Buckling of an Elastic Rod with High Intrinsic Twist

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Abstract

Motivated by the application of modelling DNA by an elastic rod, we use the technique of two-scale homogenization on a two-point boundary value problem (BVP) involving buckling of a rod with a high intrinsic twist. The basic question is to understand the errors generated in replacing a rod with a high, but finite, intrinsic twist, by an effective rod in the infinite intrinsic twist limit. For our buckling problem the effective problem is isotropic. As a consequence there is a continuous family of buckled planar solutions. We show that the buckled configurations of the rod with high intrinsic twist are close to certain special planar buckled configurations of the isotropic rod that are selected from among all the solutions to the effective problem. The selected planes are independent of the values of the (bending and twisting) stiffnesses and of the load.

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

AMS subject classifications: 74K10, 74Q15.

1 Introduction

Recently, there has been considerable interest in modeling the long length-scale (several hundred base pairs) deformations of DNA molecules using elastic rod theories (cf. the review articles [8, 9], for example). These rod models usually assume an isotropic response to bending loads, even if, on short length-scales (a few base pairs), DNA has a nonisotropic response to such loads. The reason for this approximation is the high intrinsic twist of the molecule (typically one complete turn approximately every 10.5 base pairs), which causes some "averaging" of the bending response over all directions.

It is possible to understand this "averaging" and give some justification to the use of an isotropic bending law in rod models of DNA by studying the problem of an elastic rod with a nonisotropic bending law and a high intrinsic twist. Kehrbaum and Maddocks [4] used averaging results coming from dynamical systems to show that such a rod is well approximated on relatively long length-scales by an effective rod with a particular isotropic bending law. However their treatment only considered the case of the pure initial value problem (IVP). In particular the error estimates associated with the IVP problem are not immediately applicable to the more natural problems for rods, namely two-point boundary value problems (BVPs).

In this paper we consider the same rod equations as in [3, 4], but we use a two-scale homogenization expansion. We are thereby able to treat the case of two-point BVPs. We again show that any configuration of a rod with a high intrinsic twist is well approximated by a configuration of an effective rod. However, in some cases, the effective problem has an additional continuous symmetry corresponding to isotropy, and therefore more solutions than the original problem. Then only some of the solutions to the effective problem are approximations to solutions to the original problem. We study this question in detail in the particular case of buckling of a strut. The corresponding

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effective strut is isotropic and can buckle in any direction, but we show that the strut with high intrinsic twist can only buckle in directions making a 45° angle with the direction of minimal stiffness at the clamped end.

The paper is organized as follows. In section 2 we give the definition of a rod with a high intrinsic twist. Following the treatment in [4], we write the equilibrium equations in a form suitable for homogenization by making a change of reference frame and considering a Hamiltonian formulation of the equations. More details about this approach can be found in [3]. In section 3, using a two-scale homogenization expansion, we obtain both the zeroth-order effective rod problem, and a linear BVP whose solution yields the first-order correction. In section 4 we treat the particular case of a strut with a nonisotropic cross-section and a constant high intrinsic twist. Its directions of buckling are determined by the solvability condition for the BVP associated with the first-order correction. The method builds on the approach to symmetry breaking introduced in [7].

Although in section 4 we focus on a problem with a specific set of boundary conditions, and with a specific constitutive relation, the approach developed in sections 2 and 3 is more general, and can be used to treat many different two-point BVPs involving rods with high intrinsic twist.

2 Rod with High Intrinsic Twist

We adopt the special Cosserat theory of elastic rods [1] and consider an inextensible unshearable linearly elastic rod with a high intrinsic twist. The rod is parametrized by arclength s. For convenience we choose a length-scale such that $0 \leqslant s \leqslant 1$. The configuration of the rod is represented by a centerline $\boldsymbol{r}(s) \in \mathbb{R}^3$ and an orthonormal frame of directors $\{\boldsymbol{d}_i(s) \in \mathbb{R}^3 : i = 1,2,3\}$ that describe the orientation of the rod cross-section. We assume the rod to be inextensible and unshearable, i.e. $\boldsymbol{d}_3$, the director perpendicular to the cross-section, coincides with the unit vector $\boldsymbol{r}'$ tangent to the centerline.

The functions representing the configuration of the rod in absence of applied loads (i.e. the intrinsic shape of the rod) are denoted by $\hat{\boldsymbol{r}}$, $\{\hat{\boldsymbol{d}}_i\}$. We assume the rod has a high intrinsic twist:

Definition 2.1 (cf. [3], §9.6) A rod is said to have a *high intrinsic twist* if a rapid spin of $\{\hat{\boldsymbol{d}}_1, \hat{\boldsymbol{d}}_2\}$ about $\hat{\boldsymbol{d}}_3$ is superimposed on an arbitrary (slow) variation of the directors, i.e. if $\{\hat{\boldsymbol{d}}_i\}$ are of the form

$$\hat{\boldsymbol{d}}_i(s;\epsilon) = \sum_{j=1}^{3} \Omega_{ij}(\tfrac{s}{\epsilon})\, \hat{\boldsymbol{D}}_j(s), \quad i = 1,2,3, \tag{1}$$

where ϵ is a small nonzero parameter, $\{\Omega_{ij}(\frac{s}{\epsilon})\}$ are the entries of the rotation matrix

$$\boldsymbol{\Omega}(\tfrac{s}{\epsilon}) = \begin{pmatrix} \cos\frac{s}{\epsilon} & \sin\frac{s}{\epsilon} & 0 \\ -\sin\frac{s}{\epsilon} & \cos\frac{s}{\epsilon} & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

and $\{\hat{\boldsymbol{D}}_i(s)\}$ is an orthonormal frame independent of ϵ. ■

Note that, in particular, the frame $\{\hat{\boldsymbol{D}}_i(s)\}$ is *slowly varying* in the sense that the derivatives $\{\hat{\boldsymbol{D}}_i'(s)\}$ are small compared to $\frac{1}{\epsilon}$, for ϵ sufficiently small.

Orthonormality of the directors implies the existence of a Darboux vector $\boldsymbol{u} \in \mathbb{R}^3$ satisfying $\boldsymbol{d}_i' = \boldsymbol{u} \times \boldsymbol{d}_i$, $i = 1,2,3$. The components $u_i \equiv \boldsymbol{u}^T \boldsymbol{d}_i$ of $\boldsymbol{u}$ in the frame $\{\boldsymbol{d}_i\}$ are the bending ($i = 1,2$) and twisting ($i = 3$) strains. The stresses acting across a cross-section of the rod are averaged into a net force $\boldsymbol{n}(s) \in \mathbb{R}^3$ and a net moment $\boldsymbol{m}(s) \in \mathbb{R}^3$. For a linearly elastic rod, the components $m_i \equiv \boldsymbol{m}^T \boldsymbol{d}_i$ of the moment are related to the strains u_i via a constitutive relation of the form

$$\begin{pmatrix} m_1 \\ m_2 \\ m_3 \end{pmatrix} = \boldsymbol{K} \begin{pmatrix} u_1 - \hat{u}_1 \\ u_2 - \hat{u}_2 \\ u_3 - \hat{u}_3 \end{pmatrix},$$

where the intrinsic strains $\{\hat{u}_i\}$ correspond to the directors $\{\hat{\boldsymbol{d}}_i\}$, and the 3×3 matrix $\boldsymbol{K}(s)$ is positive-definite, symmetric and independent of ϵ. We call $\boldsymbol{K}$ a stiffness matrix and $\boldsymbol{K}^{-1}$ a flexibility matrix.

Following relation (1) for the intrinsic shape, we introduce a new framing $\{\boldsymbol{D}_i\}$ for arbitrary configurations of the rod by an arclength-dependent rotation of the original frame about $\boldsymbol{d}_3$:

$$\boldsymbol{D}_i(s;\epsilon) = \sum_{j=1}^{3} \Omega_{ji}(\tfrac{s}{\epsilon})\, \boldsymbol{d}_j(s;\epsilon), \quad i = 1,2,3. \tag{2}$$

By assumption (1), the frame $\{\hat{\boldsymbol{D}}_i(s)\}$ in the reference configuration is slowly varying, and we shall seek deformed configurations in which the frame $\{\boldsymbol{D}_i(s;\epsilon)\}$ is also slowly varying.

Let $\boldsymbol{U}$ denote the Darboux vector associated with the new frame. Then the new strains $U_i \equiv \boldsymbol{U}^T\boldsymbol{D}_i$ and the components $M_i \equiv \boldsymbol{m}^T\boldsymbol{D}_i$ of the moment in the new frame are related through the constitutive relation

$$\begin{pmatrix} M_1 \\ M_2 \\ M_3 \end{pmatrix} = \boldsymbol{\Omega}\boldsymbol{K}\boldsymbol{\Omega}^T \begin{pmatrix} U_1 - \hat{U}_1 \\ U_2 - \hat{U}_2 \\ U_3 - \hat{U}_3 \end{pmatrix},$$

where $\{\hat{U}_i(s)\}$ are the intrinsic strains associated with the directors $\{\hat{\boldsymbol{D}}_i(s)\}$.

Note that the change of variable (2) used here and in [3] is slightly different from the change of variable considered in [4]. The rotation matrix relating the original and new frames considered in [4] (cf. equation (3) in [4]) is chosen in such a way that $\hat{U}_3 = 0$. In point of fact, both of these changes of variable can be used to transform the problem into a form suitable for homogenization. Moreover the two choices coincide in the particular case of a *constant* high intrinsic twist ($\hat{u}_3 = \frac{1}{\epsilon}$).

There are different ways to write the equilibrium equations for the rod described above, but the homogenization method developed in the next section only applies to first-order systems. We therefore choose the canonical Hamiltonian formulation presented in [2, 5]. Let $\{\boldsymbol{e}_i(s) \in \mathbb{R}^3 : i = 1,2,3\}$ be a fixed orthonormal frame in $\mathbb{R}^3$ and $\boldsymbol{r}$, $\boldsymbol{n}$, $\boldsymbol{D}_i$ designate the triples of components of the corresponding vectors relative to that basis. We parametrize the directors $\{\boldsymbol{D}_i\}$ by a unit quadruple $\boldsymbol{q} \in \mathbb{R}^4$ called a quaternion:

$$\text{(3)} \qquad \boldsymbol{D}_1(\boldsymbol{q}) = \begin{pmatrix} q_1^2 - q_2^2 - q_3^2 + q_4^2 \\ 2q_1q_2 + 2q_3q_4 \\ 2q_1q_3 - 2q_2q_4 \end{pmatrix}, \quad \boldsymbol{D}_2(\boldsymbol{q}) = \begin{pmatrix} 2q_1q_2 - 2q_3q_4 \\ -q_1^2 + q_2^2 - q_3^2 + q_4^2 \\ 2q_2q_3 + 2q_1q_4 \end{pmatrix}, \quad \boldsymbol{D}_3(\boldsymbol{q}) = \begin{pmatrix} 2q_1q_3 + 2q_2q_4 \\ 2q_2q_3 - 2q_1q_4 \\ -q_1^2 - q_2^2 + q_3^2 + q_4^2 \end{pmatrix}.$$

The phase variable is $\boldsymbol{x} = (\boldsymbol{r}, \boldsymbol{q}, \boldsymbol{n}, \boldsymbol{\mu}) \in \mathbb{R}^{14}$, where the force $\boldsymbol{n}$ is conjugate to the centerline $\boldsymbol{r}$ and the impetus $\boldsymbol{\mu} \in \mathbb{R}^4$ is conjugate to the quaternion $\boldsymbol{q}$. The components of the moment in the frame $\{\boldsymbol{D}_i\}$ can be written as

$$\text{(4)} \qquad M_i(\boldsymbol{q}, \boldsymbol{\mu}) = \tfrac{1}{2}\boldsymbol{\mu}^T\boldsymbol{B}_i\boldsymbol{q},$$

where

$$\boldsymbol{B}_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{B}_2 = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{B}_3 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}.$$

The Hamiltonian is

$$\text{(5)} \qquad H(\boldsymbol{x}, s, \tfrac{s}{\epsilon}) = \tfrac{1}{2}\begin{pmatrix} M_1(\boldsymbol{q},\boldsymbol{\mu}) \\ M_2(\boldsymbol{q},\boldsymbol{\mu}) \\ M_3(\boldsymbol{q},\boldsymbol{\mu}) \end{pmatrix}^T \boldsymbol{C}(s, \tfrac{s}{\epsilon}) \begin{pmatrix} M_1(\boldsymbol{q},\boldsymbol{\mu}) \\ M_2(\boldsymbol{q},\boldsymbol{\mu}) \\ M_3(\boldsymbol{q},\boldsymbol{\mu}) \end{pmatrix} + \begin{pmatrix} M_1(\boldsymbol{q},\boldsymbol{\mu}) \\ M_2(\boldsymbol{q},\boldsymbol{\mu}) \\ M_3(\boldsymbol{q},\boldsymbol{\mu}) \end{pmatrix}^T \begin{pmatrix} \hat{U}_1(s) \\ \hat{U}_2(s) \\ \hat{U}_3(s) \end{pmatrix} + \boldsymbol{n}^T\boldsymbol{D}_3(\boldsymbol{q}),$$

where

$$\text{(6)} \qquad \boldsymbol{C}(s, \tfrac{s}{\epsilon}) = \boldsymbol{\Omega}(\tfrac{s}{\epsilon})\boldsymbol{K}^{-1}(s)\boldsymbol{\Omega}^T(\tfrac{s}{\epsilon})$$

corresponds to the flexibility matrix in the new frame. The two-point BVP describing the equilibria of the rod is

$$\text{(7)} \qquad \boldsymbol{x}' = \boldsymbol{J}H_{\boldsymbol{x}}(\boldsymbol{x}, s, \tfrac{s}{\epsilon}), \quad \boldsymbol{g}(\boldsymbol{x}(0)) = \boldsymbol{0}, \quad \boldsymbol{h}(\boldsymbol{x}(1)) = \boldsymbol{0},$$

where $\boldsymbol{J} \in \mathbb{R}^{14\times14}$ is the standard symplectic matrix, $H_{\boldsymbol{x}}$ denotes the gradient of H, and $\boldsymbol{g}$, $\boldsymbol{h} \in \mathbb{R}^7$ define the boundary conditions at $s = 0$, $s = 1$.

3 Homogenization and the Effective Rod

We now develop a two-scale homogenization expansion for problem (7). We assume $\hat{U}_i(s)$, $\boldsymbol{K}^{-1}(s)$, $\boldsymbol{g}(\boldsymbol{x})$ and $\boldsymbol{h}(\boldsymbol{x})$ are smooth functions. As indicated in equations (5) and (6), $\boldsymbol{\Omega}$ is a function of the short scale variable $\frac{s}{\epsilon}$ only, while

$\hat{U}_i$ and $\boldsymbol{K}^{-1}$ are functions of the long scale variable s only. We regard the dependence of the Hamiltonian H on the variable s and on the variable $\frac{s}{\epsilon}$ as being independent, and, in the usual way leading to two-scale homogenization, we seek a solution to (7) with the same property. That is we write $\boldsymbol{x}(s;\epsilon) = \boldsymbol{z}(s,\tau)$, where $s \in [0,1]$ and $\tau \in [0, \frac{1}{\epsilon}]$ are considered as independent variables, and $\boldsymbol{z}$ is a solution to

$$\boldsymbol{z}' + \tfrac{1}{\epsilon}\dot{\boldsymbol{z}} = \boldsymbol{J}H_{\boldsymbol{x}}(\boldsymbol{z},s,\tau), \quad \boldsymbol{g}(\boldsymbol{z}(0,0)) = \boldsymbol{0}, \quad \boldsymbol{h}(\boldsymbol{z}(1,\tfrac{1}{\epsilon})) = \boldsymbol{0}, \tag{8}$$

with the notation $' \equiv \frac{\partial}{\partial s}$ and $\dot{} \equiv \frac{\partial}{\partial \tau}$. The following proposition is immediate.

Proposition 3.1 *If $\boldsymbol{z}(s,\tau)$ is a solution to problem (8), then $\boldsymbol{x}(s;\epsilon) \equiv \boldsymbol{z}(s,\frac{s}{\epsilon})$ is a solution to problem (7).*

Note that the Hamiltonian is 2π-periodic with respect to the short scale: $H(\boldsymbol{z},s,\tau+2\pi) = H(\boldsymbol{z},s,\tau)$. We therefore seek solutions to problem (8) that are also 2π-periodic in τ via an appropriate asymptotic expansion. We denote by $H_{\boldsymbol{xx}}$ the Hessian matrix of H and adopt the notation

$$H' \equiv \frac{\partial}{\partial s}H, \quad \langle H\rangle(\boldsymbol{x},s) \equiv \frac{1}{2\pi}\int_0^{2\pi} H(\boldsymbol{x},s,\sigma)\,d\sigma, \quad \widetilde{H}(\boldsymbol{x},s,\tau) \equiv \int_0^{\tau} [H(\boldsymbol{x},s,\sigma) - \langle H\rangle(\boldsymbol{x},s)]\,d\sigma.$$

Proposition 3.2 *Assume a solution $\boldsymbol{z}(s,\tau)$ to BVP (8) is 2π-periodic in τ and can be expanded in the form*

$$\boldsymbol{z}(s,\tau) = \boldsymbol{z}_0(s,\tau) + \epsilon \boldsymbol{z}_1(s,\tau) + \epsilon^2 \boldsymbol{z}_2(s,\tau) + \ldots .$$

Then $\boldsymbol{z}_0(s,\tau) = \boldsymbol{x}_*(s)$, where $\boldsymbol{x}_*(s)$ is a solution to the BVP

$$\boldsymbol{x}_*' = \boldsymbol{J}\langle H\rangle_{\boldsymbol{x}}(\boldsymbol{x}_*,s), \quad \boldsymbol{g}(\boldsymbol{x}_*(0)) = \boldsymbol{0}, \quad \boldsymbol{h}(\boldsymbol{x}_*(1)) = \boldsymbol{0}, \tag{9}$$

and

$$\boldsymbol{z}_1(s,\tau) = \boldsymbol{y}(s) + \boldsymbol{J}\widetilde{H}_{\boldsymbol{x}}(\boldsymbol{x}_*,s,\tau),$$

where $\boldsymbol{y}(s)$ is a solution to the linear BVP

$$\mathcal{L}(\boldsymbol{x}_*)\boldsymbol{y} = \boldsymbol{p}(\boldsymbol{x}_*), \quad \boldsymbol{g}_{\boldsymbol{x}}(\boldsymbol{x}_*(0))\boldsymbol{y}(0) = \boldsymbol{0}, \quad \boldsymbol{h}_{\boldsymbol{x}}(\boldsymbol{x}_*(1))\boldsymbol{y}(1) = -\boldsymbol{h}_{\boldsymbol{x}}(\boldsymbol{x}_*(1))\boldsymbol{J}\widetilde{H}_{\boldsymbol{x}}(\boldsymbol{x}_*(1),1,\xi_\epsilon). \tag{10}$$

Here

$$\mathcal{L}(\boldsymbol{x})\boldsymbol{y} \equiv \boldsymbol{J}\boldsymbol{y}' + \langle H_{\boldsymbol{xx}}\rangle(\boldsymbol{x},s)\boldsymbol{y}, \quad \boldsymbol{p}(\boldsymbol{x}) \equiv \Big(-\langle H_{\boldsymbol{xx}}\boldsymbol{J}\widetilde{H}_{\boldsymbol{x}}\rangle + \langle \widetilde{H}'_{\boldsymbol{x}}\rangle + \langle \widetilde{H}_{\boldsymbol{xx}}\rangle \boldsymbol{J}\langle H_{\boldsymbol{x}}\rangle\Big)(\boldsymbol{x},s),$$

and ξ_ϵ is defined by the condition $0 \leqslant \xi_\epsilon = \frac{1}{\epsilon} \pmod{2\pi} < 2\pi$.

We omit the proof of proposition 3.2 because of space restrictions.

As usual in two-scale homogenization theory, the zeroth-order approximation $\boldsymbol{z}_0$ depends only on the long scale variable s. Moreover, for the problem considered here, the first-order correction $\boldsymbol{z}_1$ has a particularly simple form; it is the sum of a known function $\boldsymbol{J}\widetilde{H}_{\boldsymbol{x}}(\boldsymbol{x}_*,s,\tau)$ and of a function $\boldsymbol{y}$ depending only on the variable s.

Problem (9) describes the statics of a rod similar to the original one, except that it has an effective homogenized constitutive relation defined by the averaged flexibility matrix $\langle \boldsymbol{C}\rangle(s)$. As shown in [3, 4], the homogenized constitutive relation is transversely isotropic. The results of homogenization suggest that, for ϵ small enough, any solution to the original rod BVP (7) can be approximated by a solution to the rod BVP (9), which we call the *effective rod problem.*

For the same problem, but subject only to initial conditions, it can be shown [3, 4] that the (unique) solution to the original problem tends to the (unique) solution to the effective problem as $\epsilon \to 0$. In general, in the case of two-point boundary conditions, the set of solutions to the effective problem also constitutes an approximation to the set of solutions to the original problem. However, in some cases, depending upon the precise boundary conditions, the effective problem has an additional continuous symmetry, and correspondingly more solutions than the original problem. Then, only a subset of the solutions to the effective problem constitutes an approximation to the set of solutions to the original problem. We study such an example in the next section.

4 Clamped-Free Strut with High Intrinsic Twist

Consider a rod that is vertically clamped at one end and free to move at the other end under the influence of a prescribed vertical force of magnitude λ:

$$\boldsymbol{r}(0)=\mathbf{0},\quad \boldsymbol{d}_i(0)=\boldsymbol{e}_i,\ \ i=1,2,3,\quad \boldsymbol{n}(1)=-\lambda\boldsymbol{e}_3,\quad \boldsymbol{m}(1)=\mathbf{0}.$$

We call this the Euler strut problem (cf. [6] and references therein). In the variables $\boldsymbol{x}=(\boldsymbol{r},\boldsymbol{q},\boldsymbol{n},\boldsymbol{\mu})$, these boundary conditions can be written as

$$\boldsymbol{r}(0)=\mathbf{0},\quad \boldsymbol{q}(0)=(0,0,0,1),\quad \boldsymbol{n}(1)=(0,0,-\lambda),\quad \boldsymbol{\mu}(1)=\mathbf{0}. \tag{11}$$

Assume the rod is intrinsically straight with a constant high intrinsic twist, i.e. the reference frame $\{\hat{\boldsymbol{d}}_i\}$ is defined by (1) with $\hat{\boldsymbol{D}}_i(s)=\boldsymbol{e}_i$, or $\hat{u}_1=\hat{u}_2=0$, $\hat{u}_3=\frac{1}{\epsilon}$. Suppose the rod has a diagonal constant stiffness matrix $\boldsymbol{K}=\operatorname{diag}(K_1,K_2,K_3)$, and is nonisotropic: $K_1\neq K_2$. The associated flexibility matrix is

$$\boldsymbol{C}(\tfrac{s}{\epsilon})=\begin{pmatrix}\bar{K}^{-1}+\Delta\cos(\frac{2s}{\epsilon}) & \Delta\sin(\frac{2s}{\epsilon}) & 0\\ \Delta\sin(\frac{2s}{\epsilon}) & \bar{K}^{-1}-\Delta\cos(\frac{2s}{\epsilon}) & 0\\ 0 & 0 & K_3^{-1}\end{pmatrix},$$

where $\bar{K}^{-1}=\frac{1}{2}(K_1^{-1}+K_2^{-1})$ and $\Delta=\frac{1}{2}(K_1^{-1}-K_2^{-1})\neq 0$.

The corresponding effective rod problem (9) describes an isotropic rod with flexibility matrix $\langle\boldsymbol{C}\rangle=\operatorname{diag}(\bar{K}^{-1},\bar{K}^{-1},K_3^{-1})$, subject to the same boundary conditions (11). The effective rod can buckle in any plane containing $\boldsymbol{e}_3$. The solutions $\boldsymbol{x}_0=(\boldsymbol{r}_0,\boldsymbol{q}_0,\boldsymbol{n}_0,\boldsymbol{\mu}_0)$ lying in the $(\boldsymbol{e}_1,\boldsymbol{e}_3)$-plane are of the form

$$\begin{aligned}&\boldsymbol{r}_0=\begin{pmatrix}\int_0^s\sin\phi(\sigma)\,d\sigma\\ 0\\ \int_0^s\cos\phi(\sigma)\,d\sigma\end{pmatrix},\quad \boldsymbol{q}_0=\begin{pmatrix}0\\ \sin(\frac{\phi}{2})\\ 0\\ \cos(\frac{\phi}{2})\end{pmatrix},\quad \boldsymbol{n}_0=\begin{pmatrix}0\\0\\-\lambda\end{pmatrix},\\ &\boldsymbol{\mu}_0=-2\lambda\int_s^1\cos\phi(\sigma)\,d\sigma\begin{pmatrix}0\\ \sin(\frac{\phi}{2})\\ 0\\ \cos(\frac{\phi}{2})\end{pmatrix}+2\bar{K}\phi'\begin{pmatrix}0\\ \cos(\frac{\phi}{2})\\ 0\\ -\sin(\frac{\phi}{2})\end{pmatrix},\end{aligned} \tag{12}$$

where $\phi(s)$, the angle between $\boldsymbol{D}_3(s)$ and $\boldsymbol{e}_3$, satisfies

$$\phi''=-\frac{\lambda}{\bar{K}}\sin\phi,\quad \phi(0)=0,\quad \phi'(1)=0. \tag{13}$$

Any solution to the effective problem can be written in the form $\boldsymbol{x}_\theta=\boldsymbol{R}(\theta)\boldsymbol{x}_0$, where $\boldsymbol{x}_0$ is a solution lying in the $(\boldsymbol{e}_1,\boldsymbol{e}_3)$-plane, and $\theta\in[0,\pi[$ is the angle between the plane containing the solution and $\boldsymbol{e}_1$. The transformation $\boldsymbol{R}(\theta)$ is a combination of (i) a rigid rotation of the rod by an angle θ about $\boldsymbol{e}_3$, and (ii) a rotation of $\{\boldsymbol{d}_1(s),\boldsymbol{d}_2(s)\}$ by an angle $-\theta$ about the tangent $\boldsymbol{d}_3(s)$, leaving the centerline fixed (cf. [7], §3, transformation I). Explicitly, $\boldsymbol{R}(\theta)=\operatorname{diag}(\boldsymbol{R}_3,\boldsymbol{R}_4,\boldsymbol{R}_3,\boldsymbol{R}_4)$, where

$$\boldsymbol{R}_3=\begin{pmatrix}\cos\theta & -\sin\theta & 0\\ \sin\theta & \cos\theta & 0\\ 0&0&1\end{pmatrix},\quad \boldsymbol{R}_4=\begin{pmatrix}\cos\theta & -\sin\theta & 0 & 0\\ \sin\theta & \cos\theta & 0 & 0\\ 0&0&1&0\\ 0&0&0&1\end{pmatrix}.$$

According to the results described in the previous section, each buckled configuration of the strut with high intrinsic twist is close to a buckled configuration of the effective strut. However, due to isotropy, the buckled configurations of the effective strut can lie in any vertical plane, while, since the high twist strut is not isotropic, there is no reason to expect that it can buckle close to any vertical plane. We therefore address the following question: among the one-parameter family of solutions $\{\boldsymbol{x}_\theta=\boldsymbol{R}(\theta)\boldsymbol{x}_0 : \theta\in[0,\pi[,\ \boldsymbol{x}_0 \text{ fixed}\}$ to the effective strut problem, which ones are approximations to solutions to the highly twisted problem? We will identify these special equilibria by studying the solvability condition for BVP (10) that arises in the computation of the first-order correction $\boldsymbol{z}_1$. Note that the trivial solution to the effective strut is invariant under the symmetry $\boldsymbol{R}(\theta)$ and constitutes an approximation to the trivial solution to the highly twisted strut. We therefore exclude the trivial solution from the following discussion.

Assume $\{\boldsymbol{x}_\theta = \boldsymbol{R}(\theta)\boldsymbol{x}_0 : \theta \in [0,\pi[,\ \boldsymbol{x}_0 \text{ fixed}\}$ is a family of non-trivial solutions to the effective strut problem, i.e.

$$\boldsymbol{x}_\theta' = \boldsymbol{J}\langle H\rangle_{\boldsymbol{x}}(\boldsymbol{x}_\theta, s), \quad \boldsymbol{r}_\theta(0) = \boldsymbol{0}, \quad \boldsymbol{q}_\theta(0) = (0,0,0,1), \quad \boldsymbol{n}_\theta(1) = (0,0,-\lambda), \quad \boldsymbol{\mu}_\theta(1) = \boldsymbol{0}. \tag{14}$$

Then, with the notation $\boldsymbol{y} = (\boldsymbol{y}^r, \boldsymbol{y}^q, \boldsymbol{y}^n, \boldsymbol{y}^\mu)$, BVP (10) becomes

$$\mathcal{L}(\boldsymbol{x}_\theta)\boldsymbol{y} = \boldsymbol{p}(\boldsymbol{x}_\theta), \quad \boldsymbol{y}^r(0) = \boldsymbol{0}, \quad \boldsymbol{y}^q(0) = \boldsymbol{0}, \quad \boldsymbol{y}^n(1) = \boldsymbol{0}, \quad \boldsymbol{y}^\mu(1) = \boldsymbol{0}. \tag{15}$$

It is easy to check that the linear operator $\mathcal{L}(\boldsymbol{x}_\theta)$, together with the boundary conditions in (15), is self-adjoint. Therefore, according to the standard alternative theorem (cf. e.g. [10]), problem (15) has a solution if and only if $\boldsymbol{p}(\boldsymbol{x}_\theta)$ is L_2-orthogonal to the nullspace of $\mathcal{L}$, i.e. to all $\boldsymbol{w}$ satisfying the homogeneous problem

$$\mathcal{L}(\boldsymbol{x}_\theta)\boldsymbol{w} = \boldsymbol{0}, \quad \boldsymbol{w}^r(0) = \boldsymbol{0}, \quad \boldsymbol{w}^q(0) = \boldsymbol{0}, \quad \boldsymbol{w}^n(1) = \boldsymbol{0}, \quad \boldsymbol{w}^\mu(1) = \boldsymbol{0}. \tag{16}$$

We may use the continuous symmetry present in the effective problem to directly generate solutions to (16); differentiation of (14) with respect to θ shows that $\partial\boldsymbol{x}_\theta/\partial\theta$ is a solution to (16). Thus a necessary solvability condition for problem (15) is

$$\int_0^1 \left(\frac{\partial \boldsymbol{x}_\theta}{\partial\theta}\right)^T \boldsymbol{p}(\boldsymbol{x}_\theta)\, ds = 0. \tag{17}$$

A calculation exploiting the explicit form of the Hamiltonian for the strut and the equality $\boldsymbol{x}_\theta = \boldsymbol{R}(\theta)\boldsymbol{x}_0$ yields the following expression for the integrand in (17):

$$\begin{aligned}\left(\frac{\partial \boldsymbol{x}_\theta}{\partial\theta}\right)^T \boldsymbol{p}(\boldsymbol{x}_\theta) = \cos(2\theta)\,\Delta\Big[&2\left(K_3^{-1} - \bar{K}^{-1}\right) M_1(\boldsymbol{q}_0,\boldsymbol{\mu}_0) M_2(\boldsymbol{q}_0,\boldsymbol{\mu}_0) M_3(\boldsymbol{q}_0,\boldsymbol{\mu}_0) \\ &+ M_1(\boldsymbol{q}_0,\boldsymbol{\mu}_0)\boldsymbol{D}_2(\boldsymbol{q}_0)^T\boldsymbol{n}_0 + M_2(\boldsymbol{q}_0,\boldsymbol{\mu}_0)\boldsymbol{D}_1(\boldsymbol{q}_0)^T\boldsymbol{n}_0\Big] \\ + \sin(2\theta)\,\Delta\Big[&\left(K_3^{-1} - \bar{K}^{-1}\right)\left(M_1^2(\boldsymbol{q}_0,\boldsymbol{\mu}_0) - M_2^2(\boldsymbol{q}_0,\boldsymbol{\mu}_0)\right) M_3(\boldsymbol{q}_0,\boldsymbol{\mu}_0) \\ &+ M_1(\boldsymbol{q}_0,\boldsymbol{\mu}_0)\boldsymbol{D}_1(\boldsymbol{q}_0)^T\boldsymbol{n}_0 - M_2(\boldsymbol{q}_0,\boldsymbol{\mu}_0)\boldsymbol{D}_2(\boldsymbol{q}_0)^T\boldsymbol{n}_0\Big],\end{aligned}$$

where the functions $\boldsymbol{D}_i(\boldsymbol{q})$ and $M_i(\boldsymbol{q},\boldsymbol{\mu})$ are defined in (3) and (4). Inserting expression (12) for $\boldsymbol{x}_0$, we find:

$$\left(\frac{\partial \boldsymbol{x}_\theta}{\partial\theta}\right)^T \boldsymbol{p}(\boldsymbol{x}_\theta) = \cos(2\theta)\Delta\bar{K}\lambda\phi'\sin\phi.$$

This expression can be integrated explicitly, and, with the help of (13), the solvability condition (17) becomes

$$0 = \int_0^1 \left(\frac{\partial \boldsymbol{x}_\theta}{\partial\theta}\right)^T \boldsymbol{p}(\boldsymbol{x}_\theta)\, ds = -\cos(2\theta)\Delta\bar{K}\lambda\left[\cos\phi(1) - 1\right].$$

Since we exclude the trivial solution corresponding to $\phi(s) = 0$, then, from (13), $\cos\phi(1) - 1 \neq 0$, and the solvability condition reduces to

$$\theta = \frac{\pi}{4} \text{ or } \frac{3\pi}{4}. \tag{18}$$

In conclusion, the strut with high intrinsic twist buckles close to one of the two planes characterized by (18). In other words, its approximate planes of buckling lie in directions making a 45° angle with the direction of minimal stiffness at the clamped end. In particular, this angle is independent of the values of the stiffnesses K_1, K_2, K_3, and of the load λ.

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