

Effective properties of elastic rods with high intrinsic twist

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Abstract

Motivated by applications to continuum models of tertiary structures of DNA, we use averaging theory to determine effective isotropic bending laws for non-isotropic elastic rods with high intrinsic twist.

Key words: elastic rod, high twist, homogenization, effective constitutive relation.

AMS subject classifications: 74K10, 74Q15.

1 Introduction

In this article we examine the effect of a high intrinsic twist rate on the effective bending properties of elastic rods. The elastic rod is of particular interest to us when considered as a continuum model of long length-scale deformations of DNA (see for example the recent survey articles by Schlick [1] and Olson [2]), and that is the application that motivated this investigation. (Gentle introductions, targeted at non-specialists, describing models of DNA can be found in the books by Calladine and Drew [3] and Frank-Kamenetskii [4]). It is believed that on short, base pair level, length scales DNA has an anisotropic response to loads that induce bending. However, to our knowledge, all analyses exploiting continuum models of DNA have assumed isotropic constitutive laws for bending, specifically the linearly elastic case with two equal bending stiffnesses (in the energy (1) below).

In this article we show that in a certain mathematical sense (to be made precise below), an elastic rod with locally anisotropic bending, but a high intrinsic twist, is indeed well approximated on relatively long length scales by an effective rod with an isotropic bending law. As DNA has an intrinsic twist of one complete turn approximately every 10.5 base pairs, our analysis lends mathematical credence to the assumption adopted in continuum models of DNA that there is a single effective isotropic bending stiffness on length scales involving hundreds of base pairs or more.

Our argument is constructed entirely within the framework of a continuum model. We present a rigorous asymptotic analysis of the elastic rod equilibrium equations in the limit as intrinsic twist tends to infinity. This asymptotic limit of high intrinsic twist per non-dimensionalized unit length should be interpreted within the context of DNA as consideration of deformations on length scales involving increasingly large numbers of base pairs. Our analysis can be used to show that for a rod with a locally anisotropic constitutive relation for bending, there is an effective bending law in the infinite intrinsic twist limit, and that the effective constitutive law is isotropic. For reasons of space the derivation of isotropy for a general constitutive law is not presented here. However for the particular case of the diagonal quadratic strain energy arising in standard linear elasticity the result is completely explicit; in the diagonal quadratic strain energy there are two bending stiffnesses $K_1(s)$ and $K_2(s)$ that are in general unequal, but we demonstrate that in the asymptotic limit of high intrinsic twist the two effective bending stiffnesses are equal, with the common value $\bar{K}(s)$ equal to the harmonic average:

$$\bar{K} = \frac{2}{K_1^{-1} + K_2^{-1}}.$$

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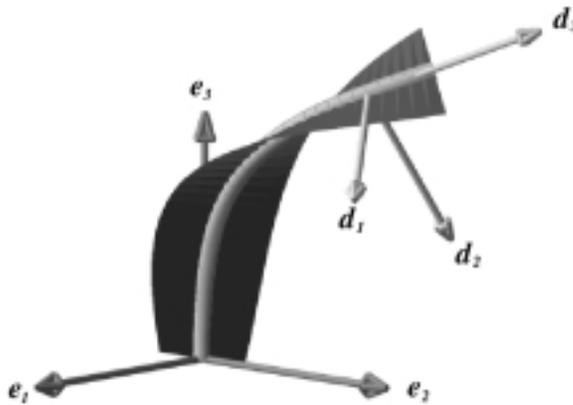


Figure 1: A configuration of an elastic rod. The tube represents the centerline $\mathbf{r}(s)$. The triad $\{\mathbf{d}_i(s)\}$ indicates the orientation of the cross-section, with \mathbf{d}_1 generating the ribbon that visualizes twist.

Averaging results are often simplest when applied to Hamiltonian systems, and here we exploit the Hamiltonian formulation of the rod equilibrium equations that is described in Dichmann et al. [5] and Li and Maddocks [6]. However to accommodate the limit of high intrinsic twist, the equilibrium equations are re-written with respect to the natural (or parallel transport) frame of the rod centerline (as introduced in the context of rod mechanics by Langer and Singer [7] and previously used for modeling DNA by Manning et al. [8]). Once the governing equations are written in an appropriate form, the existence of an effective bending law follows from a routine application of standard averaging theory. Our numerical experiments indicate that even the non-dimensional twist rate of approximately 100 that arises for the rather short (approximately 160 base pair) DNA mini-circles that were studied in [8] is effectively ‘high’.

2 The Elastic Rod Model

In this section we establish the mathematical model of an elastic rod that will be exploited in our asymptotic analysis. In subsection 2.1 we outline the elements of the (Cosserat) director theory of elastic rods (cf. Antman [9] for a more extensive discussion). Then in subsection 2.2 we introduce the concept of the *natural frame*, which plays a crucial role in our analysis (cf. [8]). An associated Hamiltonian formulation of the equilibrium conditions is introduced in subsection 2.3 (cf. [5] or [6]).

2.1 Director theory

The configuration of a rod is specified by two smooth vector-valued functions (cf. Figure 1)

$$\mathbf{r}(s), \mathbf{d}_1(s) : [0, 1] \rightarrow \mathbf{R}^3.$$

In the context of DNA, the curve $\mathbf{r}(s)$ can be interpreted as the centerline of the double helix, with $\mathbf{d}_1(s)$ being a unit vector normal to the centerline that serves to locate the orientation of the backbones. We assume that for the loadings of concern the DNA is effectively unshearable and inextensible. (The computations in [8] support this approximation for DNA mini-circles.) Mathematically, unshearability and inextensibility are expressed by setting $\mathbf{r}' = \mathbf{d}_3$ with $\mathbf{d}_3 \cdot \mathbf{d}_1 = 0$, and defining $\mathbf{d}_2 = \mathbf{d}_3 \times \mathbf{d}_1$ to obtain a right-handed orthonormal frame $\{\mathbf{d}_i\}_{i=1}^3$, called the *directors*. With the assumption of inextensibility the parameter $s \in [0, 1]$ can be interpreted as nondimensionalized arclength in any configuration of the DNA molecule.

Orthonormality of the directors $\{\mathbf{d}_i\}$ implies the existence of a *strain vector* \mathbf{u} satisfying

$$\mathbf{d}'_i = \mathbf{u} \times \mathbf{d}_i, \quad i = 1, 2, 3.$$

The components $u_i = \mathbf{u} \cdot \mathbf{d}_i$ with respect to the frame $\{\mathbf{d}_i\}$ are the bending ($i = 1, 2$) and twisting ($i = 3$) strains. We gather the three components u_i in a triple \mathbf{u} .



Figure 2: A configuration with both high intrinsic twist and natural framings.

In rod mechanics the forces and moments acting across a material cross-section are averaged into a net force $\mathbf{n}(s)$ and a net moment $\mathbf{m}(s)$. Then balance of moments and forces imply the coordinate free equilibrium equations

$$\mathbf{m}' + \mathbf{r}' \times \mathbf{n} = \mathbf{0}, \quad \mathbf{n}' = \mathbf{0}.$$

The components $m_i = \mathbf{m} \cdot \mathbf{d}_i$ are the bending and twisting moments in the rod. As above, the triple of director components (m_1, m_2, m_3) is denoted \mathbf{m} . The moments m_i must be related to the strains u_i via suitable constitutive relations. We make the assumption of hyperelasticity: for $\mathbf{v} = (v_1, v_2, v_3)$ there exists a convex strain energy density function $W(\mathbf{v}, \mathbf{s})$ such that $W_{\mathbf{v}}(\mathbf{0}, \mathbf{s}) = \mathbf{0}$, and the constitutive relations are of the form $m_i = W_{v_i}(\mathbf{u} - \hat{\mathbf{u}}, \mathbf{s})$. Here $\hat{\mathbf{u}}(s) = (\hat{u}_1(s), \hat{u}_2(s), \hat{u}_3(s))$ are the components of strain in the minimum energy unstressed configuration. Our results will be particularly explicit when the strain energy density function is assumed to be of the standard diagonal quadratic form

$$(1) \quad W(\mathbf{v}, \mathbf{s}) = \frac{1}{2} \sum_{i=1}^3 K_i(\mathbf{s}) v_i^2,$$

which generates decoupled linear constitutive relations

$$(2) \quad m_i = K_i(u_i - \hat{u}_i).$$

Then $K_1(s)$ and $K_2(s)$ are called the bending stiffnesses, and $K_3(s)$ is the twist stiffness.

2.2 The natural frame

Since we are interested in analyzing elastic rods in the limit of infinite intrinsic twist, it is important to refer the equilibrium equations to a director frame that is independent of \hat{u}_3 . To this end we shall consider the *natural* or parallel transport frame [7, 8].

The frame $\{\mathbf{d}_i\}$ can be rotated about the \mathbf{d}_3 axis through an angle $\Omega(s)$ to obtain a new set of directors $\{\mathbf{D}_i\}$ satisfying

$$\begin{pmatrix} \mathbf{D}_1^T \\ \mathbf{D}_2^T \\ \mathbf{D}_3^T \end{pmatrix} = \mathbf{R}(\Omega) \begin{pmatrix} \mathbf{d}_1^T \\ \mathbf{d}_2^T \\ \mathbf{d}_3^T \end{pmatrix},$$

where the rotation matrix $\mathbf{R}(\Omega)$ is

$$(3) \quad \mathbf{R}(\Omega) = \begin{pmatrix} \cos \Omega & \sin \Omega & 0 \\ -\sin \Omega & \cos \Omega & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The $\{\mathbf{D}_i\}$ frame has an associated strain vector \mathbf{U} satisfying

$$\mathbf{D}'_i = \mathbf{U} \times \mathbf{D}_i,$$

and the triple of components $U_i = \mathbf{U} \cdot \mathbf{D}_i$ will be denoted \mathbf{U} . Similarly we let $\hat{\mathbf{U}}$ denote the triple of components of strain of the $\{\mathbf{D}_i\}$ frame in the unstressed configuration. For any choice of angle function $\Omega(s)$, it is easily calculated (see [8]) that

$$(4) \quad \mathbf{U} = \mathbf{R}(\Omega)[\mathbf{u} + \Omega' \mathbf{e}_3],$$

where $\mathbf{e}_3 = (0, 0, 1)^T$, which can be inverted to yield

$$\mathbf{u} = \mathbf{R}^T(\Omega)[\mathbf{U} - \Omega' \mathbf{e}_3].$$

The same relation holds for the unstressed strains \hat{U}_i , i.e.

$$(5) \quad \hat{\mathbf{U}} = \mathbf{R}(\Omega)[\hat{\mathbf{u}} + \Omega' \mathbf{e}_3].$$

The frame $\{\mathbf{D}_i\}$ will be called *natural* if it has no twist in the unstressed configuration, i.e. $\hat{U}_3 = 0$. From equation (5) we see that we obtain a natural frame provided the angle function Ω is chosen to be a solution of the ordinary differential equation

$$(6) \quad \Omega' = -\hat{u}_3.$$

Accordingly we see that up to an arbitrary choice of $\Omega(0)$, the natural frame is uniquely defined by the function $\hat{u}_3(s)$. Figure 2 depicts an unstressed rod configuration with both a high intrinsic twist reference frame (representative of a frame that tracks the DNA double helix), and a natural reference frame.

In order to refer the equilibrium conditions to the natural frame it is necessary to consider the components $M_i = \mathbf{m} \cdot \mathbf{D}_i$ of the moment vector \mathbf{m} . The triple of components M_i will be denoted \mathbf{M} . Then the components \mathbf{M} in the natural frame are related to the components \mathbf{m} in the $\{\mathbf{d}_i\}$ frame via

$$\mathbf{M} = \mathbf{R}(\Omega)\mathbf{m}.$$

2.3 Hamiltonian formulation

We next describe a Hamiltonian form (with ‘evolution’ in arc-length s) of the equilibrium conditions expressed with respect to the natural frame $\{\mathbf{D}_i\}$. To formulate the equations governing rod equilibria as a canonical Hamiltonian system we need to choose a parameterization of the rotation group $SO(3)$. It should be noted however, that the form of the Hamiltonian is independent of this choice; in particular, the averaging result in section 3 is independent of the parameterization adopted.

The Euler parameter description of $SO(3)$ is a quadruple $\mathbf{q} = (q_1, q_2, q_3, q_4) \in \mathbf{R}^4$ with unit length. The directors \mathbf{D}_i can then be written, e.g.

$$\mathbf{D}_3 = \begin{pmatrix} 2(q_1 q_3 + q_2 q_4) \\ 2(-q_1 q_4 + q_2 q_3) \\ -q_1^2 - q_2^2 + q_3^2 + q_4^2 \end{pmatrix}.$$

With the notation

$$(7) \quad \mathbf{B}_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{B}_2 = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

and

$$(8) \quad \mathbf{B}_3 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix},$$

the strains U_i are

$$U_i = 2 \frac{\mathbf{B}_i \mathbf{q} \cdot \mathbf{q}'}{|\mathbf{q}|^2}.$$

We denote the strain energy density function dependent on the rotated variables $\mathbf{V} = \mathbf{R}\mathbf{v}$ by

$$W^\Omega(\mathbf{V}, s) = W(\mathbf{R}^T(\Omega)\mathbf{V}, s),$$

where $W(\mathbf{v}, s)$ is prescribed (e.g. (1) in the linearly elastic case), and furthermore define

$$\widehat{W}^\Omega(\mathbf{U}, s) = W^\Omega(\mathbf{U} - \hat{\mathbf{U}}, s) = W(\mathbf{R}^\top(\Omega)(\mathbf{U} - \hat{\mathbf{U}}), s).$$

In other words \widehat{W}^Ω is defined in terms of a given function W of the rotated and shifted variables

$$\mathbf{u} - \hat{\mathbf{u}} = \mathbf{R}^\top(\Omega)(\mathbf{U} - \hat{\mathbf{U}})$$

consistent with (4) and (5). Then the constitutive equations in the natural frame variables become

$$M_i = \widehat{W}_{U_i}^\Omega(\mathbf{U}, s).$$

A Hamiltonian formulation of the equilibrium conditions involves the Legendre transform $\widehat{W}^{\Omega*}(M, s)$ of the strain energy density function $\widehat{W}^\Omega(\mathbf{U}, s)$, which can be calculated to be

$$\widehat{W}^{\Omega*}(M, s) = W^*(\mathbf{R}^\top M, s) + \hat{\mathbf{U}} \cdot M,$$

where $W^*(\mathbf{m}, s)$ is the Legendre transform of the given function $W(\mathbf{v}, s)$. For the specific quadratic bending energy (1),

$$W^*(\mathbf{m}, s) = \frac{1}{2} \sum_{i=1}^3 K_i(s)^{-1} m_i^2,$$

so that

$$\begin{aligned} \widehat{W}^{\Omega*}(M, s) &= \frac{1}{2} \sum_{i=1}^3 a_i(s, \Omega) M_i^2 + a_{12}(s, \Omega) M_1 M_2 \\ &\quad + \hat{U}_1 M_1 + \hat{U}_2 M_2, \end{aligned}$$

where the s - and Ω -dependent coefficients are

$$\begin{aligned} a_1(s, \Omega) &= K_1(s)^{-1} \cos^2 \Omega + K_2(s)^{-1} \sin^2 \Omega, \\ a_2(s, \Omega) &= K_1(s)^{-1} \sin^2 \Omega + K_2(s)^{-1} \cos^2 \Omega, \\ a_3(s, \Omega) &= K_3(s)^{-1}, \\ a_{12}(s, \Omega) &= \left(K_2(s)^{-1} - K_1(s)^{-1} \right) \sin \Omega \cos \Omega. \end{aligned}$$

Li and Maddocks [6] derive the Euler parameter version of the rod equilibrium equations as a seven degree of freedom, canonical Hamiltonian system

$$\mathbf{z}' = \mathbf{J} \nabla H(\mathbf{z}, s, \Omega)$$

with associated Hamiltonian

$$\begin{aligned} (9) \quad H(\mathbf{z}, s, \Omega) &= \widehat{W}^{\Omega*}(M, s) + \mathbf{n} \cdot \mathbf{D}_3 \\ &= W^*(\mathbf{R}^\top(\Omega)M, s) + M \cdot \hat{\mathbf{U}} + \mathbf{n} \cdot \mathbf{D}_3, \end{aligned}$$

where $\mathbf{z} = (\mathbf{r}, \mathbf{q}, \mathbf{n}, \boldsymbol{\mu})$, and

$$\mathbf{J} = \begin{pmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{I} & \mathbf{0} \end{pmatrix}.$$

For the purposes of the following asymptotic analysis we explicitly separate the dependence of the Hamiltonian (9) on the independent variable s and the angle function Ω . In particular, because Ω only enters through the rotation matrix (3), the Hamiltonian is always 2π -periodic in Ω . Furthermore, the dependence on Ω only appears through the Legendre transform W^* of the strain energy function W , and the term $\hat{\mathbf{U}} \cdot M$ including the natural curvatures $\hat{\mathbf{U}}$ has no dependence on Ω . This will be important in our analysis of averaging over Ω , which will be seen to be a *fast* variable.

3 Homogenization

In this section we describe our main result, namely that a high intrinsic twist yields, to a first approximation, an averaged strain energy function in which any slowly varying intrinsic curvature of the unstressed rod persists. In the linearly elastic case the averaged constitutive law explicitly implies that the two effective bending stiffnesses are equal. We formulate the problem in terms of a small parameter representing the high intrinsic twist rate, and use the theory of averaging to construct a homogenized system that may be interpreted as the lowest order approximation in an asymptotic expansion.

A uniform high intrinsic twist is incorporated into the model by setting $\hat{u}_3(s) \equiv -\frac{1}{\epsilon}$ with $0 < \epsilon \ll 1$. The Hamiltonian $H(\mathbf{z}, s, \Omega)$ is dependent on the parameter ϵ through the identity $\Omega(s) = \frac{s}{\epsilon}$ obtained from integration of equation (6). We consider the limit as ϵ tends to zero, i.e. as a uniform, intrinsic twist tends to infinity. Note that this analysis requires the formulation of the problem in the natural frame $\{\mathbf{D}_i\}$, since the rod frame $\{\mathbf{d}_i\}$ is not defined in the limit.

The result is formulated as follows. Denote the solution of the Hamiltonian system

$$(10) \quad \mathbf{z}' = \mathbf{J}\nabla H\left(\mathbf{z}, s, \frac{s}{\epsilon}\right), \quad \mathbf{z}(0) = \mathbf{z}_0,$$

by $\mathbf{z}_\epsilon(s)$. Define an averaged Hamiltonian

$$\bar{H}(\mathbf{z}, s) = \frac{1}{2\pi} \int_0^{2\pi} H(\mathbf{z}, s, \Omega) d\Omega$$

by integrating over one period with respect to the fast variable Ω , and consider the corresponding averaged system

$$(11) \quad \mathbf{z}' = \mathbf{J}\nabla\bar{H}(\mathbf{z}, s), \quad \bar{\mathbf{z}}(0) = \mathbf{z}_0,$$

with solution $\bar{\mathbf{z}}(s)$. We would like to understand the sense in which the solution $\bar{\mathbf{z}}$ of (11) approximates the solution \mathbf{z}_ϵ of (10). Our conclusion is the following: if the initial data satisfy $|\mathbf{z}_0 - \bar{\mathbf{z}}_0| = O(\epsilon)$, then $|\mathbf{z}(s) - \bar{\mathbf{z}}(s)| = O(\epsilon)$ on bounded intervals. In other words as ϵ approaches zero, the solution \mathbf{z}_ϵ of (10) converges uniformly on bounded intervals to the solution $\bar{\mathbf{z}}$ of the averaged system (11).

To reach this conclusion we first cast the problem into a form suitable for standard averaging theory (cf. Hale [10, section V.3] or Guckenheimer and Holmes [11, chapter 4]). Make the substitution $t = \frac{s}{\epsilon}$ in (10) to obtain the system

$$\frac{d}{dt}\mathbf{z} = \epsilon\mathbf{J}\nabla H(\mathbf{z}, \epsilon t, t), \quad \mathbf{z}(0) = \mathbf{z}_0.$$

Introducing the new variable $\tau = \epsilon t$ then yields the augmented system

$$\frac{d}{dt}\mathbf{x} = \epsilon\mathbf{f}(\mathbf{x}, t), \quad \mathbf{x}(0) = \mathbf{x}_0,$$

where $\mathbf{x} = (\mathbf{z}, \tau)^T$, $\mathbf{x}_0 = (\mathbf{z}_0, 0)^T$ and $\mathbf{f}(\mathbf{x}, t) = (\mathbf{J}\nabla H(\mathbf{z}, \tau, t), 1)^T$. This system is now exactly in a form suitable for applying Theorem 4.1.1 of [11]. The averaged system is defined by

$$\frac{d}{dt}\bar{\mathbf{x}} = \frac{1}{2\pi} \int_0^{2\pi} \mathbf{f}(\bar{\mathbf{x}}, \sigma) d\sigma, \quad \bar{\mathbf{x}}(0) = \bar{\mathbf{x}}_0.$$

The averaging theorem implies that if $|\mathbf{x}_0 - \bar{\mathbf{x}}_0| = O(\epsilon)$ then $|\mathbf{x}(t) - \bar{\mathbf{x}}(t)| = O(\epsilon)$ on a time scale $t \sim \frac{1}{\epsilon}$. Translating back to our original variables yields the desired result, namely that $|\mathbf{z}(s) - \bar{\mathbf{z}}(s)| = O(\epsilon)$ on bounded intervals.

It remains to consider the explicit form of the averaged Hamiltonian

$$\bar{H}(\mathbf{r}, \mathbf{n}, \mathbf{q}, \boldsymbol{\mu}, s) = \bar{W}^*(M, s) + \hat{U}_1 M_1 + \hat{U}_2 M_2 + \mathbf{n} \cdot \mathbf{D}_3,$$

where

$$(12) \quad \bar{W}^*(M, s) = \frac{1}{2\pi} \int_0^{2\pi} W^*(\mathbf{R}^T(\Omega)M, s) d\Omega.$$

It is important to note that \bar{W}^* is not the Legendre transform of the average of $W(\mathbf{R}^T(\Omega)\mathbf{U}, s)$, since the averaging operator and the Legendre transform do not commute. Rather the effective strain energy function \bar{W} should be computed as the Legendre transform of the averaged transform \bar{W}^* .

In the case that the rod is linearly elastic, i.e. the bending energy is of the form (1), we can explicitly compute the averaged Hamiltonian to be

$$\begin{aligned} \overline{H}(\mathbf{r}, \mathbf{n}, \mathbf{q}, \boldsymbol{\mu}, s) &= \sum_{i=1}^2 \left\{ \frac{1}{2} \bar{K}(s)^{-1} M_i^2 + \hat{U}_i(s) M_i \right\} \\ &\quad + \frac{1}{2} K_3(s)^{-1} M_3^2 + \mathbf{n} \cdot \mathbf{D}_3, \end{aligned}$$

with the single effective isotropic bending stiffness being given by the harmonic average

$$\bar{K}(s) = \frac{2}{K_1(s)^{-1} + K_2(s)^{-1}},$$

and the associated effective strain energy

$$\begin{aligned} \overline{W}(\mathbf{U} - \hat{\mathbf{U}}, s) &= \frac{1}{2} \bar{K}(s) \left((U_1 - \hat{U}_1)^2 + (U_2 - \hat{U}_2)^2 \right) \\ &\quad + \frac{1}{2} K_3(s) U_3^2. \end{aligned}$$

It is noteworthy that while averaging over high twist eliminates anisotropy due to differing bending stiffnesses, and yields two effective equal bending stiffnesses, effects of anisotropy due to the natural curvatures of the rod, encoded by \hat{U}_1 and \hat{U}_2 , are unaffected, and persist in the averaged equations.

4 A Numerical Experiment

We now illustrate our analysis of effective constitutive relations with some computations that compare the numerical solutions of unaveraged and averaged systems. We consider only the (diagonal) linearly elastic energy (1), and further restrict ourselves to uniform rods in which the coefficient functions reduce to constants, and in which there is no intrinsic curvature. We hold the initial conditions of the Hamiltonian system fixed at values for which the equilibrium for the averaged infinite-twist limit problem is a closed circular loop. (Explicitly we take both bending stiffnesses equal to $\bar{K} = 0.1$.) We then numerically compute the equilibria for fixed $K_1 \neq K_2$, and an increasing sequence of intrinsic twist rates $\hat{u}_3 = 0, 50, 100$. (Explicitly we take $K_1 = 0.2$ and $K_2 = 0.0666$, whose harmonic average is $\bar{K} = 0.1$.) As \hat{u}_3 increases, cf. Figures 3(a), (b) and (c), the equilibria approach the circular equilibrium of the infinite intrinsic twist limit problem.

5 Conclusions

We have demonstrated that elastic rods with non-isotropic constitutive relations for bending, but with high intrinsic twist, can be well-approximated by an averaged, or homogenized, rod model corresponding to a limiting problem with an infinite intrinsic twist. The presence and significance of anisotropy due to intrinsic curvature persists through our averaging procedure. In the standard case of a linearly elastic rod with a diagonal quadratic energy, there is a single effective isotropic bending stiffness, namely the harmonic average of the two anisotropic bending stiffnesses. In the case of a more general non-linear constitutive relation for bending, the limit can again be shown to be an isotropic bending law, with the only remaining anisotropic effects being associated with natural curvature. We believe these conclusions to be of considerable interest within the context of continuum models of DNA; DNA has exactly the properties alluded to above, namely locally unequal bending stiffnesses, a high intrinsic twist rate and often nonzero unstressed curvatures (e.g. A-tracts).

Our analysis does raise further mathematical issues that remain to be resolved. First, we have in effect only computed the first term of an asymptotic expansion based on high-twist. It would also be of interest to compute higher-order correction terms as an estimate of the quality of the infinite twist limit. Second, it is important to point out that the results here are couched in terms of an initial value problem for a Hamiltonian system. But for elastic rods it is more natural to consider two-point boundary value problems, and the associated averaging theory in that context. Both of these issues are addressed in the companion article [12].

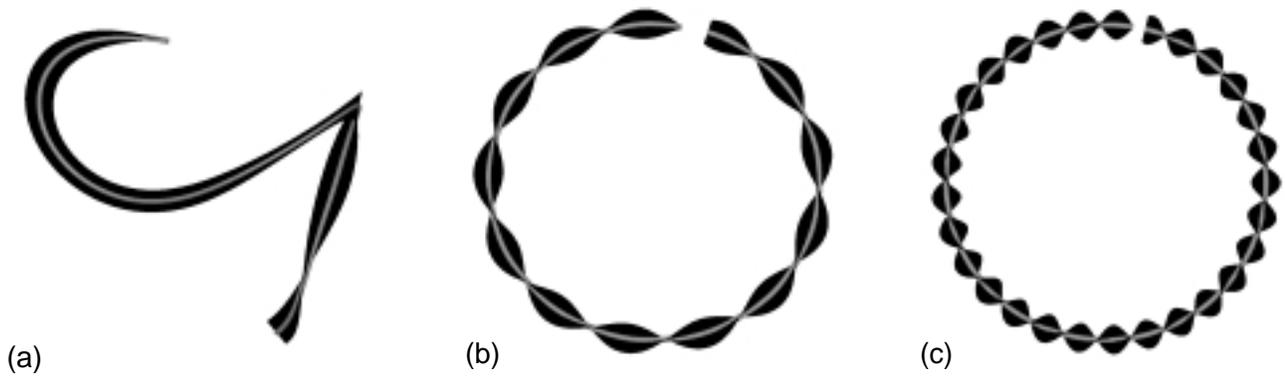


Figure 3: A sequence of equilibria of three rods with the same unequal bending stiffnesses K_1 and K_2 , but an increasing sequence of intrinsic twists. All equilibria are subject to the same initial conditions, for which the effective infinite intrinsic twist problem has as solution a closed circle. As the twist is increased, (a) $\hat{u}_3 = 0$, (b) $\hat{u}_3 = 50$, and (c) $\hat{u}_3 = 100$, the equilibria approach the equilibrium of the effective problem.

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