A Variational Characterization of a Hyperelastic Rod with Hard Self-Contact[1]

Kathleen A. Hoffman and Thomas I. Seidman

Department of Mathematics and Statistics
University of Maryland Baltimore County
Baltimore, MD 21250, USA
(khoffman, seidman@math.umbc.edu)

Abstract

We consider an elastic rod, modeled as a curve in space with an impenetrable surrounding tube of radius ρ, subject to a general class of boundary conditions. The impossibility of self-intersection is then imposed as a family of scalar constraints on the physical separation of nonlocal pairs of points on the rod. Thus, the usual variational formulation of energy minimization is considered in a context of nonconvex, nonsmooth optimization. We show existence of minimizers within suitably defined homotopy classes associated with both the centerline and the frame along the rod. The principle results are then concerned with derivation of first-order necessary conditions for optimality and some consequences of these for the contact forces and for regularity.

1 Introduction

Following Euler et seq., the classical theory of elastic rods ignores any possibility of self-intersection for the configurations considered. For rods with almost straight configurations, as were classically considered, this neglect is nugatory, but for many applications of elastic rod theory, such as fiber optic cables on the sea floor, twining of plant tendrils and plectonemically wound DNA, contact plays an important role in determining the configurations. The focus of this work is the so called *hard contact problem*, an elastic rod viewed as a framed centerline surrounded by an impenetrable tube of radius $\rho > 0$. We develop existence results, first-order optimality conditions, and regularity conclusions for a variety of boundary conditions.

Previous work by the authors [**?**] developed similar results in connection with an analysis of rods with *soft contact* in which self-intersection was avoided by the addition to the classical potential of a singular repulsive potential as an integral term

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in the variational formulation. One contribution of [?] was to distinguish between local pairs and non-local pairs of points along the rod. Nonlocal points are the points of potential self-intersections of the rod while the inevitable physical proximity of parametrically close local pairs does not represent this sort of self-intersection.

We emphasize that a major innovation of [?] and this paper is the pointwise treatment of the avoidance of self-penetration through non-local pairs: in [?] by a singular potential penalizing physical proximity and here by the formulation of self-contact through an infinite family of pointwise scalar constraints, without requiring use of any constructs of a more nonlocal nature.

In [?], local and non-local pairs of points along the rod were distinguished based on energy bounds, but for the hard contact problem our distinction between these depends solely on the tube-size; from this perspective, the hard contact problem is actually simpler than the soft contact problem. On the other hand, the potential minimized in [?] is differentiable in a neighborhood of the minimizer so finding the first order optimality conditions in the form of a pair of differential equations for the strains just follows the classical calculus of variations of Euler and Lagrange. In contrast, with the hard contact problem, the impenetrability constraint is modeled as an infinite intersection of inequality constraints. From the geometry, one easily sees that this impenetrability constraint is not a convex constraint and the resulting optimization problem involves minimizing the classical potential subject to the non-convex inequality constraints. Such problems require techniques from non-smooth analysis (e.g., [?, ?]). Indeed, since this constraint is given by an infinite family of non-convex inequalities (separating each nonlocal pair of points on the rod centerline), this problem required new results of non-smooth analysis [?] to obtain the optimality conditions.

Elastic rods with an impenetrable tube have previously been considered [?, ?, ?, ?, ?, ?] in the context of periodic boundary conditions. The most closely related work is that of Gonzalez et al. [?] and Schuricht and von der Mosel [?]. In their formulation, non-locality was addressed using a global radius of curvature function that gave rise to a nonconvex constraint in the variational formulation. Schuricht and von der Mosel [?] used Clarke's calculus of generalized derivatives [?] to formulate the optimality conditions. In contrast, we use Mordukhovich's formulation of normal cones to address the non-convex inequality constraints in our variational formulation.

A more significant difference between their analysis and the one presented here is the allowable boundary conditions. Schuricht and von der Mosel restricted their analysis to the case of a periodic centerline and were able to extend topological results involving the linking number of two closed curves to define the homotopy class for equilibrium configurations of elastic rods. In our analysis we consider more general types of boundary conditions. We assume that the centerline and orientation of the elastic rod at one end, $s = 0$, is fixed, which eliminates translation and rotational symmetries from the problem. In particular, we allow the following boundary conditions at $s = 1$: free end with no further conditions, specification of the position of the centerline, specification of the orientation of the frame, specification of the tangent vector to the centerline, or combinations of the above conditions; periodic boundary conditions are, of course, a combination of specifying the position of the centerline and specifying the orientation of the frame. With this generalization, we no longer have the notion of linking number available to define homotopy class. To this end, we have extended the idea of *rod homotopy*, first developed in [**?**], to elastic rods with impenetrable tubes in which the traditional definition of homotopy extends to both the centerline and the frame of the elastic rod.

Another challenge explicitly considered in this work is the possible kinking of the impenetrable tube since, to maintain the validity of the elastic rod model, we have a constraint that the curvature of the centerline $\kappa(s)$ satisfies $\kappa(s) \leq 1/\rho$, where ρ represents the radius of the tube surrounding the centerline; this is imposed by requiring that the elastic stored energy density becomes infinite as the curvature approaches $1/\rho$. Such a blowup of the elastic potential adds significant difficulties in deriving the optimality conditions, but seems physically appropriate. We note that Schuricht and von der Mosel refer in [**?**] to a use of similar techniques in [**?**, VII.5] and [**?**] in addressing this concern.

This article is organized as follows. Section 2 treats the geometric theory of rods: a brief description of the Cosserat description, discussion of nonlocality and constraints and the notion of rod homotopy. The following Section 3 then treats the potential energy and variational formulation, including the existence result. Section 4 uses results from Mordukhovich's books [**?**, **?**] along with Seidman's recent results [**?**] to formulate the boundary conditions and impenetrability constraints in terms of basic normal cones. The optimality results following from this, leading to regularity of the minimizer, are then presented in Section 5.

2 Problem Formulation: Geometry

2.1 The Cosserat Rod Model

As in [**?**], we continue to use the geometrically exact formulation, following the Cosserat theory specialized to large deformations of inextensible and unshearable elastic rods. A comprehensive discussion of Cosserat theory can be found in [**?**], but we briefly review here the notation and recall related results of [**?**].

The configuration of a rod is initially described by a centerline $s \mapsto \mathrm{r}(s)$, a function of arc length along the rod, choosing units so $0 \le s \le \ell = 1$. We then introduce a radius $\rho > 0$ for the impenetrable tubular neighborhood surrounding the centerline of the rod, corresponding to the hard contact formulation. For simplicity, we assume for the tube a circular cross section of constant radius, but our subsequent analysis would easily allow for a tube size slowly varying along the length of the rod and, with somewhat more effort, even for varying noncircular shape. We emphasize, however, that the present model neglects tangential forces along the rod: there is no friction.

The relationship between the tube size ρ surrounding the centerline and the curvature of that centerline helps to distinguish between parametrically *nearby* points and parametrically *nonlocal* pairs of points along the rod. The radius of curvature of the centerline at a point s is $1/\kappa(s)$ and one easily sees from the geometry that having $1/\kappa < \rho$ would have nearby cross sections of the tube actually intersecting within the tube: this is a purely local consideration leading to the condition

$$\kappa(s) \le 1/\rho \qquad \text{for each } s \in [0,1] \tag{2.1}$$

(bounding the curvature pointwise along the centerline) as a constraint necessary to ensure the validity of the rod model, although we will treat this through energy considerations rather than as an imposed constraint; see Subsubsection 2.2.2 and Remark 1. We are led to the following:

Definition 1. *A pair of points* $(s, \sigma) \in [0,1]^2$ *is called* nonlocal *if* $|s - \sigma| \ge 2\pi\rho$*; the set of such nonlocal points is denoted* $\mathcal{NL}$.

Depending on the imposed boundary conditions this may be modified at the end points: e.g., for a periodic centerline we will take $(s, \sigma) \mod 1$ in defining the set of nonlocal pairs

$$\mathcal{NL} = \{(s, \sigma) \in [0,1]^2 : |s - \sigma| \ge 2\pi\rho\}. \tag{2.2}$$

Consideration of the local geometry then shows that with the curvature bound (2.1) one can have no self-intersecting contact of centerline points closer along the rod than the minimal circumference $2\pi\rho$ of an osculating circle, i.e., the self-intersections we wish to avoid are meaningfully possible only for *nonlocal* pairs of points along the rod centerline.

For non-periodic conditions, there is still a possibility that the rod might intersect itself at an endpoint — e.g., the point at $s = 0$ could interact with the point at $s = 1/3$ — and in order to impose the same pointwise constraint we will, for convenience, think of the rod as having hemispheres of radius ρ attached at the endpoints. We recall that similar endpoint considerations applied in the soft contact problem: cf., Hoffman and Seidman [**?**, Lemma 3], where nonlocality was defined in terms of energy considerations.

Next, the Cosserat formulation attaches an orthogonal pair of unit vectors $\mathrm{d}_1, \mathrm{d}_2$ to the cross-sectional disk and sets $\mathrm{d}_3 = \mathrm{d}_1 \times \mathrm{d}_2$ so the set of *directors*

$$\mathrm{D}(s) = \{\mathrm{d}_1(s), \mathrm{d}_2(s), \mathrm{d}_3(s)\}$$

forms an orthonormal frame describing the orientation of the cross-section of the rod at each point s along the centerline. Note that $\mathrm{D}(s)$ is then a 3×3 matrix in $SO(3)$, which is viewed as a manifold embedded in the linear space $\mathcal{M} = \mathcal{M}^{3\times 3}$ of 3×3 matrices. This implies a Darboux vector $\mathrm{u}^D(s)$, defined by $\mathrm{d}_i'(s) = \mathrm{u}^D(s) \times \mathrm{d}_i(s)$ for $i = 1, 2, 3$ and we express u^D in the local rod frame with coefficients $u_i(s) \equiv \mathrm{u}^D(s) \cdot \mathrm{d}_i(s)$, giving the strains. Thus $\mathrm{u} = \Sigma_i u_i \, \mathrm{d}_i = \mathrm{D}\mathrm{u}$, with $\mathrm{u} = u_1 \mathrm{i} + u_2 \mathrm{j} + u_3 \mathrm{k} = (u_1, u_2, u_3)^{\mathsf{T}}$.

In this paper, as in [**?**], we restrict our attention to inextensible and unshearable rods for which the third director $\mathrm{d}_3 = \mathrm{D}\mathrm{k}$ coincides with the tangent vector to the centerline: $\mathrm{d}_3(s) = \mathrm{r}'(s)$. [Although this may seem a simplification from a more general problem, assuming inextensibility and unshearability imposes a pointwise constraint on the variational problem, making the problem even more challenging; however, this does allow for a consistent comparison of our results to others in the literature.] This formulation is summarized by a pair of differential equations along the rod:

$$\mathrm{D}' = (\mathrm{D}\mathrm{u}) \times \mathrm{D} = \mathrm{D}\,\mathsf{S}(\mathrm{u}) \qquad \mathrm{r}' = \mathrm{d}_3 = \mathrm{D}\mathrm{k} \qquad \text{for } 0 \le s \le 1 \tag{2.3}$$

$$\text{with} \qquad \mathsf{S}\begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} 0 & -u_3 & u_2 \\ u_3 & 0 & -u_1 \\ -u_2 & u_1 & 0 \end{pmatrix} \tag{2.4}$$

so $\mathsf{S} : \mathbb{R}^3 \to \mathcal{S}^3 = \{\text{skew}\}$; the canonical basis of $\mathbb{R}^3$ is denoted by $\{\mathrm{i}, \mathrm{j}, \mathrm{k}\}$.

Fixing $1 < p < \infty$ (and so also the conjugate index q such that $1/p + 1/q = 1$), we define the (reflexive) spaces

$$\begin{array}{llll} \mathcal{X} & = L^p([0,1] \to \mathbb{R}^3), & \hat{\mathcal{X}} & = L^p([0,1] \to \mathcal{M}^{3\times 3}), \\ \mathcal{Y} & = W^{1,p}([0,1] \to \mathcal{M}^{3\times 3}), & \mathcal{Y}_0 & = \{y \in \mathcal{Y} : y(0) = \mathbf{0}\}, \\ \mathcal{Z} & = W^{2,p}([0,1] \to \mathbb{R}^3), & \mathcal{Z}_0 & = \{z \in \mathcal{Z} : z(0) = 0 = z'(0)\} \\ & & & = \{z \in \mathcal{X} : z'' \in \mathcal{X},\ z(0) = 0 = z'(0)\}. \end{array} \tag{2.5}$$

Without loss of generality, we will assume that our coordinate system has been chosen so that

$$\mathrm{D}(0) = \mathrm{I} \qquad\qquad \mathrm{r}(0) = 0. \tag{2.6}$$

and then adjoin (2.6) to the differential equations (2.3) to define maps

$$\begin{aligned} \mathbf{D}: &\quad \mathrm{u}(\cdot) \mapsto \mathrm{D}(\cdot): \quad \mathcal{X} \to \mathcal{Y} \\ \mathbf{R}: &\quad \mathrm{D}(\cdot) \mapsto \mathrm{r}(\cdot): \quad \mathcal{Y} \to \mathcal{Z} \\ \text{so} \qquad \mathbf{R} \circ \mathbf{D}: &\quad \mathrm{u}(\cdot) \mapsto \mathrm{r}(\cdot): \quad \mathcal{X} \to \mathcal{Z}. \end{aligned} \tag{2.7}$$

Theorem 1. *We have*

1. *The composed map* $\mathbf{R} \circ \mathbf{D} : \mathrm{u}(\cdot) \mapsto \mathrm{r}(\cdot)$ *is continuous and Fréchet differentiable as a function from* $\mathcal{X}$ *to* $\mathcal{Z}$*.*
2. *The map* $\mathbf{D}$ *is continuous (and so necessarily compact) from the weak topology of* $\mathcal{X}$ *to* $C([0,1] \to \mathcal{M}^{3\times 3})$*, and correspondingly* $\mathbf{R} \circ \mathbf{D}$ *is continuous from* $\mathcal{X}_{weak}$ *to* $C^1([0,1] \to \mathbb{R}^3)$*.*

Proof. Part 1. of this Theorem was proved in [**?**, Thm 1, Cor 1] and Part 2. was proved in [**?**, Lemma 1, Cor. 1]. □

In addition to (2.5) we will also need

$$\begin{aligned} \hat{\mathcal{Y}} &= \{y \in W^{1,p}([0,1] \to \mathcal{S}^3) : \; y(0) = 0\} \\ \hat{\mathcal{Z}} &= \left\{z \in W^{2,p}([0,1] \to \mathbb{R}^3) : \; z = 0, z'(0) = 0, \; z' \cdot \bar{\mathrm{D}}\mathrm{k} \equiv 0\right\} \end{aligned} \tag{2.8}$$

where $\bar{\mathrm{D}} = \mathbf{D}(\bar{\mathrm{u}})$ for a fixed $\bar{\mathrm{u}} \in \mathcal{X}$; clearly $\hat{\mathcal{Y}}$ may be viewed as a closed subspace of $\mathcal{Y}_0$ on embedding $\mathcal{S}$ into $\mathcal{M}^{3\times 3}$ and $\hat{\mathcal{Z}}$ is a closed subspace of $\mathcal{Z}_0$

2.2 Constraints

Apart from the kinematic constraints incorporated in the map $\mathbf{R} \circ \mathbf{D}$, the admissible centerline configurations will be those that satisfy the impenetrability constraint for tube radius ρ as well as any boundary conditions imposed at $s = 0, 1$. We are here imposing both equality constraints and inequality constraints: the boundary conditions at $s = 1$ are imposed as equality constraints, but the impenetrability of the tube is imposed as a family of inequality constraints: the distance between any nonlocal pair of points along the centerline must be at least 2ρ.

2.2.1 Boundary Conditions at $s = 1$

Equation (2.6) specifies the boundary conditions at the left end of the rod ($s = 0$), but boundary conditions at the right end of the rod $s = 1$ may further be imposed to complete the formulation; any such conditions on D, r at $s = 1$ (or, perhaps, elsewhere in $(0, 1]$) remain as constraints on $\mathrm{u}(\cdot)$. There are numerous relevant possibilities:

$$
\begin{array}{ll}
\texttt{a.} & \text{a free end with no further conditions imposed} \\
\texttt{b.} & \text{specification } \mathrm{r}(1) = \mathrm{r}_1 \\
\texttt{c.} & \text{specification of } \mathrm{D}(1) = \mathrm{D}_1 \\
\texttt{d.} & \text{specification of } \mathrm{r}'(1) = \mathrm{D}(1)\mathrm{k}
\end{array}
\tag{2.9}
$$

as well as combinations of these boundary conditions. [We note that the condition (2.6) is a somewhat arbitrary coordinatization so conditions like `b.` or `c.` of (2.9) should more properly be written relatively: $\mathrm{r}(1) - \mathrm{r}(0) = \mathrm{r}_1$ or $\mathrm{D}(1)[\mathrm{D}(0)]^{-1} = \hat{\mathrm{D}}_1$; we will continue to treat these simply as boundary conditions "at $s = 1$."] Our analysis remains largely independent of any particular choice among the indicated boundary conditions at $s = 1$; whichever choice is to be made, let

$$
\Omega_1 = \{\mathrm{u} \in \mathcal{X} : \mathrm{D} = \mathbf{D}(\mathrm{u}),\ \mathrm{r} = \mathbf{R}(\mathrm{D}) \text{ satisfy the conditions at } s = 1\}. \tag{2.10}
$$

We emphasize the fact, obvious from (2.9) and further discussed in Subsection 4.3, that each of our possible choices here is an *equality constraint.*

2.2.2 Curvature Constraint

The pointwise restriction (2.1) which was used to preclude self-intersection of distinct cross-sections within the tube might be formally imposed (as an inequality constraint) in defining admissibility. It is convenient to write

$$
\tilde{\mathrm{u}} = (u_1, u_2) \in \mathbb{R}^2 \quad \text{so } \mathrm{u} = (\tilde{\mathrm{u}}, u_3) = (u_1, u_2, u_3) \in \mathbb{R}^2 \oplus \mathbb{R} = \mathbb{R}^3 \tag{2.11}
$$

and note that $\kappa(s) = |\mathrm{r}''(s)| = |\mathrm{D}'\mathrm{k}|$ so

$$
\begin{aligned}
\kappa = \kappa(s) &= |u_2 \mathrm{d}_1 - u_1 \mathrm{d}_2| = \sqrt{|u_1(s)|^2 + |u_2(s)|^2} = |\tilde{\mathrm{u}}| \\
\mathrm{u} &= [\kappa \cos\theta,\ \kappa \sin\theta,\ u_3].
\end{aligned}
\tag{2.12}
$$

At each s the set of u satisfying the condition (2.1) is the (closed) unbounded circular cylinder in $\mathbb{R}^3$ with axis k and radius $1/\rho$.

However, rather than explicitly imposing (2.1) as a constraint, we will instead treat it through the local energy functional $\mathcal{W}$ in Subsection 3.1 as an increasing resistance to infinite compression by kinking; see Remark 1 and compare the discussion in [**?**] (in a dynamic context), although some of that concern about infinite compression is here obviated by the inextensibility assumption. This way of handling (2.1) involves significant technical difficulty, but seems the physically correct treatment.

2.2.3 Impenetrability Constraint

Our principal concern in this paper is with the possibility of self-intersection of the rod. In visualizing the geometry for a tube of radius ρ it is easy to see that this *non-self-intersection constraint* just means that nonlocal pairs (s,σ) of centerline points are physically separated at least by the widths of the local tubes. Thus, impenetrability is interpreted as the family of inequality constraints

$$\begin{array}{c}\text{For each } (s,\sigma)\in\mathcal{NL} \text{ one has } \psi_{(s,\sigma)}[\mathrm{r}] \geq\ 0 \\ \text{where }\ \psi_{(s,\sigma)}[\mathrm{r}] := |\mathrm{r}(s)-\mathrm{r}(\sigma)| - 2\rho\end{array} \tag{2.13}$$

with $\mathcal{NL}$ as in (2.2), the set of nonlocal points of Definition 1.

Much as with (2.10), we let Ω_2 be the set of strains defining centerline configurations for which self-intersections do not occur, i.e.,

$$\Omega_2 = \Omega_2(\rho) = \{\mathrm{u}\in\mathcal{X} : \mathrm{r} = [\mathbf{R}\circ\mathbf{D}](\mathrm{u}) \text{ satisfies the conditions (2.13)}\}. \tag{2.14}$$

[Impenetrability could, equivalently, be enforced by a single inequality constraint

$$\phi_*[\mathrm{r}] := \min_{(s,\sigma)\in\mathcal{NL}} \{|\mathrm{r}(s)-\mathrm{r}(\sigma)|\} \quad \geq\ 2\rho, \tag{2.15}$$

but it is easier to work with (2.13).]

Note that if we fix a centerline configuration $\bar{\mathrm{r}}(\cdot)$ satisfying the constraint (2.13), then we may let $d_*(s)$ be the distance from $\bar{\mathrm{r}}(s)$ to the nearest nonlocally related point on the centerline so

$$d_*(s) = d_*(s;\bar{\mathrm{r}}) = \min_{\sigma}\{|\bar{\mathrm{r}}(s)-\bar{\mathrm{r}}(\sigma)| : (s,\sigma)\in\mathcal{NL}\}, \tag{2.16}$$

noting that this is well-defined on $[0,1]$ by the continuity of $\bar{\mathrm{r}}(\cdot)$ and the compactness of $\mathcal{NL}$ with $2\rho \leq d_*(s) \leq 2\pi\rho$. It is clear that $d_*(\cdot)$ is at least lower semicontinuous: at worst there may be jump discontinuities at $s = 2\pi\rho$ and at $s = 1-2\pi\rho$, where the number of components of $\{\sigma\in[0,1] : (s,\sigma)\in\mathcal{NL}\}$ would change. The *contact set* for this centerline will then be the closed set

$$\mathcal{C} = \mathcal{C}(\bar{\mathrm{r}}) = \{s\in[0,1] : d_*(s;\bar{\mathrm{r}}) = 2\rho\}. \tag{2.17}$$

2.3 Admissible Triples and Rod Homotopy

We now introduce the space $\mathcal{V} = \mathcal{X}_{weak}\times\mathcal{Y}\times\mathcal{Z}$ and define the set $\mathcal{A} = \mathcal{A}(\rho)$ of *admissible triples* as a subset of $\mathcal{V}$; we may then call $\mathrm{u}\in\mathcal{X}$ admissible if $\mathrm{v} = [\mathrm{u}, \mathbf{D}(\mathrm{u}), [\mathbf{R}\circ\mathbf{D}](\mathrm{u})]$ is an admissible triple.

Definition 2. *For a given* ρ, $[\mathrm{u},\mathrm{D},\mathrm{r}] \in \mathcal{V}$ *is called an* admissible triple *if it satisfies*

a. $\mathrm{u} \in \mathcal{X}$ *with* D,r *given, as in* (2.7)*, by* (2.3) *with* (2.6) *giving* $\mathrm{D} = \mathbf{D}(\mathrm{u}) \in \mathcal{Y}$ *and* $\mathrm{r} = \mathbf{R}(\mathrm{D}) \in \mathcal{Z}$,

b. $\mathrm{u} \in \Omega_1$ — *any specified boundary conditions at* $s = 1$ *are satisfied,*

c. $\mathrm{u} \in \Omega_2 = \Omega_2(\rho)$ — *there is no self-intersection for the tube, i.e.,* (2.13).

A sequence of such triples converges $[\mathrm{u}_k,\mathrm{D}_k,\mathrm{r}_k] \to [\mathrm{u}_\infty,\mathrm{D}_\infty,\mathrm{r}_\infty]$ *provided* $\mathrm{u}_k \rightharpoonup \mathrm{u}_\infty$ *(weak convergence in* $\mathcal{X}$*) with corresponding convergence of* $\mathrm{D}_k,\mathrm{r}_k$ *as in Theorem 1.*

Of course $\mathcal{A}$ depends on ρ through the imposition of the condition (2.13) in c. We further remark that it is possible for $\mathcal{A}$ to be empty, that there are no admissible triples at all, e.g., if we were to impose a boundary condition at $s = 1$ requiring $|\mathrm{r}(1)| > 1$. On the other hand, it should be noted that this notion of admissibility has not imposed the condition (2.1); as noted in Subsubsection 2.2.2, this will be imposed through finiteness of the energy functional.

It is clear from part 2. of Theorem 1 that $\mathrm{u}_k \rightharpoonup \mathrm{u}_\infty$ implies that one also has strong convergence of $\mathrm{D}_k,\mathrm{r}_k$ in $\mathcal{Y},\mathcal{Z}$, respectively so this is convergence in $\mathcal{V}$ and one has $\mathrm{D}_\infty = \mathbf{D}(\mathrm{u}_\infty)$ and $\mathrm{r}_\infty = \mathbf{R}(\mathrm{D}_\infty)$. The topology of $\mathcal{Z}$ then ensures that the constraints — both the boundary conditions as in (2.9) and the impenetrability conditions (2.13) — continue to hold in the limit where $\mathrm{r}_k \to \mathrm{r}_\infty$ uniformly. This means that Ω_1 and Ω_2 are each closed in $\mathcal{X}_{weak}$ whence the set $\mathcal{A}$ of admissible triples is closed in $\mathcal{V} = \mathcal{X}_{weak} \times \mathcal{Y} \times \mathcal{Z}$.

Following [**?**], we next use Definition 2 to define a *rod homotopy* as follows:

Definition 3. *A* rod homotopy *joining the triples* $\mathrm{v}_0 = [\bar{\mathrm{u}},\bar{\mathrm{D}},\bar{\mathrm{r}}]$ *and* $\mathrm{v}_1 = [\hat{\mathrm{u}},\hat{\mathrm{D}},\hat{\mathrm{r}}]$ *is a map* $t \mapsto [\mathrm{u}(\cdot,t),\mathrm{D}(\cdot,t),\mathrm{r}(\cdot,t)]$ *from* $[0,1]$ *to admissible triples such that*

a. $[\mathrm{u}(\cdot,0),\mathrm{D}(\cdot,0),\mathrm{r}(\cdot,0)] = [\bar{\mathrm{u}},\bar{\mathrm{D}},\bar{\mathrm{r}}]$ *and* $[\mathrm{u}(\cdot,1),\mathrm{D}(\cdot,1),\mathrm{r}(\cdot,1)] = [\hat{\mathrm{u}},\hat{\mathrm{D}},\hat{\mathrm{r}}]$,

b. *each* $[\mathrm{u}(\cdot,t),\mathrm{D}(\cdot,t),\mathrm{r}(\cdot,t)]$ *is an admissible triple,*

c. *the map is continuous in the sense of Definition 2.*

Two triples v_0, $\mathrm{v}_1 \in \mathcal{A}(\rho)$ *are* rod homotopic *if such a rod homotopy exists.*

Thus, a rod homotopy is an arc joining v_0 to v_1 within $\mathcal{A}(\rho)$, i.e., an element $\mathrm{v}(\cdot)$ of $C([0,1] \to \mathcal{A}(\rho))$ with $\mathrm{v}(0) = \mathrm{v}_0$ and $\mathrm{v}(1) = \mathrm{v}_1$ so Definition 3 just means that rod homotopic triples $[\bar{\mathrm{u}},\bar{\mathrm{D}},\bar{\mathrm{r}}]$ and $[\hat{\mathrm{u}},\hat{\mathrm{D}},\hat{\mathrm{r}}]$ are arcwise connected within the set $\mathcal{A}$ of admissible triples, viewed as a (closed) subset of $\mathcal{V} = \mathcal{X}_{weak} \times \mathcal{Y} \times \mathcal{Z}$.

We emphasize that this definition depends on the rod radius ρ and to indicate this we may say that "v_0 and v_1 are rod homotopic in the context of ρ" or that $\mathrm{v}(\cdot)$ is a "rod ρ-homotopy." Although the homotopy involves the entire triple, the dependence on ρ only involves r.

For the treatment in [**?**] it was significant that an admissible triple there (in the somewhat different soft contact setting in which impenetrability was enforced by a singular repulsion term) gave some *clearance* — each admissible triple (except the special case with $\mathrm{r}(1) = \mathrm{k}$) had a neighborhood of admissible triples — and the proof of [**?**, Thm. 2] took advantage of that fact in explicitly constructing rod homotopies within such a neighborhood. For the present setting there can be be no such neighborhood when actual hard contact occurs and we are led to introduce an apparently weaker notion:

Definition 4. *Two triples* $\mathrm{v}_0 = [\bar{\mathrm{u}}, \bar{\mathrm{D}}, \bar{\mathrm{r}}]$ *and* $\mathrm{v}_1 = [\hat{\mathrm{u}}, \hat{\mathrm{D}}, \hat{\mathrm{r}}]$ *are called* mildly rod homotopic *in the context of ρ if they are rod $\hat{\rho}$-homotopic for each* $0 < \hat{\rho} < \rho$*. It is clear that mild rod homotopy is an equivalence relation so we may say that* v_0, v_1 *are* in the same mild homotopy class*.*

Since $\mathcal{A}(\hat{\rho}) \subset \mathcal{A}(\rho)$ for $0 < \hat{\rho} \le \rho$, it is clear that any rod ρ-homotopy is also a $\hat{\rho}$-homotopy for each $\hat{\rho} < \rho$. Hence rod ρ-homotopy implies mild rod ρ-homotopy. [At this point, however, we have no proof of the converse to show that the notions are equivalent, although we know of no example of $\mathrm{v}_0, \mathrm{v}_1$ which are mildly ρ-homotopic without a ρ-homotopy existing; see Remark 2.]

3 Energy and Existence

3.1 Energy

The classical potential energy consists of the local internal potential energy $\mathcal{W}$ and the external potential energy $\mathcal{F}$. The local internal potential energy $\mathcal{W}$ is the part of the energy cost due to local deformation of the rod when one would deform to u from an unstressed reference configuration specified by $\hat{\mathrm{u}}(s)$. [For a naturally straight rod, the unstressed configuration function would be $\hat{\mathrm{u}} \equiv 0$; our formulation is general enough to include naturally anisotropic and non-uniform elastic rods for which $\hat{\mathrm{u}}(s) \not\equiv 0$.]

The external potential energy in the system is here assumed to have the form

$$\mathcal{F}[\mathrm{r}] = \int_0^1 F(s, \mathrm{r}(s))\, ds \tag{3.1}$$

where, for convenience, we have implicitly assumed some symmetry of the rod about its centerline in taking each $F(s,\cdot)$ to depend only on $\mathrm{r}(s)$ and not also on $\mathrm{D}(s)$. [Note that the function F depends on the coordinate system, which we have here specified by (2.6). Also, one might, of course, have written $\mathcal{F} = \mathcal{F}[\mathrm{u}]$ since $\mathrm{r} = \mathbf{R} \circ \mathbf{D}(\mathrm{u})$, but it is convenient to leave it as (3.1).] We assume here that:

$$F : [0,1] \times \mathbb{R}^3 \to [0,\infty) \textit{ is bounded and satisfies Carathéodory conditions.} \tag{3.2}$$

The formulation in (3.1) with the assumption (3.2) precludes any interaction with an external hard obstacle, but see Remark 4 for further comment on this possibility.

Phenomenologically, the internal potential energy $\mathcal{W}$ will be given as usual by integrating a (material-dependent) strain energy density function:

$$\mathcal{W}[\mathrm{u}] = \int_0^1 W(s, \mathrm{u}(s))\, ds. \tag{3.3}$$

[Note that $W(s,\cdot)$ at each point s along the rod is here a function only of the strain $\mathrm{u}(s)$ at that point, but we are allowing for dependence on the material properties associated with that point. This part of the formulation is essentially classical.] We will assume here that:

$$\begin{array}{ll} \texttt{a.} & W : [0,1] \times \mathbb{R}^3 \to [0,\infty] \textit{ satisfies:} \\ & \qquad W(\cdot,\mathrm{u}) \textit{ is measurable for each } \mathrm{u} \in \mathbb{R}^3, \\ & \qquad W(s,\cdot) \textit{ is continuous where finite, uniformly in } s \in [0,1] \\ \texttt{b.} & \textit{each } W(s,\cdot) \textit{ is strictly convex} \\ \texttt{c.} & \psi(|\kappa|) + b|u_3|^p \;\le\; W(s,\mathrm{u}) \;\le\; c[\psi(|\kappa|) + b|u_3|^p] \\ & \qquad \textit{for } s \in [0,1],\ \mathrm{u} = (\tilde{\mathrm{u}}, u_3) = (u_1,u_2,u_3) \in \mathbb{R}^2 \oplus \mathbb{R} = \mathbb{R}^3 \end{array} \tag{3.4}$$

where $b, c > 0$ and $\psi : [0,\infty) \to [0,\infty]$ is increasing and continuous with

$$0 \le \psi < \infty \;\text{ on } (0, 1/\rho) \quad \text{and} \quad \psi(\kappa) = \infty \;\text{ for } \kappa \ge 1/\rho. \tag{3.5}$$

Remark 1. *We consider the physical significance of the hypothesis (3.4* c*), apart from L^p coercivity of this potential. We are imposing the curvature condition* (2.1) *not merely as a constraint, but as resulting from the material's increasing resistance to the internal compression associated with kinking, i.e., as cross-sections become squeezed together when curvature approaches* $1/\rho$*; compare Subsubsection 2.2.2. This hypothesis is not really a problem for existence, but imposes significant technical difficulties for our treatment of optimality conditions; we do things this way because it seems the right way to represent the physics.* □

Combining the local and external contributions, the total classical energy $\mathcal{E}$ of the elastic rod is then given by

$$\mathcal{E}[\mathrm{u}] = \begin{array}{ccc} \mathcal{W}[\mathrm{u}] & + & \mathcal{F}[\mathrm{r}] \\ \displaystyle\int_0^1 \Big[\, W(s,\mathrm{u}(s)) & + \, F(s,\mathrm{r}(s)) & \Big]\, ds. \end{array} \tag{3.6}$$

Lemma 1. *Let F satisfy* (3.2). *Then the external energy functional* $\mathrm{u} \mapsto \mathcal{F}[\mathrm{r}]$, *defined by* (3.1) *with* $\mathbf{R} \circ \mathbf{D} : \mathrm{u} \mapsto \mathrm{r}$, *is continuous from* $\mathcal{X}_{weak}$.

Let $W : [0,1] \times \mathbb{R}^3 \to [0,\infty]$ *satisfy* (3.4). *Then the internal energy functional* $\mathcal{W}$, *defined by* (3.3), *is convex and lower semicontinuous from* $\mathcal{X}_{weak}$.

Given both (3.4) *and* (3.2), *the energy functional* $\mathcal{E} : \mathcal{X}_{weak} \to [0,\infty]$ *is lower semicontinuous and coercive. Further, for* u *with* $\mathcal{E}[\mathrm{u}] < \infty$, *one has* (2.1) *for* r.

Proof. The continuity of $\mathrm{r} \mapsto \mathcal{F} : \mathcal{Z} \to \mathbb{R}$ is standard, given (3.2). The continuity of $\mathrm{u} \mapsto \mathcal{F}[\mathrm{r}] : \mathcal{X}_{weak} \to \mathbb{R}$ then follows from part 2 of Theorem 1.

Convexity of $\mathcal{W}$ is immediate from (3.4 b). Lower semicontinuity from $\mathcal{X}_{weak}$ is less obvious since, using (3.5), the lower bound in (3.4 c) ensures that the (convex) set $\mathcal{D}_{\mathcal{W}} = \{\mathrm{u} : \mathcal{W}[\mathrm{u}] < \infty\}$ has empty interior in $\mathcal{X}$ so we shift consideration to $\mathcal{X}_{\ddagger}$, defined by using an $L^\infty[0,1]$-norm for the first two components while retaining the L^p-norm for the third. Note that $\mathcal{D}_{\mathcal{W}}$ is in $\mathcal{X}_{\ddagger}$, now with nonempty interior; further $\mathcal{X}_{\ddagger}$ embeds in $\mathcal{X}$ and is itself a dual space $[L^1([0,1] \to \mathbb{R}^2) \oplus L^q(0,1)]^*$. Thus, if there were a sequence $\mathrm{u}_k \rightharpoonup \bar{\mathrm{u}}$ in $\mathcal{X}$ with $\liminf \mathcal{W}[\mathrm{u}_k] < W[\bar{\mathrm{u}}]$ so $\mathrm{u}_k \in \mathcal{D}_{\mathcal{W}} \subset \mathcal{X}_{\ddagger}$, then we could extract a $(\mathcal{X}_{\ddagger})_{weak*}$-convergent subsequence, necessarily with the same limit $\bar{\mathrm{u}}$ and conclude that $W[\bar{\mathrm{u}}] \le \liminf \mathcal{W}[\mathrm{u}_k]$.

Combining these then gives the lower semicontinuity of $\mathcal{E} : \mathcal{X}_{weak} \to [0,\infty]$. Coercivity and (2.1) on $\mathcal{D}_{\mathcal{W}}$ are immediate from the lower bound in (3.4 c). □

3.2 Existence

Stable mechanical equilibria are usually obtained as (local) minimizers of the total energy $\mathcal{E}$, viewed as a functional defined on an appropriate set of admissible functions. In this section, we prove the existence of a minimizer of the total energy $\mathcal{E}$ and a minimizer within each mild rod homotopy class. Apart from the homotopic consideration, we are thus considering the constrained optimization problem:

$$\begin{array}{ll} \text{minimize:} & \qquad \mathcal{E}[\mathrm{u}] \qquad \text{as in (3.6)} \\ \text{subject to:} & \left\{ \begin{array}{ll} \texttt{a.} & \text{the boundary conditions at } s=1 \\ \texttt{b.} & \text{the impenetrability constraint (2.13)} \end{array} \right. \end{array} \tag{3.7}$$

[We need not include (2.1) in the constraints here since, by Lemma 1, this is implicit in the minimization.]

We then have the following existence theorem:

Theorem 2. *If the constitutive functions satisfy* (3.2) *and* (3.4) *with* (3.5) *and there is some admissible* u_0 *with finite energy, then* (3.7) *attains its minimum. If an admissible* u_0 *with finite energy is specified, then* $\mathcal{E}$ *attains its minimum over the mild rod* ρ*-homotopy class containing the admissible triple* $\mathrm{v}_0 = [\mathrm{u}_0, \mathrm{D}_0, \mathrm{r}_0]$.

Proof. The first existence assertion is entirely standard. Let $\mathrm{v}_k = [\mathrm{u}_k, \mathrm{D}_k, \mathrm{r}_k]$ be a minimizing sequence for $\mathcal{E}$ in the set $\mathcal{A}(\rho)$ of admissible triples. By the coercivity following from Lemma 1, a bound on $\mathcal{E}$ also implies a bound on the $\mathcal{X}$-norms $\{\|\mathrm{u}_k\|\}$, so we can extract a weakly convergent subsequence $\mathrm{u}_k \rightharpoonup \mathrm{u}_\infty$ whence, according to our observations above, we have convergence of v_k to an admissible triple v_∞. Lemma 1 also guarantees that $\mathrm{v} \mapsto \mathcal{E}[\mathrm{v}]$ is lower semicontinuous, which ensures that the energy infimum is actually attained at v_∞ as a global minimum.

We may next consider a minimizing sequence in the mild rod homotopy class containing v_0 and, as above, can extract a subsequence converging in $\mathcal{A}(\rho)$ to a limit $\mathrm{v}_\infty = [\mathrm{u}_\infty, \mathrm{D}_\infty, \mathrm{r}_\infty]$. Again, the energy infimum is attained at v_∞ so we again have the desired minimum provided v_∞ is itself in the mild homotopy class of v_0.

To see this we make the key observation that, for any $0 < \hat{\rho} < \rho$, the rod with tube radius $\hat{\rho}$ corresponding to the ρ-admissible centerline r_∞ must have clearance $D_* = 2(\rho - \hat{\rho}) > 0$ in the sense of [**?**, Thm. 2]. Thus r_∞ has a neighborhood in $C([0,1] \to \mathbb{R}^3)$ of $\hat{\rho}$-admissible centerlines and v_∞ has a neighborhood in $\mathcal{V}$ of triples in $\mathcal{A}(\hat{\rho})$. Convergence then gives v_k in this neighborhood for some k and so, for each of the possible cases of boundary conditions at $s = 1$, the constructions given in the proof of [**?**, Thm. 2] give a rod $\hat{\rho}$-homotopy joining this v_k to v_∞ in $\mathcal{A}(\hat{\rho})$; of course, v_∞ is then rod $\hat{\rho}$-homotopic to each other triple in that homotopy class. Since we can do this for each $0 < \hat{\rho} < \rho$, we have shown that v_∞ is itself in the specified mild rod ρ-homotopy class as desired. □

Remark 2. *Note that as* $\hat{\rho} \to \rho$ *and* $D_* \to 0$*, the neighborhoods of* v_∞ *in the proof above can be expected to shrink, forcing* $k \to \infty$ *here. [More to the point, while* v_0 *is joined to* v_∞ *by a rod* $\hat{\rho}$*-homotopy, there seems no reason to expect a compactness result within* $C([0,T] \to \mathcal{A}(\rho))$ *to suggest subsequential convergence and so existence of a rod* ρ*-homotopy joining* v_0 *to* v_∞ *as a limit. [Indeed, simple examples in compact regions in the plane show that, although the closure of a connected set is always connected, the closure of an arcwise connected set need not be arcwise connected.] In general, there seems no strong reason to expect that two arbitrary rods in the same* *mild ρ-homotopy class should actually be connectable by a rod ρ-homotopy.*

*We note the difference in the definitions of rod homotopy class for elastic rods with a repulsive potential (see [**?**]) and elastic rods with an impenetrable tube as here. Elastic rods with singular repulsive potentials have infinite energy barriers that prevent the elastic rods from actual contact, but, on the other hand, our present consideration of elastic rods with impenetrable tubes allows points of contact in which parametrically nonlocal points are exactly a distance 2ρ apart. The proof of [**?**, Theorem 2] requires "wiggle-room" not provided by nonlocal pairs with such direct contact — hence the introduction of the smaller radius $\hat{\rho}$.* □

4 Characterization of the Constraint Cone

In this section and the next we will derive first order optimality conditions for a specific (local) minimizer for the constrained minimization problem (3.7). Thus, throughout this section $\bar{\mathrm{v}} = [\bar{\mathrm{u}}, \bar{\mathrm{D}}, \bar{\mathrm{r}}]$ is a specific (local) minimizer of the energy as in (3.7) so minimization is taken over some suitable neighborhood: $\bar{\mathrm{u}} \in \mathcal{U} \subset \mathcal{X}$ or, more precisely, over the intersection of $\mathcal{U}$ with the constrained set $\Omega = \Omega_1 \cap \Omega_2$ of (2.10) and (2.14).

In our treatment we will largely follow Mordukhovich [**?**] as a basic reference, but will also note [**?**], which was developed specifically to handle aspects of the present situation as in Subsection 4.2. In particular, we will make considerable use of Mordukhovich's *basic normal cone*, denoted $N(*;*)$, as defined in [**?**, Defn.1.1]. In particular, this section is devoted to characterizing the constraint cone $N(\bar{\mathrm{u}}; \Omega_1 \cap \Omega_2)$. Note that, in parallel with the relation of Sections 2 and 3, this section depends only on the geometrical considerations of the constraints and not at all on the energy functional we will be minimizing, to which we return in Section 5.

The boundary conditions of (2.9) may each be presented as an equality constraint of the form $g(u) = 0$ and, provided the Fréchet derivative $g'(\bar{\mathrm{u}})$ is surjective, the constraint cone will then be the range of $[g'(\bar{\mathrm{u}})]^*$; a similar need for surjectivity of $\mathbf{L} = [\mathbf{R} \circ \mathbf{D}]'$ arises for the normal cone for the impenetrability constraint. This surjectivity is complicated somewhat by the hidden constraints implicit in our formulation: the frame $\mathrm{D} = \mathbf{D}(\mathrm{u})$ takes values in the manifold pointwise restricted to $SO(3) \subset \mathcal{M}^{3\times 3}$, rather than surjective to a fixed linear space, and $\mathrm{r} = \mathbf{R}\mathrm{D}$ is similarly in a manifold where r' is pointwise restricted to the unit sphere $S_2 \subset \mathbb{R}^3$. It will thus be convenient to reformulate the condition in terms of new maps $\hat{\mathbf{D}} : \mathrm{u} \mapsto \hat{\mathrm{D}} = \bar{\mathrm{D}}^{-1}\mathrm{D}$ and $\hat{\mathbf{R}} : \hat{\mathrm{D}} \mapsto \mathrm{r}$, constructed specifically with respect to the particular minimizer; Subsection 4.1 discusses these maps, their linearizations at the minimizer, the appropriate codomains, and the adjoint maps.

Following that, in Subsection 4.2 we use results of [**?**], developed specifically for this purpose, to find a cone Ξ containing $N(\bar{\mathrm{r}};\hat{\Omega}_2)$ with $\hat{\Omega}_2 = \{\mathrm{r} :(2.13)\}$. [The convex cone Ξ is associated with the contact forces resulting from the non-selfintersection constraint (impenetrability).] We use the chain rule to get $N(\bar{\mathrm{u}};\Omega_2) \subset \mathbf{L}^*\,\Xi$. In Subsection 4.3 we then find normal cones $\mathcal{T}_{\mathrm{r}}, \mathcal{T}_{\mathrm{D}}$ corresponding to boundary conditions at $s = 1$ as in (2.9). Finally, we will use the sum rule [**?**, Cor.3.5, p.268] to obtain

$$N(\bar{\mathrm{u}};\Omega_{1\mathrm{r}} \cap \Omega_{1\mathrm{D}} \cap \Omega_2\} = N(\bar{\mathrm{u}};\Omega_{1\mathrm{r}}) + N(\bar{\mathrm{u}};\Omega_{1\mathrm{D}}) + N(\bar{\mathrm{u}};\Omega_2)$$

from which we conclude that

$$N(\bar{\mathrm{u}};\Omega_1 \cap \Omega_2) \quad \subset \quad \mathcal{T}_{\mathrm{r}} + \mathcal{T}_{\mathrm{D}} + \mathbf{L}^*\Xi. \tag{4.1}$$

4.1 Linearizations and their adjoints

In this subsection, we consider the maps $\mathbf{D}' = [\nabla_{\mathrm{u}}\mathbf{D}]$ and $\mathbf{L} = \nabla_u[\mathbf{R} \circ \mathbf{D}] = \mathbf{R}\mathbf{D}'$, each taken at $\mathrm{u} = \bar{\mathrm{u}}$. Denoting the variations in $\mathrm{r}, \mathrm{D}, \mathrm{u}$ by $\mathfrak{r}, \mathfrak{D}, \mathfrak{u}$, respectively, we then have $\mathbf{D}' : \mathfrak{u} \mapsto \mathfrak{D}$ and $\mathbf{L} : \mathfrak{u} \mapsto \mathfrak{r}$. The initial condition at $s = 0$ forces $\mathfrak{D}(0) = 0$ and $\mathfrak{r}(0) = 0$ so, nominally, $\mathfrak{r} \in \mathcal{Z}_0$ and $\mathfrak{D} \in \mathcal{Y}_0$. We will later need surjectivity of these derivatives, giving corresponding injectivity for their adjoints; however, due to the hidden constraints in embedding $SO(3)$ in $\mathcal{M}^{3\times 3}$ and embedding S_2 in $\mathbb{R}^3$, surjectivity does not hold for the spaces of (2.5). It is easiest to see the appropriate codomain modifications if we compose with pointwise multiplication by $\bar{\mathrm{D}}^{-1} = \bar{\mathrm{D}}^{\mathsf{T}}$ and by $\bar{\mathrm{D}}$ to get $\hat{\mathbf{D}} : \mathrm{u} \mapsto [\bar{\mathrm{D}}]^{\mathsf{T}}\,\mathrm{D} = \hat{\mathrm{D}}$ and $\hat{\mathbf{R}} : \hat{\mathrm{D}} \mapsto \mathrm{r}$.

Lemma 2. *The maps $\hat{\mathbf{D}}$ and $\hat{\mathbf{R}} \circ \hat{\mathbf{D}} \equiv \mathbf{R} \circ \mathbf{D}$ are Fréchet differentiable with*

$$[\nabla_{\mathrm{u}}\hat{\mathbf{D}}](\bar{\mathrm{u}}) = \mathbf{K} : \mathfrak{u} \mapsto \hat{\mathfrak{D}} \qquad\qquad [\nabla_u\,(\hat{\mathbf{R}} \circ \hat{\mathbf{D}})](\bar{\mathrm{u}}) = \mathbf{L} : \mathfrak{u} \mapsto \mathfrak{r}.$$

The linear maps $\mathbf{K} : \mathcal{X} \to \hat{\mathcal{Y}}$ and $\mathbf{L} : \mathcal{X} \to \hat{\mathcal{Z}}$ with $\hat{\mathcal{Y}}, \hat{\mathcal{Z}}$ as in (2.8) are well defined through solving the differential equations:

$$\hat{\mathfrak{D}}' = [\hat{\mathfrak{D}}\mathsf{S}(\bar{\mathrm{u}}) - \mathsf{S}(\bar{\mathrm{u}})\hat{\mathfrak{D}}] + \mathsf{S}(\mathfrak{u}) \qquad \hat{\mathfrak{D}}(0) = 0 \qquad (\mathfrak{r}' = \bar{\mathrm{D}}\,\hat{\mathfrak{D}}\mathrm{k} \quad \mathfrak{r}(0) = 0) \tag{4.2}$$

with $\hat{\mathfrak{D}}(0) = 0$, $\mathfrak{r}(0) = 0 = \mathfrak{r}'(0)$. With these codomains $\mathbf{K}, \mathbf{L}$ are surjective. We also have $\hat{\mathfrak{D}} = \mathsf{S}(\mathfrak{y})$ pointwise, with $\mathfrak{y}$ satisfying the differential equation:

$$\begin{array}{lll} \mathfrak{y}' & = \mathfrak{y} \times \bar{\mathrm{u}} + \mathfrak{u} & \mathfrak{y}(0) = 0, \\ \mathfrak{r}' & = \bar{\mathrm{D}} P_2 \mathfrak{y} & \mathfrak{r}(0) = 0 \\ \textit{with} & P_2 = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} : \mathfrak{y} \mapsto \mathsf{S}(\mathfrak{y})\mathrm{k}. & \end{array} \tag{4.3}$$

[Pointwise use of S is an isomorphism of $\tilde{\mathcal{Y}} = \{y \in W^{1,p}([0,1] \to \mathbb{R}^3) : y(0) = 0\}$ with $\hat{\mathcal{Y}}$, so we will take these as effectively equivalent and note that the map: $\mathfrak{u} \mapsto \mathfrak{y}$ is surjective from $\mathcal{X}$ to $\tilde{\mathcal{Y}}$.]

Proof. Differentiating $\mathrm{D} = \bar{\mathrm{D}}\hat{\mathrm{D}}$ with respect to s, we have $\hat{\mathrm{D}}' = [\hat{\mathrm{D}}\mathsf{S}(\mathrm{u}) - \mathsf{S}(\bar{\mathrm{u}})\hat{\mathrm{D}}]$ from (2.3) and differentiating this with respect to u at $\mathrm{u} = \bar{\mathrm{u}}$ gives the first equation of (4.2). From the identity $[\mathsf{S}(u)\mathsf{S}(v) - \mathsf{S}(v)\mathsf{S}(u)] = \mathsf{S}(u \times v)$ and the invertibility of S, we then obtain (4.3). The equation $\mathfrak{r}' = \bar{\mathrm{D}}\,\hat{\mathfrak{D}}\mathrm{k}$ of (4.2) is immediate.

Pointwise, the variation $\mathfrak{D}(s)$ must lie in the tangent space to $SO(3)$ at $\bar{\mathrm{D}}(s)$ so $\hat{\mathfrak{D}} = [\bar{\mathrm{D}}(s)]^{\mathsf{T}}\mathfrak{D}$ takes its pointwise values in the tangent space to $SO(3)$ at I — i.e., in the space $\mathcal{S}^3$ of skew matrices. Noting that $[AB - BA]$ is skew for any skew matrices A, B, we see that (4.2) does keep $\hat{\mathfrak{D}}$ pointwise in $\mathcal{S}^3$ so we have $\hat{\mathfrak{D}} \in \hat{\mathcal{Y}}$. The second equation of (4.2) clearly gives $\mathrm{r}' \perp \bar{\mathrm{D}}\mathrm{k}$ since $\bar{\mathrm{D}}$ is orthogonal and $\mathsf{S}(\mathfrak{y})$ is skew. We have shown that $\hat{\mathfrak{D}} \in \hat{\mathcal{Y}}$ and $\mathrm{r} \in \hat{\mathcal{Z}}$.

To show the surjectivity of $\mathbf{K}$, let $\hat{\mathfrak{D}}$ be arbitrary in $\hat{\mathcal{Y}}$, so $\mathcal{S}^3$-valued. Then $\hat{\mathfrak{D}}'$ and $[\hat{\mathfrak{D}}\mathsf{S}(\bar{\mathrm{u}}) - \mathsf{S}(\bar{\mathrm{u}})\hat{\mathfrak{D}}]$ are also $\mathcal{S}^3$-valued so $\hat{\mathfrak{D}}' - [\hat{\mathfrak{D}}\mathsf{S}(\bar{\mathrm{u}}) - \mathsf{S}(\bar{\mathrm{u}})\hat{\mathfrak{D}}]$ is (pointwise) $\mathsf{S}(\mathfrak{u})$ for some $\mathfrak{u}(s) \in \mathbb{R}^3$, necessarily with $\mathfrak{u} \in \mathcal{X}$. One then has the differential equation defining $\mathbf{K}\mathfrak{u} = \hat{\mathfrak{D}}$ with this $\mathfrak{u}$ so this arbitrary $\hat{\mathfrak{D}} \in \hat{\mathcal{Y}}$ is in the range of $\mathbf{K}$.

To show the surjectivity of $\mathbf{L}$, let $\mathfrak{r}$ be arbitrary in $\hat{\mathcal{Z}}$ so $\bar{\mathrm{D}}\mathfrak{r}' \perp \mathrm{k}$. This gives $\bar{\mathrm{D}}\mathfrak{r}'$ of the form $a\mathrm{i} + b\mathrm{j}$ (necessarily with $W^{1,p}$ regularity) so, e.g., setting $\mathbf{x} = (-b, a, 0)^{\mathsf{T}}$ we would have $\bar{\mathrm{D}}\mathfrak{r}' = P_2\mathbf{x} = \mathsf{S}(\mathbf{x})\mathrm{k}$, with $\mathsf{S}(\mathbf{x})$ in $\hat{\mathcal{Y}}$. This gives $\mathfrak{r} = \hat{\mathbf{R}}P_2\mathbf{x}$, in the range of $\hat{\mathbf{R}}$ from $\hat{\mathcal{Y}}$ and so in the range of $\mathbf{L}$. □

We next compute the adjoints

$$\mathbf{K}^*\eta \quad (\eta \in \hat{\mathcal{Y}}^*), \qquad\qquad \mathbf{L}^*\zeta \quad (\zeta \in \hat{\mathcal{Z}}^*).$$

[It will be convenient to work with $\mathfrak{y}$ rather than with $\mathfrak{D}$, noting that $\mathfrak{y} \mapsto \mathsf{S}(\mathfrak{y}) = \mathfrak{D}$ pointwise is an isomorphism to $\hat{\mathcal{Y}}$, so we pivot on the L^2 inner product to write $\langle \eta, \mathfrak{D}\rangle = \int \hat{\eta} \cdot \mathfrak{y}\, ds$ for a suitable $\hat{\eta}$.]

Lemma 3. *The adjoint* $\mathbf{K}^*$ *is computed by solving*

$$\omega' = \omega \times \bar{\mathrm{u}} - \hat{\eta} \qquad\qquad \omega(1) = 0 \tag{4.4}$$

to get $\omega = \mathbf{K}^*\eta$. *One obtains* $\hat{\mathbf{R}}^*\zeta = \hat{\eta}$ *for* $\zeta \in \hat{\mathcal{Z}}^*$ *by*

$$\hat{\eta}(s) = {P_2}^{\mathsf{T}}[\bar{\mathrm{D}}(s)]^{\mathsf{T}} z(s) \qquad \textit{with} \quad z(s) = \int_s^1 \zeta(\sigma)\, d\sigma. \tag{4.5}$$

Then $\mathbf{L}^* = \mathbf{K}^*\mathbf{R}^* : \zeta \mapsto \mathfrak{y} \to \mathfrak{u}$ *is obtained by composing* (4.4), (4.5).

Proof. We have

$$\begin{aligned}
\langle \eta, \hat{\mathfrak{D}} \rangle &= \int_0^1 \hat{\eta} \cdot \mathfrak{y}\, ds = \int_0^1 [\omega \times \bar{\mathrm{u}} - \omega'] \cdot \mathfrak{y}\, ds \\
&= \int_0^1 (\omega \times \bar{\mathrm{u}}) \cdot \mathfrak{y}\, ds + \int_0^1 \omega \cdot \mathfrak{y}'\, ds - \omega \cdot \mathfrak{y}\Big|_0^1 \\
&= \int_0^1 [(\omega \times \bar{\mathrm{u}}) \cdot \mathfrak{y} + \omega \cdot (\mathfrak{y} \times \bar{\mathrm{u}}]\, ds + \int_0^1 \omega \cdot \mathfrak{u}\, ds \\
&= \quad \langle \omega, \mathfrak{u} \rangle
\end{aligned}$$

where we have used (4.4), (4.3) (including the boundary conditions) and the triple product identity. Thus, since $\mathfrak{D} = \mathbf{K}\mathfrak{u}$, we have $\omega = \mathbf{K}^*\eta$.

We have, from (4.5), that $z' = -\zeta$ with $z(1) = 0$ and note that $\mathfrak{r} = \mathbf{R}^*\mathfrak{D}$ gives $\mathfrak{r}' = \bar{\mathrm{D}}\hat{\mathfrak{D}}\mathrm{k} = \bar{\mathrm{D}}P_2\,\mathfrak{y}$ with $\hat{\mathfrak{D}} = \mathsf{S}(\mathfrak{y})$ as above. Thus,

$$\langle \zeta, \mathfrak{r} \rangle = -\int_0^1 z' \cdot \mathfrak{r}\, ds = \int_0^1 z \cdot \mathfrak{r}'\, ds = \int_0^1 z \cdot \bar{\mathrm{D}}P_2\,\mathfrak{y}\, ds = \int_0^1 \hat{\eta} \cdot \mathfrak{y}\, ds$$

so, indeed, $\hat{\eta}$ as given by (4.5) is $\mathbf{R}^*\zeta$. □

Remark 3. *We must be quite careful in the interpretation of the formula* (4.4) *— and its boundary condition, in particular — since* $\eta, \hat{\eta}$ *are given as distributions, not functions. For example, the functional* $\hat{\eta} = \hat{\eta}_{\mathrm{e}} : \mathfrak{y} \mapsto \mathrm{e} \cdot \mathfrak{y}(1)$ *is in* $\tilde{\mathfrak{Y}}^*$*. For this we interpret* (4.4) *as giving a jump between* $\omega(1-)$ *and* $\omega(1+)$ *with "*$\omega(1) = 0$*" applying to the latter: effectively we would have*

$$\mathbf{K}^*\hat{\eta}_{\mathrm{e}} = \omega = \omega_{\mathrm{e}} \qquad \textit{with} \quad \omega' = \omega \times \bar{\mathrm{u}}, \quad \omega(1) = \mathrm{e}. \tag{4.6}$$

The same concern also applies to (4.5)*, e.g., for* $\zeta_{\mathrm{e}} : \mathfrak{r} \mapsto \mathrm{e} \cdot \mathfrak{r}(1)$ *we would similarly get from* (4.5)

$$\mathbf{R}^*\zeta_{\mathrm{e}} = \hat{\eta} = P_2{}^{\mathsf{T}}\bar{\mathrm{D}}^{\mathsf{T}}\mathrm{e}, \tag{4.7}$$

which we can verify by noting directly that

$$\int_0^1 [P_2{}^{\mathsf{T}}\bar{\mathrm{D}}^{\mathsf{T}}\mathrm{e}] \cdot \mathfrak{y}\, ds = \int_0^1 \mathrm{e} \cdot [\bar{\mathrm{D}}P_2\mathfrak{y}]\, ds = \mathrm{e} \cdot \int_0^1 \mathfrak{r}'\, ds = \mathrm{e} \cdot \mathfrak{r}(1).$$

4.2 The cone $N(\bar{\mathrm{u}};\Omega_2)$

The set Ω_2 consists of $\mathrm{u} \in \mathcal{X}$ for which the resulting rods have no self-intersections and we easily see that this can be written, along the lines of (2.13), as an infinite intersection of simpler sets. The sum rule [**?**, Cor.3.5, p.268] considers intersections of two sets and so, by induction, finite intersections; indeed, we will use it in that form in Subsection 4.4 below. However, results have apparently been unavailable for infinite intersections as here so, motivated by the present application, Seidman [**?**] studied normal cones of certain infinite intersections and obtained abstract results directly applicable to the present situation. This enables us to follow [**?**] here in computing $N(\bar{\mathrm{r}};\hat{\Omega}_2)$ and so $N(\bar{\mathrm{u}};\Omega_2)$.

We state the principal result of [**?**] in a notation easily adaptable to this paper:

Theorem 3 (Seidman [**?**, Thm. 3.1])**.** *Let $\mathcal{Z}$ be a Banach space and Ψ a family of (nonlinear) functionals $\psi : \mathcal{Z} \supset \hat{\mathcal{U}} \to \mathbb{R}$; fix $\bar{z} \in \hat{\Omega} = \bigcap_{\psi\in\Psi}\{z \in \mathcal{Z} : \psi(z) \geq 0\}$ and, for $\omega > 0$, set $\Psi^\omega = \{\psi \in \Psi : \psi(\bar{z}) \leq \omega\}$. Suppose*

- `a.` *each $\psi \in \Psi$ is differentiable on the open set $\hat{\mathcal{U}} \subset \mathcal{Z}$ with the derivatives $\{\psi' : \hat{\mathcal{U}} \to \mathcal{Z}^* : \psi \in \Psi\}$ equicontinuous at $\bar{z}$ and*
- `b.` *for some $\omega > 0$ and some space $\hat{\mathcal{Z}}$ with $\mathcal{Z} \hookrightarrow \hat{\mathcal{Z}}$, the $\hat{\mathcal{Z}}$-closure of $\mathcal{B}^\omega := \{z \in \hat{\mathcal{Z}} : \langle\psi'(\bar{z}), z\rangle \geq 0$ for all $\psi \in \Psi^\omega\}$ has nonempty interior in $\hat{\mathcal{Z}}$.*

Then the basic normal cone to $\hat{\Omega}$ at $\bar{z}$ satisfies

$$N(\bar{z};\hat{\Omega}) \quad \subset \quad \bigcap_{\omega>0} \overline{\mathrm{cone}}\,\{\psi'(\bar{z}) \in \hat{\mathcal{Z}}^* : \psi \in \Psi^\omega\} \tag{4.8}$$

with N computed for $\hat{\Omega} \subset \mathcal{Z}$, but the closure of each $\overline{\mathrm{cone}}$ taken in $\hat{\mathcal{Z}}^*$.

[We have denoted by $\overline{\mathrm{cone}}(\mathcal{S})$ the closed conical hull of $\mathcal{S}$, i.e., the closed convex hull of $\{a\xi : \xi \in \mathcal{S},\ a > 0\}$, although that notation does not explicitly indicate the norm used for this closure.]

Proof. This actually combines material presented in [**?**] as Theorem 3.1, Corollary 4.1, and Theorem 4.3. □

Theorem 4. *Under our hypotheses on the constitutive functions, let $\bar{\mathrm{r}} = [\mathbf{R}\circ\mathbf{D}](\bar{\mathrm{u}})$ for a local minimizer $\bar{\mathrm{u}}$ of (3.7) and let $\hat{\Omega}_2 = \{\mathrm{r} \in \mathcal{Z} : (2.13)\}$. Then*

$$N(\bar{\mathrm{r}};\hat{\Omega}_2) \;\subset\; \Xi = \bigcap_{\omega>0} \overline{\mathrm{cone}}\,\{\psi'_{(s,\sigma)} \in \hat{\mathcal{Z}}^* : (s,\sigma) \in \mathcal{NL}_\omega\} \tag{4.9}$$

where $\mathcal{NL}_\omega = \{(s,\sigma) \in \mathcal{NL} : |\mathrm{r}(s) - \mathrm{r}(\sigma)| \le 2\rho + \omega\}$ *and* $\hat{\mathcal{Z}} = C([0,1] \to \mathbb{R}^3)$*. [Note that* $\Xi \subset \hat{\mathcal{Z}}^*$*, a space of* $\mathbb{R}^3$*-valued Borel measures on* $[0,1]$*.] Also*

$$N(\bar{\mathrm{u}}; \Omega_2) \;\subset\; \mathbf{L}^* \,\Xi. \tag{4.10}$$

Finally, each $\xi \in \Xi$ *is orthogonal to constants in* $\mathcal{X}$ *and is (pointwise in* s*) orthogonal to the centerline.*

Proof. Most of this result is a corollary to Theorem 3: we need only check the hypotheses `a,b` of that theorem for this setting. With $\psi = \psi_{(s,\sigma)}$ as in (2.13), an easy calculation gives

$$\psi'(\mathrm{r}) = \frac{d\psi}{d\mathrm{r}} : \;\mathfrak{r} \;\longmapsto\; \frac{\mathrm{r}(s) - \mathrm{r}(\sigma)}{|\mathrm{r}(s) - \mathrm{r}(\sigma)|} \,\cdot\, [\mathfrak{r}(s) - \mathfrak{r}(\sigma)]. \tag{4.11}$$

so

$$\|\psi'(\mathrm{r}) - \psi'(\bar{\mathrm{r}})\| \le 2 \left\| \frac{\mathrm{r}(s) - \mathrm{r}(\sigma)}{|\mathrm{r}(s) - \mathrm{r}(\sigma)|} - \frac{\bar{\mathrm{r}}(s) - \bar{\mathrm{r}}(\sigma)}{|\bar{\mathrm{r}}(s) - \bar{\mathrm{r}}(\sigma)|} \right\|.$$

Noting that $\bar{\mathrm{r}} \in \hat{\Omega}_2$ so $|\bar{\mathrm{r}}(s) - \bar{\mathrm{r}}(\sigma)| \ge 2\rho$ for each pair $(s,\sigma) \in \mathcal{NL}$, we see that the denominators are bounded away from 0 uniformly on the compact set $\mathcal{NL} \subset [0,1]^2$ and for all r close to $\bar{\mathrm{r}}$ in $\mathcal{Z}$ or $\hat{\mathcal{Z}}$. Thus we have the equicontinuity condition `a` even for the $\hat{\mathcal{Z}}$-norm.

We note next that $\psi \in \Psi^\omega$ just means that $\psi = \psi_{(s,\sigma)}$ with $(s,\sigma) \in \mathcal{NL}_\omega$. For any $\omega > 0$ one gets from (4.11) that, using the $\hat{\mathcal{Z}}$-norm,

$$\langle \psi'(\bar{\mathrm{r}}), z\rangle = \frac{\bar{\mathrm{r}}(s) - \bar{\mathrm{r}}(\sigma)}{|\bar{\mathrm{r}}(s) - \bar{\mathrm{r}}(\sigma)|} \cdot [z(s) - z(\sigma)] \ge |\bar{\mathrm{r}}(s) - \bar{\mathrm{r}}(\sigma)| - 2\|z - \bar{\mathrm{r}}\|_{\hat{\mathcal{Z}}}.$$

Thus, noting that $\bar{\mathrm{r}}$ satisfies the constraint so $|\bar{\mathrm{r}}(s) - \bar{\mathrm{r}}(\sigma)| \ge 2\rho$ for (s,σ) nonlocal, we see that the convex set $\mathcal{B}^\omega$ contains the (open) $\hat{\mathcal{Z}}$-ball of radius ρ and center $\bar{\mathrm{r}}$, giving the qualification condition `b`. Applying Theorem 3 gives $N(\bar{\mathrm{r}}; \hat{\Omega}_2) \subset \Xi$ and then $N(\bar{\mathrm{u}}; \Omega_2) = \mathbf{L}^* \, N(\bar{\mathrm{r}}; \hat{\Omega}_2) \subset \mathbf{L}^* \,\Xi$ by the chain rule.

If $\mathfrak{r}$ is constant one has $[\mathfrak{r}(s) - \mathfrak{r}(\sigma)] = 0$ so then $\langle \psi'(\mathrm{r}), \mathfrak{r}\rangle = 0$ for any $\psi = \psi_{(s,\sigma)}$ by (4.11). Each such $\xi = \psi'_{(s,\sigma)} \in \Xi_\omega$ is thus orthogonal to the 3-dimensional subspace of constants in $\mathcal{X}$; we note that this then holds for multiples, sums and limits so $\langle \xi, \mathfrak{r}\rangle = 0$ for each $\xi \in \Xi$ and each constant $\mathfrak{r}$.

Finally, we wish to show pointwise orthogonality to the centerline, i.e., that one has $\xi(s) \perp \bar{\mathrm{r}}'(s)$ for each $s \in [0,1]$ and each $\xi \in \Xi$. If $\xi \in \Xi$ were of the special form $\psi'_{(s,\sigma)}$ with the constraint active so $|\bar{\mathrm{r}}(s) - \bar{\mathrm{r}}(\sigma)| = 2\rho$ for this pair $(s,\sigma) \in \mathcal{NL}$, the fact that $|\bar{\mathrm{r}}(\hat{s}) - \bar{\mathrm{r}}(\sigma)| \ge 2\rho$ for nearby $\hat{s}$ makes s a minimizer of the distance from $\bar{\mathrm{r}}(\sigma)$ so

$\bar{\mathrm{r}}'(s)\cdot[\bar{\mathrm{r}}(s)-\bar{\mathrm{r}}(\sigma)]=0$, i.e., $\xi(s)\perp\bar{\mathrm{r}}'(s)$; in view of (4.11), we are treating the measure ξ near s as a vector delta function with direction $[\bar{\mathrm{r}}(s)-\bar{\mathrm{r}}(\sigma)]$. More generally, for $(s,\sigma)\in\mathcal{NL}_\omega$, a slightly more delicate argument along the same lines shows that, in the presence of a bound on $\bar{\mathrm{r}}''=\kappa$ we have an estimate $|\bar{\mathrm{r}}'(s)\cdot[\bar{\mathrm{r}}(s)-\bar{\mathrm{r}}(\sigma)]|=\mathcal{O}(\omega)$ uniform as $\omega\to 0$ which gives a corresponding estimate for ξ in the cone generated by such $\psi'_{(s,\sigma)}$ for $\psi\in\Psi^\omega$. Taking limits and then letting $\omega\to 0$ gives the desired result. $\square$

Remark 4. *As noted,* (3.2) *does not permit external hard obstacles, but this possibility could be treated much as the prohibition against self-intersection was treated here. Any hard external obstacle $\mathcal{O}$, taken as a closed subset of $\mathbb{R}^3$, may be viewed as a constraint: no point of the tube is to coincide with $\mathcal{O}$. We then enforce this by imposing a family of scalar constraints*

$$\begin{array}{c}\textit{For each } [s,\mathbf{x}]\in[0,1]\times\mathcal{O} \textit{ one has } \psi_{[s,\mathbf{x}]}[\mathrm{r}]\geq\ 0\\ \textit{where}\ \ \psi_{[s,\mathbf{x}]}[\mathrm{r}]:=|\mathrm{r}(s)-\mathbf{x}|-\rho\end{array}\tag{4.12}$$

much like (2.13) *but now parametrized by $s\in[0,1],\mathbf{x}\in\mathcal{O}$. If we let $\hat\Omega_3=\{\mathrm{r}:(4.12)\}$ and $\Omega_3=\{\tilde{\mathrm{u}}:\mathrm{r}=[\mathbf{R}\circ\mathbf{D}](\mathrm{u})\in\hat\Omega_3\}$, then one would expect to apply Theorem 3 as above. We do not address here any regularity requirements on the set $\mathcal{O}$ which might be needed for this to be possible or the verification of a modified Lemma 4, below.* $\square$

4.3 The cones $N(\bar{\mathrm{u}};\Omega_{1\mathrm{r}})$ and $N(\bar{\mathrm{u}};\Omega_{1\mathrm{D}})$

This subsection is concerned with constraints arising from the possible imposition of boundary conditions at $s=1$ as in (2.9). We consider separately constraints involving $\mathrm{D}(1)$ and those involving $\mathrm{r}(1)$, with the obvious treatment of mixed cases in which some combinations or partial specifications might be imposed.

If one were to specify $\mathrm{D}(1)=\mathrm{D}_1$, then $\bar{\mathrm{D}}$ satisfies this so we are always specifying $\hat{\mathrm{D}}(1)=I$. Except that we are viewing this as a constraint, this is much like the initial condition at $s=0$ and requires that variations $\hat{\mathfrak{D}}$ vanish at $s=1$ or, equivalently, that each $\langle\hat\eta_{\mathrm{e}},\mathbf{K}\mathfrak{u}\rangle=\mathrm{e}\cdot\mathfrak{y}(1)$ should vanish for $\mathrm{e}\in\mathbb{R}^3$. Letting $\Omega_{1,\mathrm{D}}=\{\mathrm{u}:\hat{\mathbf{D}}(\mathrm{u})=I\}$, corresponding to this specification, then gives the normal cone

$$N(\bar{\mathrm{u}};\Omega_{1,\mathrm{D}})=[\Omega_{1,\mathrm{D}}]^{\mathsf{T}}=\mathrm{span}\,\{\mathbf{K}^*\hat\eta_e:\mathrm{e}\in\mathbb{R}^3\}\ =\mathcal{T}_{\mathrm{D}}\tag{4.13}$$

if we impose such a condition. We then have $\mathcal{T}_{\mathrm{D}}=\mathrm{span}\,\{\omega_e:\mathrm{e}=\mathrm{i},\mathrm{j},\mathrm{k}\}$, using (4.6) from Remark 3.

Similarly,if one were to specify $\mathrm{r}(1) = \mathrm{r}_1$, then the variations $\mathfrak{r}$ must vanish at $s = 1$, i.e., $\langle \zeta_{\mathrm{e}}, \mathbf{L}\mathfrak{u}\rangle = e \cdot \mathfrak{r}(1) = 0$ for each $\mathrm{e} \in \mathbb{R}^3$. Letting $\Omega_{1,\mathrm{r}} = \{\mathrm{u} : \mathbf{RD}(\mathrm{u}) = \mathrm{r}_1\}$, corresponding to this specification, then gives the normal cone

$$N(\bar{\mathrm{u}}; \Omega_{1,\mathrm{r}}) = [\Omega_{1,\mathrm{r}}]^{\mathsf{T}} = \mathrm{span}\,\{\mathbf{L}^*\zeta_e : \mathrm{e} \in \mathbb{R}^3\} \; = \mathcal{T}_{\mathrm{r}} \tag{4.14}$$

if we impose such a condition. We then have $\mathcal{T}_{\mathrm{r}} = \mathrm{span}\,\{\mathbf{L}^*\zeta_e : \mathrm{e} = \mathrm{i}, \mathrm{j}, \mathrm{k}\}$, for which we use (4.7) from Remark 3.

4.4 The Sum Rule

In this subsection, we relate the separate cones to the normal cone $N(\bar{\mathrm{u}}; \Omega)$ with the constrained set $\Omega = \Omega_{1\mathrm{r}} \cap \Omega_{1\mathrm{D}} \cap \Omega_2$ and show that (4.1) holds. To this end we will apply the sum rule [**?**, Cor.3.5,p.268] to get

$$N(\bar{\mathrm{u}}; \Omega_{1\mathrm{r}} \cap \Omega_{1\mathrm{D}} \cap \Omega_2) = N(\bar{\mathrm{u}}; \Omega_{1\mathrm{r}}) + N(\bar{\mathrm{u}}; \Omega_{1\mathrm{D}}) + N(\bar{\mathrm{u}};\ \Omega_2), \tag{4.15}$$

noting that we have already shown that

$$N(\bar{\mathrm{u}}; \Omega_{1\mathrm{r}}) = \mathcal{T}_{\mathrm{r}}, \qquad N(\bar{\mathrm{u}}; \Omega_{1\mathrm{D}}) = \mathcal{T}_{\mathrm{D}}, \qquad N(\bar{\mathrm{u}}; \Omega_2) \subset \mathbf{L}^*\Xi \tag{4.16}$$

in the previous subsections. Allowing for the various possibilities in (2.9), we write $\mathcal{T} = \mathcal{T}_{\mathrm{r}} + \mathcal{T}_{\mathrm{D}}$.

Lemma 4. $\quad N(\bar{\mathrm{u}}; \Omega) \;\subset\; \mathcal{T} + \mathbf{L}^*\Xi.$

Proof. To apply [**?**, Cor.3.5] for (4.15), it is sufficient to verify the qualification condition:

$$\begin{array}{ll} \textit{If} & \omega^\dagger \in N(\bar{\mathrm{u}}; \Omega_{1\mathrm{r}}),\ \ \omega^\ddagger \in N(\bar{\mathrm{u}}; \Omega_{1\mathrm{D}}),\ \ \omega \in N(\bar{\mathrm{u}}; \Omega_2) \\ \quad \textit{with} & \qquad \omega^\dagger + \omega^\ddagger + \omega = 0, \\ \textit{then} & \qquad \omega^\dagger = 0,\ \ \omega^\ddagger = 0,\ \ \omega = 0. \end{array} \tag{4.17}$$

Given (4.16) we have

$$\omega^\dagger = L^*\zeta_{\mathrm{e}^\dagger}, \qquad \omega^\ddagger = K^*\hat{\eta}_{\mathrm{e}^\ddagger}, \qquad \omega = \mathbf{L}^*\xi$$

for some $\mathrm{e}^\dagger, \mathrm{e}^\ddagger \in \mathbb{R}^3$ and some $\xi \in \Xi$. Since $\mathbf{K}^*$ is injective by (4.2), we have $\hat{\eta}_{\mathrm{e}^\ddagger} + \hat{\mathbf{R}}^*[\zeta_{\mathrm{e}^\dagger} + \xi] = 0$ as we know $0 = \omega^\dagger + \omega^\ddagger + \omega = \mathbf{K}^*\left(\hat{\eta}_{\mathrm{e}^\ddagger} + \hat{\mathbf{R}}^*[\zeta_{\mathrm{e}^\dagger} + \xi]\right)$. Note that anything in the range of $\hat{\mathbf{R}}^*$ is a continuous function whereas $\hat{\eta}_{\mathrm{e}^\ddagger} : \mathfrak{y} \mapsto \mathrm{e}^\ddagger \cdot \mathfrak{y}(1)$ cannot be a function unless $\mathrm{e}^\ddagger = 0$. Thus $\omega^\ddagger = 0$ and $0 = \omega^\dagger + \omega = \mathbf{L}^*(\zeta_{\mathrm{e}^\dagger} + \xi)$. By the injectivity of $\mathbf{L}^*$, we then have $\zeta_{\mathrm{e}^\dagger} + \xi = 0$. Taking $\mathfrak{r}$ =constant= $\mathrm{e}^\dagger$, we have $\langle \xi, \mathfrak{r}\rangle = 0$ by Theorem 4 while $\langle \zeta_{e^\dagger}, \mathfrak{r}\rangle = |e^\dagger|^2$ so $e^\dagger = 0$ and $\omega^\dagger = 0,\ \omega = 0$. This gives (4.17) whence [**?**, Cor.3.5] applies to give (4.15) and so the desired result by (4.16). □

5 Optimality Conditions and Regularity

In this section, we derive necessary first-order optimality conditions

$$-W_{\mathrm{u}} = \mathrm{t}_* + \mathbf{L}^*[F_{\mathrm{r}} + \xi_*] \qquad \text{some } \mathrm{t}_* \in \mathcal{T}, \text{ some } \xi_* \in \Xi, \tag{5.1}$$

(much like the KKT conditions for constrained optimization problems in finite-dimensional settings) for an elastic rod with an impenetrable tube surrounding the centerline, i.e., for (3.7).

We begin by computing $\mathcal{E}'$,for which the major new challenge is that our treatment of (2.1) requires (3.4)c so, unlike the situation in [**?**] where $\mathcal{W}$ was finite everywhere in $\mathcal{X}$, the domain of the functional $\mathcal{W}$ now has empty interior. We then use these conditions to show regularity of the minimizer along the lines of [**?**, Theorem 5].

5.1 Computation of $\mathcal{E}'$

Lemma 5. *Assume, in addition to* (3.4), (3.2)*, that $F(s,x)$ is smooth (in the variables $s \in [0,1]$ and $x \in \mathbb{R}^3$) and that W is locally smooth where finite. Then $\mathcal{F}$ is Fréchet differentiable with $\mathcal{F}' = \nabla_{\mathrm{u}}\mathcal{F}$ given, as in [**?**, Lemma 7], by*

$$\nabla_{\mathrm{u}}\mathcal{F} = \mathbf{L}^*[\nabla_{\mathrm{r}}\mathcal{F}] = \mathbf{L}^*[F_{\mathrm{r}}] \tag{5.2}$$

where F_{r} is given pointwise as $F_{\mathrm{r}}(s, \bar{\mathrm{r}}(s))$. The subdifferential $\partial\mathcal{W}$ of the convex function $\mathcal{W}$ is a singleton at each point where $\mathcal{W}$ is finite, and this is given pointwise by $W_{\mathrm{u}} = W_{\mathrm{u}}(s, \mathrm{u}(s))$. Then

$$\mathcal{E}' := \nabla_{\mathrm{u}}\mathcal{E} \;=\; W_{\mathrm{u}} + \mathbf{L}^*[F_{\mathrm{r}}] \tag{5.3}$$

with the right hand side interpreted as an $\mathbb{R}^3$-valued function of $s \in [0,1]$.

Proof. Since the argument of $F(s, \bar{\mathrm{r}}(s))$ is uniformly bounded, the assumed smoothness easily justifies bringing differentiation under the integral sign so

$$\langle \nabla_{\mathrm{r}}\mathcal{F}, \mathfrak{r} \rangle := \lim_{t\to 0} \int_0^1 t^{-1}[F(s, \mathrm{r}(s) + t\mathfrak{r}(s)) - F(s, \mathrm{r}(s))]\, ds = \int_0^1 \left[\frac{\partial F}{\partial \mathrm{r}}(s, \mathrm{r}(s))\right] \mathfrak{r}(s)\, ds$$

and this is continuous in $\mathrm{r}, \mathfrak{r}$ so we have a Fréchet derivative $\nabla_{\mathrm{r}}\mathcal{F} = F_{\mathrm{r}}$. In considering $\mathcal{F}[\mathrm{r}] = \mathcal{F}[\mathbf{R}(\mathbf{D}(\mathrm{u}))]$, the chain rule then gives $\nabla_{\mathrm{u}}\mathcal{F} = \mathbf{L}^*[\nabla_{\mathrm{r}}\mathcal{F}]$.

From [**?**, Thm.1.93], we have $\partial\mathcal{W}[\mathrm{u}] = \{\xi \in \mathcal{X} : \mathcal{W}[\mathrm{u} + \mathfrak{u}] - \mathcal{W}[\mathrm{u}] \geq \langle \xi, \mathfrak{u} \rangle\}$. We then easily verify that $W_{\mathrm{u}}(s) = [\partial W/\partial \mathrm{u}](s, \hat{\mathrm{u}}(s))$ is in $\partial\mathcal{W}[\hat{\mathrm{u}}]$ when $\mathcal{W}(\hat{\mathrm{u}}) < \infty$, much as for the computation above of $\nabla_{\mathrm{r}}\mathcal{F}$ (noting that the condition on $\xi \in \partial\mathcal{W}[\mathrm{u}]$

is vacuous when $\mathfrak{u}$ is such that $\mathcal{W}[\mathrm{u}+\mathfrak{u}]=\infty$). To see that this is the only element of $\partial\mathcal{W}[\mathrm{u}]$, we note that we can always find subsets of $\mathcal{X}$ with dense span consisting of $\mathfrak{u}$ for which $\mathcal{W}[\mathrm{u}+t\mathfrak{u}]<\infty$ for small $|t|$, e.g., bounded $\mathfrak{u}$ with support where $|\tilde{\mathrm{u}}|$ (the first two components of u) is bounded below $1/\rho$. The limit argument shows that $\langle \xi - W_{\mathrm{u}}, \pm\mathfrak{u}\rangle \leq 0$ for all such $\mathfrak{u}$ whence, in view of the strict convexity of each $W(s,\cdot)$, $\xi = W_{\mathrm{u}}$ and $\partial\mathcal{W}[\mathrm{u}]$ is that singleton. Note that (3.4)c ensures that the domain of $\mathcal{W}$ has empty interior in $\mathcal{X}$ so we cannot, at this point, claim that $\mathcal{W}'[\bar{\mathrm{u}}]$ is continuous as a functional on $\mathcal{X}$: we have only identified it pointwise as a function of $s\in[0,1]$.

Finally, since $\mathcal{F}$ is certainly strictly differentiable in the sense of [?, Defn.1.13], the sum rule [?, Prop.1.107(ii)] gives $\partial\mathcal{E}=\partial\mathcal{W}+\nabla_{\mathrm{u}}\mathcal{F}$ and so (5.3). □

5.2 First order necessary conditions

In this subsection we show that the optimization condition

$$-\mathcal{E}'[\bar{\mathrm{u}}] \;\in\; N(\bar{\mathrm{u}};\Omega) \tag{5.4}$$

holds at the constrained minimizer. Since we have already calculated $\mathcal{E}'[\bar{\mathrm{u}}]$ and $N(\bar{\mathrm{u}};\Omega)$, this will provide the first order necessary conditions we desire.

This standard optimality condition (5.4) would be given by [?, Thm. 5.1, p.4] if $\mathcal{E}[\mathrm{u}]$ would be Fréchet differentiable near $\bar{\mathrm{u}}\in\mathcal{X}$ or by [?, Prop.1.107(ii)] provided we had strict differentiability. However, even strict differentiability (which would imply a local Lipschitz condition) is impossible in the present context in view of (2.1) as imposed by (3.4)c. [Our approach will be to replace the $\mathcal{X}$-norm by a stronger $\mathcal{X}_\ddagger$-norm temporarily. This would be simpler if we already knew here that $\bar{\mathrm{u}}$ satisfied (2.1) as a uniform strict inequality; this, indeed, will later be shown in Theorem 6, but that proof relies on (5.4).]

Theorem 5. *Under the hypotheses of Lemma 5 one has the first order necessary condition* (5.4) *at the constrained minimizer* $\bar{\mathrm{u}}$.

Proof. We begin by setting $\mathcal{E}_\ddagger[\mathfrak{u}]=\mathcal{E}[\bar{\mathrm{u}}+\mathfrak{u}]$ and similarly shifting the constraint set. It is immediate that $\mathcal{E}_\ddagger[\mathfrak{u}]$ is finite when

$$|\tilde{\mathfrak{u}}(s)|<\alpha_0(s)=1/\rho-|\tilde{\bar{\mathrm{u}}}(s)|$$

(where we note that $\alpha_0(s)>0$ except perhaps on some set of measure 0) with $u_3(\cdot)\in L^p$. For each s where $\alpha_0\neq 0$ it is possible to take $0<\alpha(s)<\alpha_0(s)$ small enough to get differentiability of $\mathfrak{u} \mapsto \mathcal{W}_\ddagger[\mathfrak{u}] = \mathcal{W}[\bar{\mathrm{u}} + \mathfrak{u}]$ at 0 (i.e., at $\mathrm{u} = \bar{\mathrm{u}}(s)$) uniformly in s with perturbations relative to $\alpha(s)$. We now define a norm

$$\|\mathfrak{u}\|_\ddagger = \sup_{s\in[0,1]} \left\{ \frac{|\tilde{\mathfrak{u}}(s)|}{\alpha(s)} \right\} + \|\mathfrak{u}_3\|_{L^p(0,1)} \tag{5.5}$$

and the corresponding space $\mathcal{X}_\ddagger$. This choice of the function α ensures that we have strict differentiability of $\mathcal{W}$ with respect to this $\mathcal{X}_\ddagger$-norm and already had Fréchet differentiability of $\mathcal{F}$ with respect to the weaker $\mathcal{X}$-norm. Thus, using [**?**, Prop.1.107(ii)], we have (5.4) at the constrained minimizer $\bar{\mathrm{u}}$ in this context — noting that the basic normal cone $N(0; \Omega - \bar{\mathrm{u}})$ is now computed in the context of the dual space to $\mathcal{X}_\ddagger$. On the other hand, we recall from Theorems 3 and 4 that the cone $N(\bar{\mathrm{r}}; \hat{\Omega})$ can be equivalently computed in C^* as noted in the analysis of Section 4. □

An immediate consequence of this and the analyses of Section 4 and Lemma 5 is the first order necessary condition (5.1) for optimality.

5.3 Regularity

We continue to consider some specific (local) energy minimizer $\bar{\mathrm{u}}$. In this subsection we show some consequences of the first order necessary condition (5.1) obtained above under the assumptions, in addition to (3.2), (3.4), that F is smooth and that W is smooth where finite. In some sense, our principal result will be that the curvature assumption (2.1) is never active as a constraint: the minimizer $\bar{\mathrm{u}}(\cdot)$ is continuous, with (3.4 c) ensuring that $\kappa(\cdot)$ remains uniformly bounded away from $1/\rho$. Further regularity of $\bar{\mathrm{u}}$, up to a point, then follows from a more careful look at the cone Ξ and the usual bootstrap argument as in [**?**, Theorem 5].

We next wish to show that (2.1) will be satisfied with a (uniform) strict inequality.

Theorem 6. *Assume* (3.2), (3.4)*, that F is smooth and that W is smooth where finite with invertible Hessian at each such s, u. Let $\bar{\mathrm{u}}$ be a solution of the constrained minimization problem* (3.7)*. Then $\bar{\mathrm{u}}(\cdot)$ is a continuous function with* (2.1) *holding uniformly on* $[0, 1]$*: κ is bounded below $1/\rho$.*

Proof. Looking at $W(s, \cdot)$ on the infinite cylinder in $\mathbb{R}^3$ where it is finite, and set $\mu = \min\{W\}$ so $\mu \le c\psi(0)$. In view of the assumed convexity, we have (for large values of W) that

$$|\nabla_{\mathrm{u}} W| \ge \left| \frac{\partial W}{\partial u_3} \right| \ge \frac{W - \mu}{|u_3|} \ge \frac{b|u_3|^p - \mu}{|u_3|} \quad \to \infty \text{ as } |u_3| \to \infty$$

with growth uniform in $s, \tilde{u}$, whence bounding $|W_{\mathrm{u}}|$ bounds $|u_3|$. Similarly,

$$|\nabla_{\mathrm{u}} W| \geq \left|\frac{\partial W}{\partial \kappa}\right| \geq \frac{W-\mu}{\kappa} \geq \frac{\psi(\kappa)-\mu}{\kappa} \quad \to \infty \text{ as } \kappa \to 1/\rho$$

uniformly in s, θ, u_3 so bounding $|\nabla_{\mathrm{u}} W|$ also implies a (computable) bound away from $1/\rho$ for κ.

Letting $w(s) = W_u(s, \bar{u}(s))$, we have, from (5.1), that $w = t_* + \mathbf{L}^*[F_{\mathrm{r}} + \xi_*]$ with $t_* \in \mathcal{T}$ and $\xi_* \in \Xi$. From (4.13), (4.14), it is clear that $t_*(\cdot)$ must be (at least) Lipschitzian and one also has at least this regularity for $[\mathbf{L}^* F_{\mathrm{r}}](\cdot)$. Since Theorem 4 gives $\Xi \subset [C([0,1] \to \mathbb{R}^3)]^*$, a space of finite Borel measures, one must have $\mathbf{R}^*\xi$ bounded for any measure $\xi \in \Xi$ so $L^*\xi_*$ is again Lipschitzian. It follows that $w(\cdot)$ must be a (Lipschitz) continuous function on $[0,1]$. In particular, this bounds $w = \nabla_{\mathrm{u}} W$ on $[0,1]$ so the estimates above apply to bound u_3 and to bound κ below $1/\rho$.

Thus we have shown that (2.1) is never active as a constraint and that $\bar{u}$ takes its values in a compact set where W is smooth. At each $s \in [0,1]$ the invertibility of the Hessian ensures, by the Implicit Function Theorem, that we can locally solve the defining equation $w(s) = W_{\mathrm{u}}(s, \bar{u}(s))$ for $\bar{u}(s)$ as a continuous function of $s, w(s)$ so $\bar{u}$ is a continuous function of s as asserted. $\square$

We next note that ξ_* in (5.1) has the interpretation of forces on the rod due to the constraint against self-intersection, i.e., contact forces. It should not, then, be surprising that they are restricted to the contact set $\mathcal{C} = \mathcal{C}(\bar{r})$ of (2.17).

Lemma 6. *Each $\xi \in \Xi$ is a vector Borel measure whose support (in the sense of distributions) lies in the contact set.*

Proof. From Theorem 4 we have that Ξ is in $\hat{\mathcal{Z}}^* = [C([0,1] \to \mathbb{R}^3)]^*$, a space of vector Borel measures and we must localize the support of $\xi \in \Xi$. To this end, let $\mathcal{I}$ be any open subinterval in the complement of $\mathcal{C}$ and let ϕ be any (vector-valued) smooth function with (compact) support $\mathcal{I}_* \subset \mathcal{I}$. We must show that $\langle \xi, \phi \rangle = 0$ for such ϕ.

Let $\omega_* = [\inf\{d_*(s) : s \in \mathcal{I}_*\} - 2\rho]$ with d_* as in (2.16); this is attained as a minimum since d_* is lower semicontinuous and $\mathcal{I}_*$ is compact. Since $\mathcal{I}_*$ is disjoint from $\mathcal{C}(\bar{r})$, we must have $\omega_* > 0$. For any $(s, \sigma) \in \mathcal{NL}_\omega$ with $0 < \omega < \omega_*$ we will then have $s, \sigma \notin \mathcal{I}_*$ so $\phi(s) = 0$, $\phi(\sigma) = 0$ so we have $\langle \psi', \phi \rangle = 0$ for each such $\psi' \in \{\psi'_{(s,\sigma)} : (s,\sigma) \in \mathcal{NL}_\omega\}$. As in the proof of Theorem 4, we note that this orthogonality then also holds for multiples, sums and limits so $\langle \xi, \phi \rangle = 0$ for all $\xi \in \Xi$. Since ϕ is an arbitrary test function with support in the complement of $\mathcal{C}$, we have demonstrated that the support of ξ lies in $\mathcal{C}$. $\square$

In [**?**, Theorem 5] a bootstrapping argument was used to obtain further regularity of the minimizer $\bar{\mathrm{u}}$ in that setting. While we again use an argument of that nature, we are now limited by the localized regularity of $\xi_* \in \Xi$ as above.

Theorem 7. *Under the hypotheses of Theorem 6, the minimizer $\bar{\mathrm{u}}$ will be will be a continuously differentiable function on $[0,1]$, indeed, with $\bar{\mathrm{u}}' \in BV$. Further, $\bar{\mathrm{u}}$ will be infinitely differentiable (to the extent that the regularity of F, W supports this) on the complement of the contact set, i.e., on the open intervals between contact points. In each case there will be corresponding regularity of the frame $\bar{\mathrm{D}}$ and of the centerline $\bar{\mathrm{r}}$.*

Proof. This is essentially a corollary to Theorem 6 and Lemma 6 and a continuation of the proof of Theorem 6, from which we recall, in particular, that the standard bootstrapping argument gives regularity of $\bar{\mathrm{u}}$ to be the same (supported by the regularity of W) as the regularity of

$$W_u(\cdot, \bar{\mathrm{u}}(\cdot)) = w(\cdot) = t_* + \mathbf{L}^*[f_* + \xi_*].$$

Using (5.4), we have here $t_* \in \mathcal{T}$ given by (4.6), (4.7) and $f_* = F_{\mathrm{r}}(\cdot, \bar{\mathrm{r}}(\cdot))$ with, finally, the self-contact forces $\xi_* \in \Xi$.

From (4.6), (4.7) we have $t_*' = t_* \times \bar{\mathrm{u}} - \hat{\eta}$ — with $\hat{\eta} = 0$ and $t_*(1) = \mathrm{e}$ or with $\hat{\eta} = P_2{}^{\mathsf{T}}\bar{\mathrm{D}}^{\mathsf{T}}\mathrm{e}$ and $t_*(1) = 0$ or a combination, so t_*' is at least as smooth as $\bar{\mathrm{u}}$. Thus, the t_* term does not limit regularity. Also, since f_* has regularity comparable to that of $\bar{\mathrm{r}} = \mathbf{R}(\mathbf{D}(\bar{\mathrm{u}}))$, the regularity of $(f_* + \xi_*)$ is dominated by that of $\xi_* \in \Xi$.

Globally on $[0,1]$ we note from Theorem 4 that $\xi_* \in \Xi \subset [C([0,1] \to \mathbb{R}^3)]^*$, a space of vector Borel measures. Using (4.5) (and noting Remark 3 in case the measure ξ_* might have an atom at $s = 1$), we get the integral $z(\cdot)$ in BV so, as $\bar{\mathrm{D}}$ is at least in $\mathcal{Y}$, $\hat{\eta} = \mathbf{R}^*\xi_*$ is also in BV. Using (4.4) gives $\omega = \mathbf{K}^*\hat{\eta}$ satisfying $\omega' = \omega \times \bar{\mathrm{u}} - \hat{\eta}$ and we have seen that the regularity of $\bar{\mathrm{u}}$ matches that of $\omega = \mathbf{L}^*\xi_*$, hence gives $\bar{\mathrm{u}}'$ with the regularity of $\hat{\eta} \in BV$ as asserted.

This argument localizes as the differential equations involved can be restricted to any open set. In particular, the contact set is closed so its complement consists of open intervals and we have $\xi_* \equiv 0$ on each of these by Theorem 4. Thus, the same argument used above can there proceed indefinitely, subject only to the regularity of the constitutive functions W, F, to give an arbitrary level of differentiability for the restriction of $\bar{\mathrm{u}}$. □

Remark 5. *Observe that Theorem 4 has shown that, pointwise, these forces are orthogonal to the centerline and also, since they are orthogonal to constants, that the total internal force must vanish. These results and Theorem 7 are consistent* *with previous work by Schuricht and von der Mosel [**?**] on this problem with periodic boundary conditions.* $\square$

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