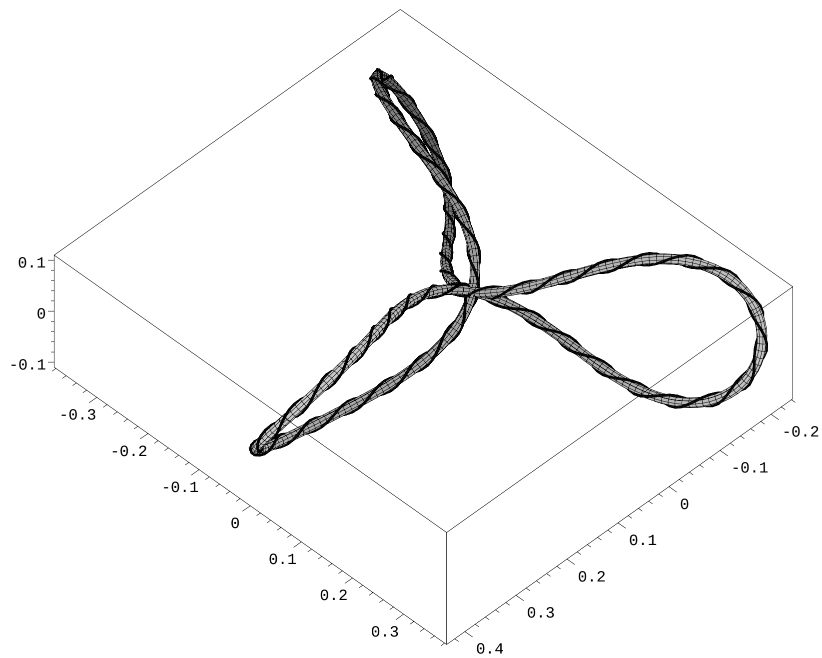

Figure 1: An example of a 3-leaf shape with the self-interacting force; $m_0 = 3, m_1 = -1$.

and identity of all element loops provide for both the constantness of the internal force and the continuity of the internal moment. Note that although the solutions obtained have a point of self-contact, there is no interaction between the remote fragments.

The inclination of each loop (which turns out to be somewhat flat) to the $\xi\eta$-plane may be estimated by using Eq. (11). At the initial and end points of each loop the angle between the tangent and the ζ-axis can be found from

$$-\cos\theta_0 = g_2 = \frac{\mathrm{E} - (1-k^2)\,\mathrm{K}}{\sqrt{(1-k^2)\,\mathrm{K}(\mathrm{K} - 2\,\mathrm{E}) + \mathrm{E}^2}}$$

and at the middle point of the loop, where the polar radius ρ takes on its maximal value,

$$-\cos\theta_m = g_1 = \frac{\mathrm{E} - \mathrm{K}}{\sqrt{(1-k^2)\,\mathrm{K}(\mathrm{K} - 2\,\mathrm{E}) + \mathrm{E}^2}}.$$

For $k = 0$, the loop entirely lies in the plane $\zeta = 0$ and its shape is a circle of radius $\frac{1}{2\pi m_0}$. With increase of the modulus k, the loop becomes "steeper" and, for $k = k_{max}$, its plane is perpendicular to the $\xi\eta$-plane.

It is interesting to follow the evolution of such shapes with a multi-contact point taking into account the contact forces. For the slender rod, the region of self-interaction is idealized to be a point. Therefore, we assume that the contact forces are pointwise and frictionless, i.e., they act only in the normal plane in the point of the contact. We also keep on considering the symmetric configurations only. These rose shapes with self-interaction were considered by Le Bret [9] though no example of them was presented.

As in the forceless case, the whole closed shape is assembled from m_0 identical leaves. Note that the individual loops are solutions of the more general BVP, for which the initial and end points coincide to each other, but not to the origin: $\boldsymbol{r_0}=\boldsymbol{r_1}$. The end forces and moments acting on each loop are to be in the accordance to each other. Every loop is to be smoothly joined to its neighbours. These constraints result in a set of one-parameter families of the solutions. The simplest solutions of this type, the warped figures-8 ($m_0 = 2$), are computed numerically by Jülicher [10]. However, there exist such configurations with larger number of leaves, an example is shown in Fig. 1 for $m_0 = 3$ (the length of each elementary loop is taken 1). The whole assembling procedure reduces essentially to solving an extra non-linear algebraic equation.

The calculations in this paper were carried out with the help of *Maple* program [11].

4 Conclusions

1. A one-parameter family of analytical solutions of the BVP for the simple loop is obtained. These solutions widen the set of the known analytically described configurations of a closed rod.

2. These solutions serve simultaneously as basic elements of the symmetric multi-leafed shapes of the rod with the single self-contact point.

3. The further evolution of these symmetric multi-leafed configurations may be followed taking into account the pointwise and frictionless contact forces in the point of multi-contact by using an assemling procedure.

4. The solutions considered may be used as basic shapes by numerical computation of more complex configurations, described also by more elaborated models. The results presented may be readily applied to other physical objects that obey the equilibrium equations of thin elastic rods.

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