Elasticity of Thin Rods with Spontaneous Curvature and Torsion—Beyond Geometrical Lines

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Abstract

We study three-dimensional deformations of thin inextensible elastic rods with non-vanishing spontaneous curvature and torsion. In addition to the usual description in terms of curvature and torsion which considers only the configuration of the centerline of the rod, we allow deformations that involve the rotation of the rod's cross-section around its centerline. We derive new expressions for the mechanical energy and for the force and moment balance conditions for the equilibrium of a rod under the action of arbitrary external loads. Several illustrative examples are studied and the connection between our results and recent experiments on the stretching of supercoiled DNA molecules is discussed.

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1. Introduction

Recent experimental advances in the art of manipulation of single DNA molecules and of rigid protein assemblies such as actin filaments, etc., have led to an outbreak of theoretical activity connected with the elasticity of thin rods\textsuperscript{1−19}. One of the most intriguing theoretical...
questions related to the deformation of DNA concerns the coupling between bending and twist in the mechanical energy of the polymer. The problem is usually considered in the following terms: at the first step, the thin rod which models the molecule is replaced by its centerline. With each point of the line (specified by its position along the contour $\xi$) one associates a triad of unit vectors: the tangent to the line ($t$), the principal normal ($n$) which lies in the plane defined by the tangents at points $\xi$ and $\xi + d\xi$, and the binormal ($b$) which is orthogonal to both $t$ and $n$. As one moves along the line, the triad rotates and this rotation is described by the Frenet–Serret equations in which the “rate” of rotation of each unit vector is determined by two parameters: the local curvature $\kappa$ and the local torsion $\omega$ (sometimes referred to as writhe). In order to relate this purely geometrical picture to the elastic response of real rods, one has to specify the physical properties of the rod in a stress–free (undeformed) reference state and to write the energy as a quadratic expansion in deviations from this state. In the classical theories of thin elastic rods one usually assumes that the reference state corresponds to a straight untwisted rod (with vanishing spontaneous curvature $\kappa_0$ and spontaneous torsion $\omega_0$) and the mechanical energy density is written as a sum of terms proportional to $\kappa^2$ and $\omega^2$. The generalization to the case of non–vanishing spontaneous curvature and torsion is then done by requiring that the strain energy density per unit length $U$ is minimized for $\kappa = \kappa_0$ and $\omega = \omega_0$ which leads to the expression

$$U = \frac{1}{2} \left[ A_1(\kappa - \kappa_0)^2 + A_2(\omega - \omega_0)^2 \right].$$

(1)

Here $A_1$ and $A_2$ are material parameters (products of elastic moduli and moments of inertia).

Although Eq. (1) has been employed in a number of studies, its validity has been questioned by several authors, who argued that it fails to describe, even qualitatively, the experimental data on torsionally constrained DNA. To account for the coupling between bending and twist observed in experiment, extra terms are conventionally added to the mechanical energy density, Eq. (1), by hand.

The objective of this work is to derive an expression for the mechanical energy and obtain the equations which determine the mechanical equilibrium of a rod subjected to arbitrary
forces and moments. This is done using a new form of the displacement field, which accounts for both the deformation of the centerline and the rotation of the cross-section around this line (i.e., twist). Instead of using ad hoc assumptions about the form of the coupling between bending and twist, we will use standard methods of the theory of elasticity in order to derive the correct form of the coupling.

In this work we will consider cylindrical rods with circular cross-sections. Although, at first sight, this case appears to be simpler than that of rods with asymmetric cross-sections, the reverse is true: while in the asymmetric case one can introduce a triad of vectors associated with the principal axes of inertia, which can rotate at a different rate than the Frenet triad, no such natural choice is possible in the symmetric case which therefore requires a more careful analysis.

The exposition is organized as follows. Section 2 deals with geometry of deformation. The strain energy density of a rod is introduced in Section 3. Stress-strain relations are developed in Section 4. In Section 5, force and moment balance equations which describe the mechanical equilibrium of thin rods are derived. Several examples which illustrate the different aspects of the interaction between elongation, torsion and twist, are discussed in Section 6. Finally, in Section 7 we discuss the connection between our results and other theoretical and experimental works and outline directions for future research.

2. Geometry of deformation

A long chain is modeled as an elastic rod with length $L$ and a circular cross-section $S$ with radius $a \ll L$. Denote by $\xi$ the arc-length of the centerline of the rod in the reference (stress-free) configuration. Let $\mathbf{R}_0(\xi)$ be the radius vector of the longitudinal axis and $\mathbf{t}_0(\xi) = d\mathbf{R}_0/d\xi$ the unit tangent vector in the reference state. The unit normal vector $\mathbf{n}_0(\xi)$ and the unit binormal vector $\mathbf{b}_0(\xi)$ are introduced by the conventional way. These vectors obey the Frenet-Serret equations with given spontaneous curvature $\kappa_0(\xi)$ and torsion $\omega_0(\xi)$:
\[ \frac{dt_0}{d\xi} = \kappa_0 n_0, \quad \frac{dn_0}{d\xi} = \omega_0 b_0 - \kappa_0 t_0, \quad \frac{db_0}{d\xi} = -\omega_0 n_0. \]  

(2)

Points of the rod refer to Lagrangian coordinates \( \{\xi_i\} \), where \( \xi_1, \xi_2 \) are Cartesian coordinates in the cross-sectional plane with unit vectors \( n_0 \) and \( b_0 \) and \( \xi_3 = \xi \),

\[ r_0(\xi_1, \xi_2, \xi) = R_0(\xi) + \xi_1 n_0(\xi) + \xi_2 b_0(\xi). \]  

(3)

It follows from Eqs. (2) and (3) that the covariant base vectors in the reference configuration, \( g_{0k} = \partial r_0 / \partial \xi_k \) are given by

\[ g_{01} = n_0, \quad g_{02} = b_0, \quad g_{03} = (1 - \kappa_0 \xi_1) t_0 + \omega_0 (\xi_1 b_0 - \xi_2 n_0). \]  

(4)

The position of the longitudinal axis of the rod in the actual (deformed) configuration is determined by the radius vector \( R(\xi) \). Following the conventional theories of rods, see, e.g.,\,[25] we assume that the longitudinal axis is inextensible, which means that \( \xi \) remains the arc-length in the actual configuration (for attempts to account for the extensibility of the longitudinal axis, see\,[7,10,11,15]). The unit tangent vector in the actual configuration \( t = dR / d\xi \) together with the unit normal vector \( n \) and the unit binormal vector \( b \) satisfy the Frenet–Serret equations

\[ \frac{dt}{d\xi} = \kappa n, \quad \frac{dn}{d\xi} = \omega b - \kappa t, \quad \frac{db}{d\xi} = -\omega n. \]  

(5)

For Kirchhoff rods\,[4], the radius vector of an arbitrary point is represented as an expansion in the coordinates \( \xi_1 \) and \( \xi_2 \):

\[ r(\xi_1, \xi_2, \xi) = R(\xi) + \xi_1 n(\xi) + \xi_2 b(\xi). \]  

(6)

The functional form of Eq. (6) implies that any cross-section remains planar and perpendicular to the centerline of the rod, even in the actual deformed configuration. Furthermore, it also implies that any cross-section rotates rigidly with the longitudinal axis and therefore Eq. (6) does not allow for the possibility of a twist of the cross-section with respect to the centerline of the rod. Since the latter assumption has no physical basis\,[2], we relax it by introducing a more general displacement field.
\( \mathbf{r}(\xi_1, \xi_2, \xi) = \mathbf{R}(\xi) + (\xi_1 \cos \alpha - \xi_2 \sin \alpha) \mathbf{n}(\xi) + (\xi_1 \sin \alpha + \xi_2 \cos \alpha) \mathbf{b}(\xi), \) 

(7)

where \( \alpha(\xi) \) is the rotation angle around the centerline of the rod. From here on we will refer to this rotation as “twist” and will reserve the terms “torsion” and “writhe” to describe the three-dimensional geometry of bending of the centerline of the rod.

The covariant base vectors \( \mathbf{g}_k = \frac{\partial \mathbf{r}}{\partial \xi_k} \) are given by

\[
\mathbf{g}_1 = \cos \alpha \mathbf{n} + \sin \alpha \mathbf{b}, \quad \mathbf{g}_2 = -\sin \alpha \mathbf{n} + \cos \alpha \mathbf{b}, \\
\mathbf{g}_3 = \left[ 1 - \kappa (\xi_1 \cos \alpha - \xi_2 \sin \alpha) \right] \mathbf{t} \\
+ (\omega + \frac{d\alpha}{d\xi}) \left[ - (\xi_1 \sin \alpha + \xi_2 \cos \alpha) \mathbf{n} + (\xi_1 \cos \alpha - \xi_2 \sin \alpha) \mathbf{b} \right].
\]

(8)

The contravariant base vectors \( \mathbf{g}^k \) are found from Eq. (8) and the equality \( \mathbf{g}_i \cdot \mathbf{g}^j = \delta^j_i \), where the dot stands for inner product and \( \delta^j_i \) is the Kronecker delta. Simple calculations result in

\[
\mathbf{g}^1 = \cos \alpha \mathbf{n} + \sin \alpha \mathbf{b} + C_1 \mathbf{t}, \quad \mathbf{g}^2 = -\sin \alpha \mathbf{n} + \cos \alpha \mathbf{b} + C_2 \mathbf{t}, \quad \mathbf{g}^3 = C_3 \mathbf{t},
\]

(9)

where

\[
A_n = - \left( \frac{d\alpha}{d\xi} + \omega \right) (\xi_1 \sin \alpha + \xi_2 \cos \alpha), \quad A_b = \left( \frac{d\alpha}{d\xi} + \omega \right) (\xi_1 \cos \alpha - \xi_2 \sin \alpha), \\
A_t = 1 - \kappa (\xi_1 \cos \alpha - \xi_2 \sin \alpha), \quad C_1 = - \frac{1}{A_t} (A_n \cos \alpha + A_b \sin \alpha), \\
C_2 = \frac{1}{A_t} (A_n \sin \alpha - A_b \cos \alpha), \quad C_3 = \frac{1}{A_t}.
\]

(10)

One can proceed to calculate the energy of deformation using the displacement gradient either in the deformed, \( \nabla \mathbf{r}_0 \), or in the reference, \( \nabla_0 \mathbf{r} \), state. Both approaches result in the same expression for the mechanical energy. We will use the displacement gradient in the actual configuration \( \nabla \mathbf{r}_0 \), because the corresponding strain tensor is connected with the stress tensor (always defined with respect to the coordinates in the deformed state) by conventional constitutive equations. It follows from Eqs. (4) and (9) that the tensor \( \nabla \mathbf{r}_0 = \mathbf{g}^k \mathbf{g}_{0k} \) is given by
\( \nabla r_0 = \cos \alpha (nn_0 + bb_0) + \sin \alpha (bn_0 - nb_0) \)
\( + (C_1 - C_3 \omega_0 \xi_2) tn_0 + (C_2 + C_3 \omega_0 \xi_1) tb_0 + C_3 (1 - \kappa_0 \xi_1) tt_0. \) \end{equation}

As a measure of deformation, the Almansi tensor \( \mathbf{A} = \nabla r_0 \cdot \nabla r_0^\top \) is employed, where \( \top \) stands for transpose. The tensor \( \mathbf{A} \) is connected with the strain tensor \( \mathbf{\epsilon} \) in the deformed state by the equality \( \mathbf{\epsilon} = \frac{1}{2} (\mathbf{I} - \mathbf{A}) \), where \( \mathbf{I} \) is the unit tensor. It follows from Eq. (11) that the non–zero components of \( \mathbf{\epsilon} \) are given by

\begin{align*}
\epsilon_{13} &= \epsilon_{31} = -\frac{1}{2} (\xi_1 \sin \alpha + \xi_2 \cos \alpha) \left( \frac{d\alpha}{d\xi} + \omega - \omega_0 \right), \\
\epsilon_{23} &= \epsilon_{32} = \frac{1}{2} (\xi_1 \cos \alpha - \xi_2 \sin \alpha) \left( \frac{d\alpha}{d\xi} + \omega - \omega_0 \right), \\
\epsilon_{33} &= -\kappa (\xi_1 \cos \alpha - \xi_2 \sin \alpha) + \kappa_0 \xi_1,
\end{align*}

where we kept only terms up to first order in \( \xi_1 \) and \( \xi_2 \). The neglect of second and higher order terms follows from the standard small local deformation assumption, which implies that all the length scales associated with bending, torsion and twist (e.g., radii of curvature) are much larger than the diameter of the rod. Note that this approximation is consistent with the form of the displacement field, Eqs. (3) and (7), where only terms up to linear order in the transverse coordinated \( \xi_1 \) and \( \xi_2 \) were kept.

3. Strain energy density

For a linear anisotropic elastic medium, the mechanical energy of elongation per unit volume in the deformed state is calculated as

\( u_{el} = \frac{1}{2} E_1 \epsilon_{33}^2, \)

and the mechanical energy of shear is

\( u_{sh} = E_2 (\epsilon_{13}^2 + \epsilon_{31}^2 + \epsilon_{23}^2 + \epsilon_{32}^2), \)

where \( E_1 \) and \( E_2 \) are the appropriate elastic moduli. It follows from Eqs. (12) to (14) that the mechanical energy density
\[ u = u_{el} + u_{sh} \]  

is can be written as

\[ u = \frac{1}{2} \left\{ E_1 \left[ \kappa^2 (\xi_1 \cos \alpha - \xi_2 \sin \alpha)^2 + \kappa_0^2 \xi_1^2 \right] + E_2 (\xi_1^2 + \xi_2^2) \left( \frac{d\alpha}{d\xi} + \omega - \omega_0 \right)^2 \right\}. \]  

(15)

(16)

The mechanical energy per unit length is given by

\[ U = \int_S u d\xi_1 d\xi_2, \]

which yields, upon integration

\[ U = \frac{1}{2} \left[ A_1 (\kappa^2 - 2\kappa \kappa_0 \cos \alpha + \kappa_0^2) + A_2 \left( \frac{d\alpha}{d\xi} + \omega - \omega_0 \right)^2 \right] \]

(17)

with

\[ A_1 = E_1 I, \quad A_2 = 2E_2 I, \quad I = \int_S \xi_1^2 d\xi_1 d\xi_2 = \int_S \xi_2^2 d\xi_1 d\xi_2, \quad \int_S \xi_1 \xi_2 d\xi_1 d\xi_2 = 0. \]

Comparison of Eqs. (1) and (17) shows that the two expressions coincide in the absence of rotation of the cross-section with respect to the centerline (no twist, \( \alpha = 0 \)). In the general case, when \( \alpha \neq 0 \), Eq. (17) differs from Eq. (1) in several important ways:

1. The torsion \( \omega \) is replaced by \( \omega + d\alpha/d\xi \). This correction has a simple intuitive meaning: the rotation of a point on the surface of a rod is the sum of the rotation in space of the centerline of the rod and of the twist of the cross-section about this centerline. Notice that this correction may always be present, independent of whether the rod has a non-vanishing spontaneous curvature (\( \kappa_0 \)) and spontaneous torsion (\( \omega_0 \)) or not. Such a correction was, in fact, proposed by previous investigators.

2. The term \( 2\kappa \kappa_0 \) is replaced by \( 2\kappa \kappa_0 \cos \alpha \), introducing a non-trivial coupling between the spontaneous and the actual curvatures of the rod, and the twist of its cross-section with respect to the centerline. Note that this term appears only when the rod has a non-vanishing spontaneous curvature and therefore while it has no effect on the elasticity of straight rods (\( \kappa_0 = 0 \)), it has a dramatic effect on the elasticity of helices and other curved (\( \kappa_0 \neq 0 \)) rods.
3. The usual expression for the energy, Eq. (1), is minimized when the curvature ($\kappa$) and torsion ($\omega$) recover their spontaneous values ($\kappa_0$ and $\omega_0$, respectively) in the stress–free reference state. Although this appears to be no longer true for our energy, Eq. (17), the difference stems from the fact that we have introduced a new independent variable ($\alpha$) that describes the twist of the cross–section with respect to the centerline of the rod. In the absence of externally applied torques and tensile forces, minimizing the energy with respect to $\kappa$, $\omega$ and $\alpha$ yields their values in the stress–free reference state, i.e., $\kappa_0$, $\omega_0$ and $\alpha = 0$, respectively.

4. Stress–strain relations

Denote by $\sigma$ the Cauchy stress tensor and by $\sigma^{ij}$ its contravariant components in the basis of the actual configuration. Substitution of Eqs. (13) to (15) into the equality

$$\sigma^{ij} = \frac{\partial u}{\partial \epsilon_{ij}},$$

results in

$$\sigma^{13} = \sigma^{31} = -E_2(\xi_1 \sin \alpha + \xi_2 \cos \alpha)(\frac{d\alpha}{d\xi} + \omega - \omega_0),$$

$$\sigma^{23} = \sigma^{32} = E_2(\xi_1 \cos \alpha - \xi_2 \cos \alpha)(\frac{d\alpha}{d\xi} + \omega - \omega_0),$$

$$\sigma^{33} = E_1[-\kappa(\xi_1 \cos \alpha - \xi_2 \sin \alpha) + \kappa_0 \xi_1].$$

Equation (19) does not take into account the inextensibility of the longitudinal axis. In order to enforce this constraint, we add an unknown parameter $p$ (a Lagrange multiplier analogous to pressure for incompressible solids) to Eq. (19):

$$\sigma^{33} = -p + E_1[-\kappa(\xi_1 \cos \alpha - \xi_2 \sin \alpha) + \kappa_0 \xi_1].$$

Equation (20)

Since the unit normal to a cross-section of the rod coincides with $t$, the internal force (per unit area) $f$ that acts on the cross–section of the rod is given by

$$f = t \cdot \sigma = \sigma^{13}n + \sigma^{23}b + \sigma^{33}t.$$
It follows from Eq. (7) that the radius vector $\rho$ from the center point of the cross-section (its intersection with the centerline) to an arbitrary point of the cross-section is

$$\rho = (\xi_1 \cos \alpha - \xi_2 \sin \alpha)n + (\xi_1 \sin \alpha + \xi_2 \cos \alpha)b.$$  \hfill (22)

The moment (per unit area) $\mu$ of the internal force with respect to the center point of the cross-section is defined as

$$\mu = \rho \times f,$$  \hfill (23)

where $\times$ stands for vector product. Combining Eqs. (21) to (23) and using the equalities

$$\mathbf{t} \times \mathbf{n} = \mathbf{b}, \quad \mathbf{n} \times \mathbf{b} = \mathbf{t}, \quad \mathbf{b} \times \mathbf{t} = \mathbf{n},$$  \hfill (24)

we find that

$$\mu = \left[(\xi_1 \sin \alpha + \xi_2 \cos \alpha)n - (\xi_1 \cos \alpha - \xi_2 \sin \alpha)b\right]\sigma^{33}$$

$$+ \left[(\xi_1 \cos \alpha - \xi_2 \sin \alpha)\sigma^{23} - (\xi_1 \sin \alpha + \xi_2 \cos \alpha)\sigma^{13}\right]t.$$ \hfill (25)

The internal moment $\mathbf{M}$ is obtained by integrating $\mu$ over the cross-section of the rod,

$$\mathbf{M} = \int_S \mu d\xi_1 d\xi_2 = M_n\mathbf{n} + M_b\mathbf{b} + M_t\mathbf{t}.$$ \hfill (26)

In principle, one could proceed in similar fashion and obtain the internal force

$$\mathbf{F} = F_n\mathbf{n} + F_b\mathbf{b} + F_t\mathbf{t}$$ \hfill (27)

by integrating $\mathbf{f}$ over the cross-section of the rod. However, inspection of Eqs. (18)–(21) shows that since our expression for $\mathbf{f}$ is linear in the transverse coordinates $\xi_1$ and $\xi_2$, the integral over the cross-section vanishes. The source of the problem can be traced back to our choice of the displacement fields, Eqs. (3) and (7), where only linear terms in the transverse coordinates $\xi_1$ and $\xi_2$ were taken into account. Note, however, that even if we were to keep higher order terms in $\xi_1$ and $\xi_2$ in these equations, the unknown function $\mathbf{F}$ would be expressed in terms of new unknown functions (coefficients of quadratic contributions in $\xi_1$.
and $\xi_2$ to the displacement fields). Instead, we will follow the standard approach and treat the vector $\mathbf{F}$ as an additional unknown that is found from the equilibrium equations (force and moment balance conditions).

We now proceed to calculate the internal moment by substituting expressions (18) and (21) into Eqs. (25) and (26). Upon integration we obtain the constitutive relation between the parameters that characterize the deformation ($\kappa$, $\omega$ and $\alpha$) and the internal moment $\mathbf{M}$

\[
\mathbf{M} = A_1 \kappa_0 \sin \alpha \mathbf{n} + A_1 (\kappa - \kappa_0 \cos \alpha) \mathbf{b} + A_2 \left(\omega + \frac{d\alpha}{d\xi} - \omega_0\right) \mathbf{t}.
\]  

Equation (28) is a new expression for the moment of internal forces which accounts for the twist of the cross-section with respect to the centerline of the rod. As expected, the internal moment vanishes in the stress-free reference state: $\kappa = \kappa_0$, $\omega = \omega_0$, $\alpha = 0$. In the absence of twist, $\alpha = 0$, Eq. (28) reduces to the conventional expression for Kirchhoff rods

\[
\mathbf{M} = A_1 (\kappa - \kappa_0) \mathbf{b} + A_2 \left(\omega - \omega_0\right) \mathbf{t}.
\]  

5. Equilibrium equations

Consider an element of the rod bounded by two cross-sections with longitudinal coordinates $\xi$ and $\xi + d\xi$. Forces acting on this element consist of the internal force $-\mathbf{F}(\xi)$ applied to the cross-section $\xi$, the internal force $\mathbf{F}(\xi + d\xi)$ applied to the cross-section $\xi + d\xi$, and the external force $\mathbf{q}(\xi)d\xi$ proportional to the length of the element $d\xi$. Balancing the forces on the element yields

\[
\mathbf{F}(\xi + d\xi) - \mathbf{F}(\xi) + \mathbf{q}(\xi)d\xi = 0.
\]  

Expanding the vector function

\[
\mathbf{F}(\xi + d\xi) = F_n(\xi + d\xi)\mathbf{n}(\xi + d\xi) + F_b(\xi + d\xi)\mathbf{b}(\xi + d\xi) + F_t(\xi + d\xi)\mathbf{t}(\xi + d\xi)
\]

into the Taylor series, using Eq. (5), and neglecting terms of second order in $d\xi$, we find that
\[ \mathbf{F}(\xi + d\xi) - \mathbf{F}(\xi) = \left[ (\frac{dF_n}{d\xi} + \kappa F_t - \omega F_b) \mathbf{n} + (\frac{dF_b}{d\xi} + \omega F_n) \mathbf{b} + (\frac{dF_t}{d\xi} - \kappa F_n) \mathbf{t} \right] d\xi. \] (31)

Substitution of Eq. (31) into Eq. (30) results in the equilibrium equations
\[ \frac{dF_n}{d\xi} + \kappa F_t - \omega F_b + q_n = 0, \quad \frac{dF_b}{d\xi} + \omega F_n + q_b = 0, \] (32)
\[ \frac{dF_t}{d\xi} - \kappa F_n + q_t = 0. \] (33)

where \( q_n, \ q_b, \) and \( q_t \) are the components of the external force per unit length, \( \mathbf{q} = q_n \mathbf{n} + q_b \mathbf{b} + q_t \mathbf{t}. \)

The moments acting on the element of the rod consist of the internal moment \(-M(\xi)\) applied to the cross-section \( \xi \), the internal moment \( M(\xi + d\xi) \) applied to the cross-section \( \xi + d\xi \), the moments of internal forces \(-\mathbf{F}(\xi)\) and \( \mathbf{F}(\xi + d\xi)\), and the external moment \( \mathbf{md} \) proportional to the length \( d\xi \), where \( \mathbf{m} = m_n \mathbf{n} + m_b \mathbf{b} + m_t \mathbf{t} \) is the external moment per unit length. To first order in \( d\xi \), the moment of internal forces with respect to the center of the cross-section with coordinate \( \xi \) is
\[ [\mathbf{R}(\xi + d\xi) - \mathbf{R}(\xi)] \times \mathbf{F}(\xi + d\xi) = \mathbf{t}(\xi) \times \mathbf{F}(\xi) d\xi. \]

The balance equation for the moments reads
\[ \mathbf{M}(\xi + d\xi) - \mathbf{M}(\xi) + \mathbf{t}(\xi) \times \mathbf{F}(\xi) d\xi + \mathbf{m}(\xi) d\xi = 0. \] (34)

It follows from Eqs. (24) and (26) that \( \mathbf{t} \times \mathbf{F} = -F_b \mathbf{n} + F_n \mathbf{b}. \) By analogy with Eq. (31), one can write
\[ \mathbf{M}(\xi + d\xi) - \mathbf{M}(\xi) = \left[ \left( \frac{dM_n}{d\xi} + \kappa M_t - \omega M_b \right) \mathbf{n} + \left( \frac{dM_b}{d\xi} + \omega M_n \right) \mathbf{b} + \left( \frac{dM_t}{d\xi} - \kappa M_n \right) \mathbf{t} \right] d\xi. \]

Substitution of these expressions into Eq. (34) results in the equations
\[ \frac{dM_n}{d\xi} + \kappa M_t - \omega M_b - F_b + m_n = 0, \quad \frac{dM_b}{d\xi} + \omega M_n + F_n + m_b = 0, \] (35)
\[ \frac{dM_t}{d\xi} - \kappa M_n + m_t = 0. \] (36)

Given the vectors \( \mathbf{M} \) and \( \mathbf{m} \), Eqs. (35) can be used to determine the forces \( F_n \) and \( F_b \).

Eliminating the unknown functions \( F_n \) and \( F_b \) from Eqs. (32) and (35), we obtain
\[
\frac{dF_t}{d\xi} + \kappa \left( \frac{dM_b}{d\xi} + \omega M_n + m_b \right) + q_t = 0, \\
\frac{d}{d\xi} \left( \frac{dM_b}{d\xi} + \omega M_n + m_b \right) + \omega \left( \frac{dM_n}{d\xi} + \kappa M_t - \omega M_b + m_n \right) - \kappa F_t - q_n = 0, \\
\frac{d}{d\xi} \left( \frac{dM_n}{d\xi} + \kappa M_t - \omega M_b + m_n \right) - \omega \left( \frac{dM_b}{d\xi} + \omega M_n + m_b \right) + q_b = 0.
\]

Equations (36) to (38) together with constitutive relation (28) are a set of four nonlinear differential equations which determine the four unknown functions \(F_t, \alpha, \kappa\) and \(\omega\). The neglect of \(\alpha\) (that is the use of conventional formula (6) instead of Eq. (7) for the displacement field \(r\)) is acceptable only when special restrictions are imposed on external forces and moments. In the general case, this simplification is not correct, and Eq. (7) should be employed for the analysis of deformations.

6. Examples

A. Twist of a closed loop

Consider a rod whose stress-free shape is a planar circular loop with radius \(a_0\), under the action of a constant twisting moment \(m_t\). It is assumed that the moments \(m_n\) and \(m_b\), as well as the forces \(q_n\), \(q_b\) and \(q_t\) vanish. The solution of Eqs. (36) to (38) reads

\[
\kappa = \kappa_0 = a_0^{-1}, \\
\omega = \omega_0 = 0, \quad F_t = 0, \quad \alpha = \arcsin \frac{m_t a_0^2}{A_1}.
\]

According to these equalities, any cross-section of the rod twists around its centerline by a constant angle \(\alpha\). This solution is not described by the Kirchhoff theory of thin rods. It exists as long as the moment \(m_t\) satisfies the condition \(|m_t| \leq A_1 a_0^{-2}\). If the latter restriction is not fulfilled, the planar shape of the loop becomes unstable.
B. Torsion of a disconnected ring

We analyze the deformation of a disconnected ring (no contact between the points $\xi = 0$ and $\xi = L$). The end $\xi = 0$ is fixed, and a torque $T$ is applied to the free end $\xi = L$. The centerline of the rod in the stress–free reference state describes a planar circle with radius $a_0 = \kappa_0^{-1}$ and no spontaneous torsion, $\omega_0 = 0$. Similar problems were recently studied and their solutions were applied to the analysis of kink transitions in short DNA rings.

We assume that in the deformed state the centerline becomes a non-planar curve whose radius of curvature remains unchanged, see Eq. (39). For simplicity, we confine ourselves to small displacements, and neglect terms of order $\alpha^2$ in the constitutive equations (28). This yields

\[ M_n = A_1 \kappa_0 \alpha, \quad M_b = 0, \quad M_t = A_2 \left( \frac{d\alpha}{d\xi} + \omega \right). \tag{41} \]

Substitution of these expressions into the equilibrium equations (36) to (38) implies that the longitudinal force $F_t$ vanishes, whereas the functions $\alpha$ and $\omega$ obey the equations

\[ A_2 \left( \frac{d^2\alpha}{d\xi^2} + \frac{d\omega}{d\xi} \right) - A_1 \kappa_0^2 \alpha = 0, \quad \frac{d}{d\xi} \left[ A_1 \frac{d\alpha}{d\xi} + A_2 \left( \frac{d\alpha}{d\xi} + \omega \right) \right] = 0. \tag{42} \]

It follows from the second equality in Eq. (42) that

\[ (A_1 + A_2) \frac{d\alpha}{d\xi} + A_2 \omega = c, \tag{43} \]

where $c$ is a constant to be found. Excluding $\omega$ from Eqs. (42) and (43), we obtain

\[ \frac{d^2\alpha}{d\xi^2} + \kappa_0^2 \alpha = 0. \tag{44} \]

The solution of Eq. (44) is given by

\[ \alpha = c_1 \sin \kappa_0 \xi + c_2 \cos \kappa_0 \xi, \tag{45} \]

where $c_1$ and $c_2$ are arbitrary constants. Substitution of Eqs. (43) and (45) into the boundary conditions at the clamped end $\xi = 0$
\( \alpha(0) = 0, \quad \omega(0) = 0 \)

implies that
\[
\alpha = c_1 \sin \kappa_0 \xi, \quad \omega = \frac{A_1 + A_2}{A_2} \kappa_0 c_1 (1 - \cos \kappa_0 \xi).
\]  

Equating the moment \( M_t \) at the end \( \xi = L \) to the external torque \( T \) and using Eqs. (41) and (46), we obtain
\[
c_1 = \frac{T}{A_2 \kappa_0},
\]
which results in the formulas
\[
\alpha = \frac{T}{A_2 \kappa_0} \sin(\kappa_0 \xi), \quad \omega = \frac{T(A_1 + A_2)}{A_2^2} \left(1 - \cos(\kappa_0 \xi)\right).
\]  

Equations (41) and (47) provide an explicit solution to the torque problem, which cannot be obtained in the framework of the Kirchhoff theory of rods. When the radius of the ring tends to infinity, i.e. for a prismatic rod, Eq. (47) implies that
\[
\alpha = \frac{T}{A_2} \xi, \quad \omega = 0.
\]  

In this limit, the solution (48) coincides with the classical displacement field for the twist of a circular cylinder.  

C. Helix under tension and torque

A helix–shaped rod whose stress–free reference state is characterized by spontaneous curvature \( \kappa_0 \) and torsion \( \omega_0 \), is deformed by tensile forces \( P \) and torques \( T \) applied to its ends. All other forces \( \mathbf{q} \) and moments \( \mathbf{m} \) are assumed to vanish. We introduce Cartesian coordinates \( \{x_k\} \) with unit vectors \( \mathbf{e}_k \) and describe the configuration of the centerline of the rod in the stress–free reference state by the vector
\[
\mathbf{R}_0 = a_0 \cos \frac{\xi}{\sqrt{a_0^2 + b_0^2}} \mathbf{e}_1 + a_0 \sin \frac{\xi}{\sqrt{a_0^2 + b_0^2}} \mathbf{e}_2 + \frac{b_0 \xi}{\sqrt{a_0^2 + b_0^2}} \mathbf{e}_3.
\]  

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The parameters $a_0$ and $b_0$ are expressed in terms of the spontaneous curvature $\kappa_0$ and torsion $\omega_0$ by the formulas
\[
\kappa_0 = \frac{a_0}{a_0^2 + b_0^2}, \quad \omega_0 = \frac{b_0}{a_0^2 + b_0^2}.
\]  
(50)

1. Fixed force and torque on ends

Consider a rod whose centerline describes one complete turn of a helix (the angle between tangent vectors at the two ends of the undeformed rod equals $2\pi$). The contour length of the rod is
\[
l = 2\pi(\kappa_0^2 + \omega_0^2)^{\frac{3}{2}}.
\]  
(51)

We assume the following boundary conditions at the ends of the rod:
\[
M_n(0) = M_n(l) = 0, \quad M_b(0) = M_b(l) = 0,
\]
\[
M_t(0) = M_t(l) = T, \quad F_t(0) = F_t(l) = P.
\]  
(52)

Equations (52) imply that the torque $T$ and the tensile force $P$ are the only external loads applied to the segment. Assuming the parameters $P$ and $T$ to be rather small and neglecting the deviation of torsion from its value in the stress–free state, we look for a solution of the equilibrium equations in the form
\[
\alpha = \Delta \alpha, \quad \kappa = \kappa_0 + \Delta \kappa, \quad \omega = \omega_0,
\]  
(53)

where $\Delta \alpha$ is small compared to unity, and $\Delta \kappa$ is small compared to $\kappa_0$.

Neglecting terms of the second order in the perturbations of twist angle and curvature ($\Delta \alpha$ and $\Delta \kappa$, respectively), we find from Eq. (28) that
\[
M_n = A_1 \kappa_0 \Delta \alpha, \quad M_b = A_1 \Delta \kappa, \quad M_t = A_2 \frac{d \Delta \alpha}{d \xi}.
\]  
(54)

We substitute expressions (53) and (54) into Eqs. (36) to (38), neglect terms of the second order in $\Delta \alpha$ and $\Delta \kappa$, and arrive at the equations
\[
\frac{dM_t}{d\xi} - \kappa_0 M_n = 0, \tag{55}
\]
\[
\frac{dF_t}{d\xi} + \kappa_0 \left( \frac{dM_b}{d\xi} + \omega_0 M_n \right) = 0, \tag{56}
\]
\[
\frac{d^2 M_b}{d\xi^2} + 2\omega_0 \frac{dM_n}{d\xi} + \kappa_0 \omega_0 M_t - \omega_0^2 M_b - \kappa_0 F_t = 0, \tag{57}
\]
\[
\frac{d^2 M_n}{d\xi^2} + \kappa_0 \frac{dM_t}{d\xi} - 2\omega_0 \frac{dM_b}{d\xi} - \omega_0^2 M_n = 0, \tag{58}
\]
where the longitudinal force \( F_t \) is assumed to be small as well. It follows from Eqs. (55) and (58) that
\[
\frac{dM_b}{d\xi} = \frac{1}{2\omega_0} \left[ \frac{d^2 M_n}{d\xi^2} + (\kappa_0^2 - \omega_0^2) M_n \right]. \tag{59}
\]
Substitution of Eq. (59) into Eq. (56) results in
\[
\frac{dF_t}{d\xi} + \frac{\kappa_0}{2\omega_0} \left[ \frac{d^2 M_n}{d\xi^2} + (\kappa_0^2 + \omega_0^2) M_n \right] = 0. \tag{60}
\]
Equations (55), (57) and (59) imply that
\[
\frac{dF_t}{d\xi} = \frac{1}{\kappa_0} \left( \frac{d^3 M_b}{d\xi^3} + 2\omega_0 \frac{d^2 M_n}{d\xi^2} + \kappa_0 \omega_0 \frac{dM_t}{d\xi} - \omega_0^2 \frac{dM_b}{d\xi} \right)
\]
\[
= \frac{1}{2\kappa_0 \omega_0} \left[ \frac{d^4 M_n}{d\xi^4} + (\kappa_0^2 + 2\omega_0^2) \frac{d^2 M_n}{d\xi^2} + \omega_0^2 (\kappa_0^2 + \omega_0^2) M_n \right]. \tag{61}
\]
Excluding the function \( F_t \) from Eqs. (60) and (61), we obtain a closed equation for the internal moment \( M_n \)
\[
\frac{d^4 M_n}{d\xi^4} + 2(\kappa_0^2 + \omega_0^2) \frac{d^2 M_n}{d\xi^2} + (\kappa_0^2 + \omega_0^2)^2 M_n = 0. \tag{62}
\]
The solution of Eq. (62) reads
\[
M_n = (c_1 + c_1' \xi) \sin \left( \sqrt{\kappa_0^2 + \omega_0^2} \xi \right) + (c_2 + c_2' \xi) \cos \left( \sqrt{\kappa_0^2 + \omega_0^2} \xi \right), \tag{63}
\]
where \( c_k, c_k' \) are constants to be found. It follows from the boundary conditions (52) for the function \( M_n \) and Eq. (63) that
\[
c_2 = c_2' = 0. \tag{64}
\]
Integrating Eq. (59) from 0 to \( l \) and using boundary conditions (52) for the function \( M_b \), we obtain

\[
\int_0^l \left[ \frac{d^2 M_n}{d\xi^2} + (\kappa_0^2 - \omega_0^2) M_n \right] d\xi = 0.
\]

Substitution of expressions (63) and (64) into this equality results in

\[ c'_1 = 0. \quad (65) \]

Combining Eqs. (54) and (63) to (65), we find that

\[
\Delta\alpha(\xi) = \frac{c_1}{A_1\kappa_0} \sin\left(\sqrt{\kappa_0^2 + \omega_0^2} \xi\right), \quad (66)
\]

Note that although the twist angle vanishes at the ends and in the middle of the rod \( (\Delta\alpha(0) = \Delta\alpha(l) = \Delta\alpha(l/2) = 0) \), it does not vanish elsewhere. Differentiating Eq. (66) and using Eq. (54) and the boundary conditions (52) for \( M_t \), we arrive at the equality

\[
c_1 = \frac{A_1 T \kappa_0}{A_2 \sqrt{\kappa_0^2 + \omega_0^2}}. \quad (67)
\]

Substitution of Eqs. (64), (65) and (67) into Eqs. (54), (63) and (66) implies that

\[
M_n = \frac{A_1 T \kappa_0}{A_2 \sqrt{\kappa_0^2 + \omega_0^2}} \sin\left(\sqrt{\kappa_0^2 + \omega_0^2} \xi\right), \quad M_t = T \cos\left(\sqrt{\kappa_0^2 + \omega_0^2} \xi\right). \quad (68)
\]

It follows from Eqs. (59) and (68) that

\[
\frac{dM_b}{d\xi} = -\frac{A_1 T \kappa_0 \omega_0}{A_2 \sqrt{\kappa_0^2 + \omega_0^2}} \sin\left(\sqrt{\kappa_0^2 + \omega_0^2} \xi\right).
\]

Integrating this equality with the boundary conditions (52) and substituting in Eq. (54) yields

\[
\Delta\kappa(\xi) = \frac{M_b}{A_1} = -\frac{T \kappa_0 \omega_0}{A_2 (\kappa_0^2 + \omega_0^2)} \left[ 1 - \cos\left(\sqrt{\kappa_0^2 + \omega_0^2} \xi\right) \right]. \quad (69)
\]

Note that the sign of \( \Delta\kappa \) vanishes at the ends of the rod; inside it, its sign is opposite to that of the torque \( T \) (positive torque means overtwisting). Substitution of Eqs. (68) and (69) into Eq. (57) gives the internal tensile force.
\[ F_t = T\omega_0\left[\left(1 + \frac{A_1}{A_2}(1 + \frac{\omega_0^2}{\kappa_0^2 + \omega_0^2})\right)\cos\left(\sqrt{\kappa_0^2 + \omega_0^2}\xi\right) - \frac{A_1\omega_0^2}{A_2(\kappa_0^2 + \omega_0^2)}\right]. \]  

(70)

It follows from Eq. (70) that our solution \(\kappa(\xi), \omega\) and \(\alpha(\xi)\) under boundary conditions (52) is valid if the tensile force \(P\) and the torque \(T\) applied to the ends of the rod satisfy the relation

\[ P = T\omega_0\left(1 + \frac{A_1}{A_2}\right). \]  

(71)

Equations (68) to (70) provide an explicit solution to the problem of combined tension and torsion of a helical segment. The main results are as follows:

1. The application of positive torque \(T\) at the ends (overtwist) leads to axial compression of the helix which is maximal at the center and vanishes at the ends of the rod;

2. The ratio of the tensile force \(P\) and the torque \(T\) is independent of the initial curvature \(\kappa_0\) (and, therefore, of the length of the rod) and depends only on the initial torsion \(\omega_0\) and the ratio of elastic moduli \(A_1/A_2 = E_1/(2E_2)\);

3. The force \(P\) is proportional to the torque \(T\). This result is markedly different from that obtained for a similar deformation of a circular incompressible cylinder, where \(P\) can be shown to be proportional to \(T^2\) (the Poynting effect[24]).

Note that our solution corresponds to a helical rod (with constant \(\kappa_0\) and \(\omega_0\)) which, upon application of external forces and torques, is deformed into a new, non-helical shape. It is natural to ask under which boundary conditions a helix will deform into another helix (with constant \(\kappa\) and \(\omega\)), and derive the corresponding force–elongation relation. This is done in the following.

2. Elongation and winding of a helix

Consider a helix made of an arbitrary number of repetitive units \(L_0\) (\(L_0\) is the smallest segment for which the angle between tangent vectors at its ends is \(2\pi\)) such that its stress–free reference state is characterized by the parameters \(\kappa_0\) and \(\omega_0\). We allow deformations
that satisfy the following conditions: (i) the rod becomes a helix with constant curvature \( \kappa \) and constant torsion \( \omega \), and (ii) the twist \( \alpha \) vanishes. Under the action of combined tensile force \( P \) and torque \( T \), any repetitive unit \( L_0 \) of the helix in the reference state is transformed into an element with the angle between tangent vectors at the ends \( 2\pi(1 + \varphi) \), where the angle \( 2\pi\varphi \) can take positive or negative values. The radius vector of the centerline of the rod in the deformed state can be written in the form

\[
R = a \cos(S\xi)e_1 + a \sin(S\xi)e_2 + S_1\xi e_3, \tag{72}
\]

where \( a, S \) and \( S_1 \) are constants which will be calculated in the following. Differentiating Eq. (72) with respect to \( \xi \) and bearing in mind that \( |t| = 1 \), we obtain

\[
a^2S^2 + S_1^2 = 1. \tag{73}
\]

According to the definition of \( \varphi \),

\[
S l = 2\pi(1 + \varphi). \tag{74}
\]

The projected distances (along the \( x_3 \)-axis) between the ends of the repetitive unit in the reference and deformed states are

\[
\Pi_0 = 2\pi b_0, \quad \Pi = S_1 l, \tag{75}
\]

respectively. The axial elongation \( \eta \) is defined as the ratio of these distances,

\[
\eta = \frac{\Pi}{\Pi_0} = \frac{S_1 l}{2\pi b_0} = \frac{l}{2\pi b_0} \sqrt{1 - a^2S^2}. \tag{76}
\]

Simple calculations result in the formulas

\[
\kappa = aS^2, \quad \omega = S\sqrt{1 - a^2S^2}. \tag{77}
\]

It follows from Eq. (72) that the projection of the force \( F_t \) on the axis \( x_3 \) is \( F_t \cdot e_3 = F_t S_1 \). Equating this expression to the tensile force \( P \) and using Eq. (73), we arrive at the relation

\[
F_t = \frac{P}{\sqrt{1 - a^2S^2}}. \tag{78}
\]
which means that \( F_t \) is independent of \( \xi \). Equation (28) implies that components of the
moment \( \mathbf{M} \) are independent of \( \xi \) as well,

\[
M_n = 0, \quad M_b = A_1(\kappa - \kappa_0), \quad M_t = A_2(\omega - \omega_0). \tag{79}
\]

The only equilibrium equation reads

\[
\omega(\kappa M_t - \omega M_b) = \kappa F_t.
\]

Substitution of expressions (78) and (79) into this equality yields

\[
\omega \left[ A_2 \kappa (\omega - \omega_0) - A_1 \omega (\kappa - \kappa_0) \right] = \frac{\kappa P}{\sqrt{1 - a^2 S^2}}, \tag{80}
\]

Excluding the parameters \( a, S, \kappa \) and \( \omega \) from Eqs. (73), (74), (76), (77) and (80), we express
the tensile force \( P \) in terms of the axial elongation of the helix \( \eta \):

\[
P_0 = \frac{\lambda(1 + \varphi)\eta^2}{\sqrt{1 + \lambda^2}} \left[ (1 + \varphi)\eta - 1 - A\eta \left( (1 + \varphi) - \frac{1}{\sqrt{1 + \lambda^2(1 - \eta^2)}} \right) \right], \tag{81}
\]

where

\[
A = \frac{A_1}{A_2}, \quad \lambda = \frac{\omega_0}{\kappa_0}, \quad P_0 = \frac{P}{A_2\omega_0^2}.
\]

Comparing Eq. (52) with Eqs. (78) and (79) we find that the only difference between the
boundary conditions for the two problems is that in the former case we have neglected the
moment \( M_b \). The fact that a minor change of boundary conditions can drastically change
the character of deformation is quite remarkable and indicates that these conditions should
be chosen with care.

Since various variants of the theory of elastic rods were applied to interpret the experimental
force–elongation curves for stretched DNA molecules at large deformations, we will
present plots of some of the results of this section and comment on their qualitative features.
The graph \( P_0 = P_0(\eta) \) for extension without torsion, \( \varphi = 0 \), is plotted in Figure 1. In the
calculation we used \( A = 0.67 \), in agreement with conventional data on DNA \( \tilde{A}_1 = 50 \) nm,
\( \tilde{A}_2 = 75 \) nm\(^{15} \), where \( \tilde{A}_k = A_k/(k_BT) \), \( k_B \) is Boltzmann’s constant and \( T \) is temperature.
No detailed comparison with experiment is attempted here, but Figure 1 captures rather well the qualitative features of the experimental data for DNA molecules.

In order to check whether our theory captures the qualitative features of experimental data on the elasticity of supercoiled DNA, the dependence $\eta = \eta(\varphi)$ is depicted in Figure 2 for various tensile forces $P_0$. This figure also shows qualitative agreement with observations on the DNA chains: for small tensile forces, there is pronounced asymmetry with regard to the sign of $\varphi$, but the $\eta = \eta(\varphi)$ curve becomes nearly flat at large tensile forces. Throughout the parameter range, the elongation decreases nearly linearly with degree of supercoiling. All these features were observed experimentally and were interpreted as a proof for the existence of a new type of twist–stretch coupling. Note, however, that in the analysis that led to Figure 2 we assumed that the deformation of the helix takes place with no twist of its cross–section around the centerline of the rod ($\alpha = 0$). Therefore, our solution can be derived using the standard theory of elastic rods, based on the elastic energy of Eq. (1), in which no such coupling appears. Inspection of the derivation of Eq. (81) leads to the conclusion that the strong dependence of elongation on the degree of supercoiling has a simple physical meaning: when an inextensible helical rod is subjected to torque that produces supercoiling, each new turn has non-vanishing projection on the $x_1 - x_2$ plane and the projection of the deformed helix on the $x_3$ axis (i.e., its elongation) decreases as the result. This can be fully described by Eq. (1) and does not require the introduction of new coupling into the mechanical energy of elastic rods.

7. Concluding remarks

In this work we have extended the theory of elasticity of thin inextensible rods beyond that of three–dimensional space curves which can be completely described by local curvature $\kappa$ and geometric torsion $\omega$. We have shown that in order to describe the displacement of a point in a rod of arbitrarily small but non–vanishing thickness, one has to account for deformations that produce a rotation of the cross–section of the rod about its centerline.
The modified displacement field was then used to calculate the strain tensor. The resulting expression for the mechanical energy of rods with non-vanishing spontaneous curvature contains a new coupling term between the curvature of the rod and the twist of its cross-section with respect to the centerline, which does not appear in any of the previous theories. We derived the complete set of non-linear differential equations which describe the conditions of mechanical equilibrium and which can be solved for the parameters of deformation $\kappa$, $\omega$ and $\alpha$ for arbitrary external forces and moments acting on the rod. In order to illustrate the physical consequences of our theory, we proceeded to analyze several illustrative examples. In particular, we have analyzed the deformation of a helical rod subjected to a combination of tension and torque and showed that the theory captures the qualitative features of the recent observations on the connection between supercoiling and elongation of strongly stretched DNA molecules.

Note that we have described the deformation of thin rods by three independent functions $\alpha$, $\kappa$ and $\omega$. This is reminiscent of the conventional approach\textsuperscript{9} where the deformation is described in terms of the three components of the, so called, “twist” vector, $\kappa_1$, $\kappa_2$ and $\kappa_3$. Although this was not mentioned by the above authors, such an approach goes beyond the purely geometric description of an elastic line in which only two functions are necessary\textsuperscript{20} and describes a line with some “internal structure”. With each point of this line one can associate a “physical” triad of vectors that differs, in general, from the “geometric” (Frenet) triad. While the two triads have one common vector (the tangent to the line), the other two pairs of vectors rotate at different rates as one moves along the line contour and therefore the rotation of the physical triad can not be completely described by the two Frenet parameters $\kappa$ and $\omega$. It is important to realize that the introduction of a physical triad is necessary whenever some asymmetry of the cross-section, either geometric or physical\textsuperscript{14}, is present. However, even though the procedure is not unique, one may also introduce the physical triad by hand even for a rod with a circular cross-section. For example, we may draw a line on the surface of a rod which describes the intersection of the normal vector with this surface. When the rod is deformed, the deformation of this line will, in general, be different from
that of the centerline. We can now connect the corresponding points of the two lines (having the same contour parameter $\xi$) and define the resulting vector as one of the vectors of the physical triad. The remaining vector is then defined as the normal to the plane formed by the above vector and the tangent to the centerline. This procedure is completely equivalent to what we have done here, by introducing the rotation $\alpha(\xi)$ and explains the appearance of an $\alpha-$dependent term ($\kappa \kappa_0 \cos \alpha$) in the expression for the mechanical energy, that couples the curvatures in the stress–free and the deformed states of the rod. Note that while for rods with asymmetric cross–sections, three independent parameters are needed in order to characterize the stress–free reference state, only two such parameters (e.g., $\kappa_0$ and $\omega_0$) are necessary in the degenerate case of rods with circular cross–sections.

There are several possible directions in which the work presented here can be extended. For example, throughout this work we assumed that the conditions of mechanical equilibrium can be satisfied and considered only stable configurations of the deformed rods. However, the introduction of a new type of deformations is expected to have a profound effect on various instabilities (e.g., buckling under torsion and twist, plectoneme formation, etc.) and we are now studying these questions. Another direction for future research involves the extension of the present, purely mechanical, analysis to include the effects of thermal fluctuations. This leads naturally to a new class of physical models for rigid biopolymers and protein assemblies which can account for the spontaneous curvature of these objects.

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FIGURES

Fig. 1. The dimensionless tensile force $P_0$ versus the axial elongation $\eta$ for a helix with $A = 0.67$ and $\varphi = 0$. Curve 1: $\lambda = 0.5$; curve 2: $\lambda = 0.6$; curve 3: $\lambda = 0.7$

Fig. 2. The axial elongation $\eta$ versus the overtwist $\varphi$ for a helix with $A = 0.67$ and $\lambda = 0.6$. Curve 1: $P_0 = 0.1$; curve 2: $P_0 = 1.0$; curve 3: $P_0 = 10.0$
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