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## Global curvature and self-contact of nonlinearly elastic curves and rods

Received: 19 January 2001 / Accepted: 23 January 2001 /

Published online: 23 April 2001 – © Springer-Verlag 2001

**Abstract.** Many different physical systems, e.g. super-coiled DNA molecules, have been successfully modelled as elastic curves, ribbons or rods. We will describe all such systems as *framed curves*, and will consider problems in which a three dimensional framed curve has an associated energy that is to be minimized subject to the constraint of there being no self-intersection. For closed curves the knot type may therefore be specified a priori. Depending on the precise form of the energy and imposed boundary conditions, local minima of both open and closed framed curves often appear to involve regions of self-contact, that is, regions in which points that are distant along the curve are close in space. While this phenomenon of self-contact is familiar through every day experience with string, rope and wire, the idea is surprisingly difficult to define in a way that is simultaneously physically reasonable, mathematically precise, and analytically tractable. Here we use the notion of global radius of curvature of a space curve in a new formulation of the self-contact constraint, and exploit our formulation to derive existence results for minimizers, in the presence of self-contact, of a range of elastic energies that define various framed curve models. As a special case we establish the existence of *ideal shapes* of knots.

*Mathematics Subject Classification (2000):* 49J99, 53A04, 57M25, 74B20, 92C40

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### 1. Introduction

The basic question we address is the existence of curves that minimize one of a variety of prescribed elastic energies, all subject to the constraint that some tube surrounding the curve does not intersect itself. Elastic curves subject to this type of constraint provide a model for physical objects that exhibit self-contact, such as those illustrated in Fig. 1. Figure 1a is an image of a bacterium which appears to exhibit extended regions of self-contact between nearly helical segments and circular arcs. Figure 1b is an electron-micrograph of a DNA fragment which, after drying onto a planar substrate, exhibits a small overhand knot and regions of both

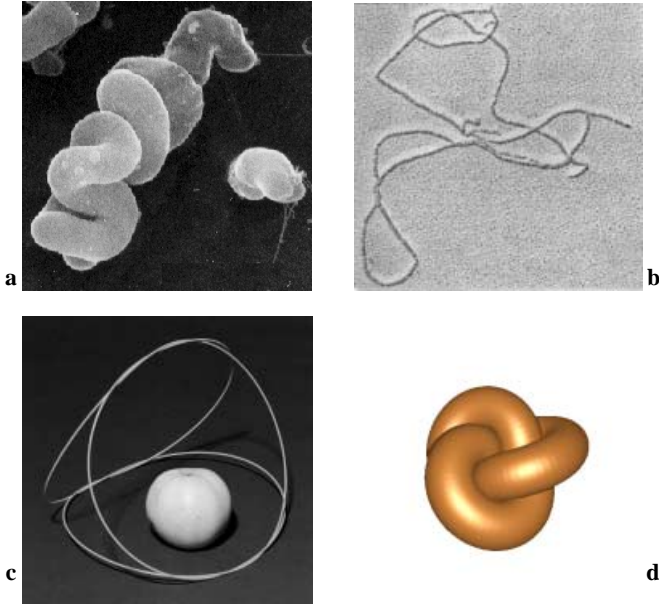
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**Fig. 1.** Images of four different physical systems exhibiting the phenomenon of self-contact of a tube-like object: **(a)** an image of the bacteria *B. subtilis* (courtesy of M.J. Tilby [28]), **(b)** an electron-micrograph of a DNA fragment (courtesy of A. Stasiak [27]), **(c)** a photograph of a knotted metal wire loop (actually a ‘Jumping Knot’ of J. Langer, with the apple included for scale and enhanced three-dimensionality), **(d)** a numerically computed *ideal* shape of a trefoil knot (image generated by smoothing data of [16]).

point and extended self-contact. Figure 1c is a photograph of a knotted metal wire loop which apparently exhibits three regions of line contact, and Fig. 1d illustrates a numerically computed *ideal shape* of a knotted closed loop which exhibits self-contact along its entire length (see Section 5 for further explanation of this problem). Perhaps the most familiar example of all is the tightly coiled, helical cord used on many telephones. The objective of this article is to develop a mathematically precise model of the phenomenon of self-contact of such tubular objects, which we describe as framed curves, and to use this characterization to demonstrate the existence of minimizers, in appropriate function spaces, for various elastic energies, all subject to our self-contact constraint.

For our purposes, the dominant feature in all four of the examples depicted in Fig. 1 is the phenomenon of self-contact of a physical object that has the geometrical properties of a tube. When such a tube is described by its centreline curve, points of self-contact on the tubular surface correspond to pairs of points along the centreline that are close in space, but not necessarily close in arclength. The condition that the tube not pass through itself, or self-intersect, is transferred to the centreline curve; in particular, the centreline is kept suitably far from self-intersection.

There are various ways to prevent a curve from self-intersecting. One intuitive mechanical approach is to introduce explicit repulsive forces between pairs of points along the curve; for example, a repulsive force which is inversely proportional to

some power of the pairwise Euclidean distance. Such forces certainly discourage self-intersection, and can even be made to prevent it, but they typically need to be regularized in some way to account for points immediately adjacent in arc-length. The necessity for this regularization can lead to non-trivial mathematical and computational difficulties (see for example [10], [22], [31]). Natural choices for repulsive forces may be available depending on the detailed physics of the system, for example electrically charged polymers such as DNA, and the study of discretized curves subject to these types of forces has been the subject of several investigations (see for example [24], [32]).

An alternative, purely geometrical, way to prohibit self-intersections of a curve can also be considered. Supposing that the curve is the centreline of a solid tube of uniform diameter, the physical volume occupied by the tube material keeps the curve from self-intersecting at a global level, and also restricts how tightly the curve can bend at a local level. Such a model certainly seems pertinent for the macroscopic wire example illustrated in Fig. 1c, where the hard surface of the wire touches itself. For the bacterium shown in Fig. 1a it is possible to imagine that both the local and global effects of self-avoidance are active at different places. In this viewpoint the obstruction to self-intersection is purely geometrical; the finite volume of the tube imposes a constraint on the configuration of the centreline curve. This condition is typically referred to as an excluded volume, hardcore or steric constraint in the polymer physics literature; the estimation of its effects on the statistical properties of polymer chains is a classic problem that has been studied within the context of piece-wise linear chain models [8]. Various forms of a geometric excluded volume constraint have also been used specifically in the mechanical modelling of DNA, for example [4], [6], [29]. The geometrical notion of self-avoidance also lies at the heart of the study of ideal shapes of knotted curves as discussed for example in [2], [16] and [21].

In this article we present a new mathematical characterization of the geometric excluded volume constraint, and study the set of admissible curves that it defines. Moreover, we prove the existence of minimizers within our admissible set for a range of curve energies pertinent to modelling physical systems such as those illustrated in Fig. 1. Such existence results are of independent mathematical interest, but in addition they indicate that a particular mathematical formulation of a physical model is well-posed, and they also contribute to the efficient design of associated numerical algorithms by providing *a priori* information on the regularity of the solutions that are being sought.

While the geometric excluded volume constraint is physically appealing and intuitively clear, it is surprisingly difficult to formulate in an analytic way that is sufficiently tractable for existence studies. We believe the concept from differential geometry of normal injectivity radius (see, for example, [7, p. 271]) to be the only prior, precise definition of the self-avoidance condition for curves that have not been discretized in some way. Both the global and local properties of the excluded volume constraint are captured in the idea of the normal injectivity radius, which can be outlined as follows. At each point along a sufficiently smooth curve  $\gamma$  one constructs a circle in the normal plane to the curve, centred on the curve and of constant radius along the curve. For a sufficiently small radius, the tubular envelope

of these circles will be smooth. The normal injectivity radius, here denoted  $\text{Inj}[\gamma]$ , is then the smallest radius at which the envelope develops a singularity. The first singularity may be local, when the radius of the circle equals the local radius of curvature of the curve, or non-local, when two circles centred on non-adjacent points touch.

For a physical tube of uniform radius  $\theta > 0$ , the excluded volume constraint on its centreline  $\gamma$  can then be expressed as the lower bound  $\text{Inj}[\gamma] \geq \theta$ . That is, the normal injectivity radius of the centreline must be at least as large as the radius of the tube, and equality is achieved when the tube is in self-contact, or is locally bent as severely as allowed. For example, in Fig. 1c, the geometrical self-avoidance condition for a tube of uniform small radius seems to be an excellent physical approximation for modelling self-contact of the wire. In the configuration shown, the centreline satisfies  $\text{Inj}[\gamma] = \theta$  because the tube actually achieves self-contact at a number of distinct points. If the wire were to be mildly deformed so as to avoid self-contact, then the centreline would satisfy  $\text{Inj}[\gamma] > \theta$ , but then the configuration would presumably no longer minimize the elastic energy of bending and twisting of the wire.

For our objective of deriving existence results, the difficulty with the classic definition of normal injectivity radius is that it is implicit, i.e. only given through a geometrical construction, and it has no apparent, simple analytic representation. We therefore extend to a class of curves  $\gamma$  sufficiently large to obtain existence results, the observation of [12] that for sufficiently smooth curves  $\gamma$  the normal injectivity radius  $\text{Inj}[\gamma]$  can be given an alternative characterization in terms of a quantity called *global radius of curvature*. Our most general definition of global radius of curvature is deferred until Section 2, but the central ideas can be explained within the context of curves  $\gamma$  that are twice differentiable, and which have only transversal crossings (i.e. wherever the curve intersects itself the two tangent vectors are distinct). For such curves we define

$$\Delta[\gamma] := \inf_{\substack{x, y, z \in \gamma \\ x \neq y \neq z \neq x}} r(x, y, z) \quad (1)$$

where  $r(x, y, z)$  denotes the radius of the unique circle through the three distinct points  $x, y$  and  $z$ . Then it is straightforward to argue, as in [12], that the infimum in (1) corresponds to one of three cases: (i) In the limit, all three points in a minimizing sequence coalesce at a point  $\zeta$  at which the radius of curvature is minimal along the curve, the limiting circle is the osculating circle at  $\zeta$ , and  $\Delta[\gamma]$  is the radius of curvature at  $\zeta$ . (ii) In the limit, two points coalesce to a point  $\zeta_1$  with the third converging to a different point  $\zeta_2$ , and the circle is tangent to the curve at both  $\zeta_1$  and  $\zeta_2$ , with both tangents orthogonal to the chord  $\zeta_1 - \zeta_2$ . In other words,  $\Delta[\gamma]$  is half of the distance between a pair of points  $(\zeta_1, \zeta_2)$  of closest approach. This possibility of a pair of points of closest approach includes the case in which the curve  $\gamma$  has a transversal self-intersection, for then there is a sequence of circles whose radius approaches zero, i.e.  $\Delta[\gamma] = 0$ . (iii) Or, for open curves, there are various other possibilities involving an end-point. Given these remarks it is then apparent that, neglecting any end-point effects,  $\Delta[\gamma] = \text{Inj}[\gamma]$ . In particular, cases

(i) and (ii) are just the two possible ways, local and global, in which the normal injectivity radius can be achieved.

In fact for each point  $x \in \gamma$  we may define the *global radius of curvature* function

$$\rho_G(x) = \inf_{\substack{y, z \in \gamma \\ x \neq y \neq z \neq x}} r(x, y, z). \quad (2)$$

Then the contact set can be interpreted as points  $x$  at which the global radius of curvature achieves its minimal value, i.e. the infimum defined in (1). For example, in Fig. 1d, (a numerical discretization of) a tube of uniform radius and prescribed knot type has been made as short as possible, that is, the knot has been made very tight. Such a configuration is called an *ideal shape* of the knot [16]; a mathematically precise, defining property is that the arclength of the centreline  $\gamma$  is minimal amongst curves of the prescribed knot type when subject to the excluded volume constraint  $\Delta[\gamma] \geq \theta$ . In Fig. 1d the tube is (up to computational tolerance) everywhere in self-contact, so that the global radius of curvature is constant, which satisfies a necessary condition for ideality derived in [12]. (The numerics indicate that the usual *local* radius of curvature on this ideal shape is far from being constant.)

One of the main objectives of the present article is to extend appropriately the definitions (1) and (2) to curves  $\gamma$  that are not *a priori* smooth, and thereby to obtain an analytic characterization of normal injectivity radius in a manner that is largely independent of curve regularity. This objective is achieved in Section 2. More precisely, working in the space of closed curves  $\gamma$  with a parameterization in  $W^{1,q}$  ( $q \geq 1$ ) we find that the constraint

$$\Delta[\gamma] \geq \theta > 0 \quad (3)$$

actually implies the existence of an arclength parameterization in  $W^{2,\infty}$  (or equivalently  $C^{1,1}$ ) for  $\gamma$ , and that the set of curves satisfying (3) is closed under weak convergence in  $W^{1,q}$  ( $q > 1$ ). Consequently, by standard direct methods we obtain existence of constrained minimizers for a variety of physically pertinent energies, including those arising in the usual elastic rod theories, and the integral of squared curvature on curves of prescribed arclength. Moreover, for closed curves in the set (3), knot types (along with a prescribed link in the case of framed curves) are also preserved under weak convergence, which implies existence of constrained minimizers for each type.

The presentation is structured as follows. In Section 2 we define global radius of curvature precisely, and develop properties of the constraint set (3) as discussed above. In Section 3 we introduce the concept of a framed curve and establish an abstract existence theorem for minimizers of a general class of energy functions defined on framed curves lying in weakly closed sets. This result can be applied to many models involving elastic strings and rods because we show that link classes and typical boundary conditions for framed curves are weakly closed. In Sections 4 and 5 we specialize the general result to some particular models and boundary conditions. In Section 4 we consider the closed configurations of a wide class of elastic rods, that, for example, provide a model of the system illustrated in Fig. 1c. Specifically, we establish the existence of constrained minimizers of the elastic

energy within each prescribed knot and link class. In Section 5 we consider the ideal knot problem underlying Fig. 1d, and establish the existence of  $C^{1,1}$  curves minimizing arclength within each knot class subject to the constraint (3). Proofs of all of our results are deferred, without further comment, until Section 6.

## 2. Global curvature and weak closure

Here we introduce for a rather general space curve  $\gamma$  the global radius of curvature functions  $\rho_G$  and  $\Delta$ , and the tubular neighbourhood  $B_\theta$  of radius  $\theta > 0$ . We study various implications of the constraint  $\Delta[\gamma] \geq \theta$  and show that it provides a geometrically exact model for the excluded volume constraint on  $\gamma$  imposed by  $B_\theta$  when considered as a material tube. To avoid discussion of many special cases associated with end-points, we consider only closed curves. However, many of the results carry over to the open case. As some of the arguments justifying our claims are quite lengthy, we present here a detailed development and explanation of our conclusions, but all proofs are deferred to Section 6.

### 2.1. Preliminaries

Throughout our developments we consider the set  $\mathcal{G}$  of continuous closed curves  $\gamma : \bar{I} \rightarrow \mathbb{R}^3$  that possess a Lipschitz continuous arclength parameterization  $\Gamma_\gamma : S_L \rightarrow \mathbb{R}^3$ . Here  $I = (a, b)$  is an interval,  $L \geq 0$  denotes the length of  $\gamma$  and  $S_L$  is the circle with perimeter  $L$ ; in particular,  $S_L \cong \mathbb{R}/(L \cdot \mathbb{Z})$ . To simplify notation, we mostly omit the subscript  $\gamma$  and agree that  $\Gamma, \Gamma_k, \tilde{\Gamma}$  correspond to  $\gamma, \gamma_k, \tilde{\gamma}$  and so on. In our analysis we will also consider the Sobolev spaces  $W^{1,q}(I, \mathbb{R}^3)$  with  $q \geq 1$ , and we note that closed curves in these spaces are also in  $\mathcal{G}$ . In particular, every curve  $\gamma \in W^{1,q}(I, \mathbb{R}^3)$  has bounded variation and one can find a Lipschitz continuous arclength parameterization (see [11, vol.II, p. 255]).

A curve  $\gamma \in \mathcal{G}$  will be called *simple* if it has no self-intersections, that is, if its arclength parameterization  $\Gamma : S_L \rightarrow \mathbb{R}^3$  is injective. Otherwise, the curve  $\gamma$  will be called *non-simple*. In this case there exist pairs  $s, t \in S_L$  ( $s \neq t$ ) for which  $\Gamma(s) = \Gamma(t)$ . Any such pair will be called a *double point* of  $\gamma$ .

We use  $\langle \cdot, \cdot \rangle$  to denote the standard Euclidean inner product in  $\mathbb{R}^3$ , and  $|\cdot|$  to denote the (intrinsic) distance between two points in  $\mathbb{R}^3$  or  $S_L$  depending on the context. To denote the angle between two non-zero vectors  $u$  and  $v$  in  $\mathbb{R}^3$  we use  $\angle(u, v) \in [0, \pi]$ . The distance between a point  $x \in \mathbb{R}^3$  and a subset  $\Sigma \subset \mathbb{R}^3$  will be denoted by  $\text{dist}(x, \Sigma)$  and the diameter of  $\Sigma$  will be denoted by  $\text{diam}(\Sigma)$ . For any  $r > 0$  we define open neighbourhoods of  $x$  and  $\Sigma$  by

$$B_r(x) = \{y \in \mathbb{R}^3 \mid |y - x| < r\} \quad \text{and} \quad B_r(\Sigma) = \{y \in \mathbb{R}^3 \mid \text{dist}(y, \Sigma) < r\}.$$

When  $\Sigma$  is the image of a curve  $\gamma \in \mathcal{G}$ , or equivalently its corresponding arclength parameterization  $\Gamma : S_L \rightarrow \mathbb{R}^3$ , we call  $B_r(\Sigma) = B_r(\Gamma(S_L))$  the *tubular neighbourhood* of  $\gamma$  with radius  $r > 0$ . We say that  $B_r(\Gamma(S_L))$  is *non-self-intersecting* or *regular* if the closest-point projection map  $\Pi_\Gamma : B_r(\Gamma(S_L)) \rightarrow \Gamma(S_L)$  is single-valued and continuous. That is to say, for any  $x \in B_r(\Gamma(S_L))$  there is exactly one  $s(x) \in S_L$  such that  $\Pi_\Gamma(x) := \Gamma(s(x))$  satisfies

$$\text{dist}(x, \Gamma(S_L)) = |\Gamma(s(x)) - x|,$$

and  $\Pi_\Gamma(x)$  is a continuous function of  $x \in B_r(\Gamma(S_L))$ . For further justification of this notion of non-self-intersecting see the discussion following Lemmas 3 and 7.

## 2.2. Global radius of curvature functions

Motivated by, but also modifying, the analysis presented in [12], we define the global radius of curvature functions  $\rho_G$  and  $\Delta$  for space curves  $\gamma$  as follows.

**Definition 1.** Consider a curve  $\gamma \in \mathcal{G}$  with arclength parameterization  $\Gamma(s)$ ,  $s \in S_L$ . Then the global radius of curvature of  $\gamma$  at the point  $\Gamma(s)$  is given by

$$\rho_G[\gamma](s) := \begin{cases} \inf\{R(\Gamma(s), \Gamma(\sigma), \Gamma(\tau)) \mid \sigma, \tau \in S_L \setminus \{s\}, \sigma \neq \tau\}, & \text{if } L > 0, \\ 0, & \text{if } L = 0, \end{cases} \quad (4)$$

and we denote its infimum by

$$\Delta[\gamma] := \inf_{s \in S_L} \rho_G[\gamma](s). \quad (5)$$

Here  $R(x, y, z) \geq 0$  is the radius of the *smallest* circle containing  $x, y$  and  $z$ . When  $x, y$  and  $z$  are non-collinear (and thus distinct) there is a unique circle passing through them and

$$R(x, y, z) = \frac{|x - y|}{|2 \sin[\angle(x - z, y - z)]|}. \quad (6)$$

When  $x, y$  and  $z$  are collinear and distinct there is no circle passing through all three points and we define  $R(x, y, z)$  to be infinite, but if two points coincide, say  $x = z$  or  $y = z$ , then there are many circles through the three points and we take  $R(x, y, z)$  to be the smallest possible radius namely the distance  $|x - y|/2$ . With this choice the function  $R(x, y, z)$  is not continuous at coincident arguments. Notice nevertheless that, by definition,  $R(x, y, z)$  is symmetric in its arguments.

The difference between the global radius of curvature function  $\rho_G[\gamma]$  introduced in [12] and the one presented above is as follows. In [12], the function  $R(x, y, z)$  is considered directly only for distinct points  $x, y$  and  $z$  in the image of  $\gamma$ , and the various coalescent cases are considered as limits as the points move along the image of  $\gamma$ . Then in the case of smooth curves that are either simple or have only transversal crossings,  $R(x, y, z)$  is well-defined and continuous in any of the limits  $x \rightarrow y$  etc., because the direction of approach along the curve singles out a unique limiting value of  $R(x, y, z)$ . However, the case of parameterized curves with double-covered regions is problematic. For example, in the definition of [12], a single-covered and a double-covered circle of radius one each have a global radius of curvature one everywhere. In contrast, in Definition 1 above, the infimum is over distinct arclength parameters  $s, \sigma$  and  $\tau$  in  $S_L$  and  $y(\sigma) = z(\tau)$  is an allowed competitor provided  $\sigma \neq \tau$ . Then a double-covered circle of radius one has a global radius of curvature zero everywhere (while a single-covered circle still has global radius of curvature one everywhere). In particular, with Definition 1 we have the following

**Lemma 1.** *If  $\gamma$  has a double point at the pair  $s, t \in S_L$  ( $s \neq t$ ), then  $\rho_G[\gamma](s) = \rho_G[\gamma](t) = 0$ . If  $\Delta[\gamma] > 0$ , then  $\gamma$  is simple.*

When a closed curve  $\gamma$  is both smooth and simple, the functions  $\rho_G[\gamma]$  and  $\Delta[\gamma]$  are known to be related to the standard local radius of curvature  $\rho[\gamma]$ , and to the thickness or normal injectivity radius  $\text{Inj}[\gamma]$  of  $\gamma$  as defined, for example, in [2] and [7, p. 271]. In particular, one has  $0 \leq \rho_G[\gamma](s) \leq \rho[\gamma](s)$  for all  $s \in S_L$  ( $L > 0$ ) and  $\Delta[\gamma] = \text{Inj}[\gamma]$ , [12]. In this case  $\Delta[\gamma] > 0$  is the radius of the thickest smooth tube that can be centred on  $\gamma$  as discussed in Section 1. In the following developments we generalize this result to the case where  $\gamma$  may be non-smooth.

### 2.3. Regularity results

Here we examine various implications of the condition  $\Delta[\gamma] \geq \theta > 0$  where  $\theta$  is a given constant. Our first result is:

**Lemma 2.** <sup>1</sup> *Let  $\gamma \in \mathcal{G}$  and  $\Delta[\gamma] \geq \theta > 0$  for some constant  $\theta$ . Then the corresponding arclength parameterization  $\Gamma$  has a Lipschitz continuous tangent  $\Gamma'$  with Lipschitz constant  $\theta^{-1}$ , i.e.,  $\Gamma \in C^{1,1}(S_L, \mathbb{R}^3)$  and*

$$|\Gamma'(s_1) - \Gamma'(s_2)| \leq \theta^{-1}|s_1 - s_2| \quad \forall s_1, s_2 \in S_L. \quad (7)$$

Thus a positive lower bound on  $\Delta[\gamma]$  imposes a certain amount of regularity on the curve  $\gamma$ . In particular, while an arbitrary curve  $\gamma \in \mathcal{G}$  may not even admit a continuous unit tangent field, those curves satisfying  $\Delta[\gamma] \geq \theta > 0$  are guaranteed to admit a Lipschitz continuous unit tangent field. The existence of this field will play a central role in many of the following arguments.

Our second result establishes the fact that if a curve  $\gamma \in \mathcal{G}$  satisfies  $\Delta[\gamma] \geq \theta > 0$ , then  $\gamma$  is restricted on how tightly it can bend locally, and on how close it can come to self-intersection globally.

**Lemma 3.** *Consider  $\gamma \in \mathcal{G}$  such that  $\Delta[\gamma] > 0$  and let  $\Gamma \in C^{1,1}(S_L, \mathbb{R}^3)$  denote its corresponding arclength parameterization. For a given constant  $\theta > 0$  let  $D_\theta(z, z')$  denote the open planar disk of radius  $\theta$  centred at  $z \in \mathbb{R}^3$  perpendicular to  $z' \in \mathbb{R}^3 \setminus \{0\}$  and for any  $s_0 \in S_L$  let*

$$C(s_0, \theta) = \partial D_\theta(\Gamma(s_0), \Gamma'(s_0)) \quad \text{and} \quad M(s_0, \theta) = \bigcup_{z \in C(s_0, \theta)} B_\theta(z).$$

Then

- (i)  $\Gamma(S_L) \cap M(s_0, \theta) = \emptyset$  for all  $s_0 \in S_L$  iff  $\Delta[\gamma] \geq \theta$ ,
- (ii)  $\text{diam}(\Gamma(S_L)) \geq 2\theta$  if  $\Delta[\gamma] \geq \theta$ ,
- (iii)  $B_\theta(\Gamma(S_L))$  is regular iff  $\Delta[\gamma] \geq \theta$ ,
- (iv)  $\Pi_\Gamma$  has the property  $\Pi_\Gamma^{-1}(\Gamma(s_0)) \cap B_\theta(\Gamma(S_L)) = D_\theta(\Gamma(s_0), \Gamma'(s_0))$  if  $B_\theta(\Gamma(S_L))$  is regular.

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<sup>1</sup> We are grateful to T. Ilmanen who first suggested to us that a result of this nature should be available.



Item (i) of the above result implies that if  $\Delta[\gamma] \geq \theta$ , then an open ball of radius  $\theta$  placed tangent at any point  $\Gamma(s_0)$  may be rotated around the tangent vector  $\Gamma'(s_0)$  without intersecting the curve. On the other hand, if  $\Delta[\gamma] < \theta$ , then there is a point on the curve about which a similar rotation of such a ball could not be effected. Thus  $\Delta[\gamma]$  is the radius of the largest ball that can be rotated tangentially about every point of a curve  $\gamma$  without intersecting it. The proof of item (i) actually shows that a stronger, local version of this result holds; namely,  $\Gamma(S_L) \cap M(s_0, \rho_0) = \emptyset$  if  $\rho_0 := \rho_G[\gamma](s_0) > 0$ . The above interpretations also suggest that the inequality  $\Delta[\gamma] \geq \theta$  imposes a lower bound on the overall size of  $\gamma$ , which is the essence of item (ii).

Items (iii) and (iv) imply that the regularity of the tubular neighbourhood  $B_\theta(\Gamma(S_L))$  is equivalent to the condition  $\Delta[\gamma] \geq \theta$ , and that  $B_\theta(\Gamma(S_L))$  is the envelope of disjoint disks  $D_\theta(\Gamma(s_0), \Gamma'(s_0))$ . Since each point  $x \in B_\theta(\Gamma(S_L))$  is in a unique disk  $D_\theta(\Gamma(s_0), \Gamma'(s_0))$  normal to the curve, we deduce that  $B_\theta(\Gamma(S_L))$  has the structure of a uniform tube of radius  $\theta$  centred on  $\gamma$ . Moreover, according to item (iii), any tubular neighbourhood of radius larger than  $\Delta[\gamma]$  would fail to have this structure. Thus the condition  $\Delta[\gamma] \geq \theta$  provides a geometrically exact model for the excluded volume constraint on  $\gamma$  imposed by the tubular neighbourhood  $B_\theta(\Gamma(S_L))$  when considered as a material tube. This idea will be developed further in Section 3.

#### 2.4. Weak closedness results

Here we study various implications of the condition  $\Delta[\gamma] \geq \theta > 0$  for closed curves  $\gamma$  in the Sobolev spaces  $W^{1,q}(I, \mathbb{R}^3)$ ,  $q \in (1, \infty)$ . Notice that, because such curves are also in  $\mathcal{G}$ , a positive lower bound on  $\Delta[\gamma]$  retains its interpretation as an excluded volume constraint.

Our first result states that, as a subset of  $W^{1,q}(I, \mathbb{R}^3)$ , the set of closed curves satisfying  $\Delta[\gamma] \geq \theta > 0$  is weakly closed.

**Lemma 4.** *Let  $\{\gamma_n\} \subset W^{1,q}(I, \mathbb{R}^3)$ ,  $q \in (1, \infty)$ , be a sequence of closed curves such that  $\gamma_n \rightharpoonup \gamma \in W^{1,q}(I, \mathbb{R}^3)$  and*

$$\Delta[\gamma_n] \geq \theta, \quad \forall n \in \mathbb{N} \quad (8)$$

*for some constant  $\theta > 0$ . Then  $\gamma$  is a closed curve and*

$$\Delta[\gamma] \geq \theta. \quad (9)$$

This result will be particularly useful when studying energy functionals defined on closed curves in  $W^{1,q}(I, \mathbb{R}^3)$ . In particular, it suggests that standard direct methods may be used to establish the existence of constrained minimizers.

In our applications we will consider energy functionals defined on closed curves in a fixed isotopy class or knot type in the following sense.

**Definition 2.** *Two continuous closed curves  $K_1, K_2 \subset \mathbb{R}^3$  are isotopic, denoted as  $K_1 \simeq K_2$ , if there are open neighbourhoods  $N_1$  of  $K_1$ ,  $N_2$  of  $K_2$ , and a continuous mapping  $\Phi : N_1 \times [0, 1] \rightarrow \mathbb{R}^3$  such that  $\Phi(N_1, \tau)$  is homeomorphic to  $N_1$  for all  $\tau \in [0, 1]$ ,  $\Phi(x, 0) = x$  for all  $x \in N_1$ ,  $\Phi(N_1, 1) = N_2$ , and  $\Phi(K_1, 1) = K_2$ .*

Roughly speaking, two curves are in the same isotopy class if one can be continuously deformed onto the other. The next result states that, as a subset of  $W^{1,q}(I, \mathbb{R}^3)$ , the set of closed curves in any fixed isotopy class satisfying  $\Delta[\gamma] \geq \theta > 0$  is weakly closed.

**Lemma 5.** *Let the sequence  $\{\gamma_n\} \subset W^{1,q}(I, \mathbb{R}^3) \cap \mathcal{G}$ ,  $q \in (1, \infty)$ , satisfy*

- (i)  $\gamma_n(\bar{I}) \simeq \gamma_1(\bar{I}), \quad \forall n \in \mathbb{N},$
- (ii)  $\Delta[\gamma_n] \geq \theta > 0, \quad \forall n \in \mathbb{N},$
- (iii)  $\gamma_n \rightharpoonup \gamma \in W^{1,q}(I, \mathbb{R}^3) \quad \text{as } n \rightarrow \infty.$

*Then  $\gamma(\bar{I}) \simeq \gamma_1(\bar{I})$ .*

Thus, the excluded volume constraint  $\Delta[\gamma_n] \geq \theta > 0$  prevents a change in knot type along weakly convergent sequences. The construction of the isotopy map  $\Phi$  between  $\gamma$  and  $\gamma_n$  for  $n$  sufficiently large is based on the fact that the corresponding projection onto the image of  $\gamma_n$  restricted to  $\gamma$  is bijective. This result is important for the study of energy functionals defined on closed, knotted curves in  $W^{1,q}(I, \mathbb{R}^3)$ . In particular, it may be used to establish the existence of constrained minimizers among curves of a fixed knot type.

### 3. Framed curves and general existence result

Here we introduce the notion of a framed curve  $(\gamma, D)$ , where  $D$  is a field of orthonormal frames along a space curve  $\gamma$ , as a geometric model for physical objects such as those illustrated in Fig. 1. Then we discuss interpretations of the excluded volume constraint  $\Delta[\gamma] \geq \theta > 0$  and establish a general existence result concerning the minima of energy functionals defined on framed curves subject to this constraint. In Sections 4 and 5 we apply our result to models of elastic rods and strings, which can be interpreted as framed curves with particular energy functionals. Again proofs are deferred to Section 6.

#### 3.1. Preliminaries

By a *framed curve*  $(\gamma, D)$  we mean a curve  $\gamma : \bar{I} \rightarrow \mathbb{R}^3$  equipped with a frame field  $D : \bar{I} \rightarrow SO(3)$ , where  $D(s) = (d_1(s)|d_2(s)|d_3(s))$  consists of three orthonormal column-vectors  $d_i(s)$  ( $i = 1, 2, 3$ ) for each  $s \in \bar{I} = [a, b]$ . We view the function  $D$  as a frame field defined along  $\gamma$ . Thus, the right-handed orthonormal frame  $D(s)$  is attached to the point  $\gamma(s)$ . By a *closed framed curve* we mean a framed curve  $(\gamma, D)$  such that  $\gamma$  is closed and  $d_3(a) = d_3(b)$ . For our analysis we find it convenient to work with the Sobolev spaces  $W^{1,q}(I, \mathbb{R}^3)$  and  $W^{1,p}(I, \mathbb{R}^{3 \times 3})$  with  $q, p \geq 1$ , where  $\gamma \in W^{1,q}$  and  $D \in W^{1,p}$ . As before, closed curves in  $W^{1,q}$  are also in  $\mathcal{G}$ .

A framed curve  $(\gamma, D) \in W^{1,q} \times W^{1,p}$  may be uniquely determined from shape and placement variables  $w = (u, v, \gamma_0, D_0) \in X_0^{p,q}$  with  $u = (u_1, u_2, u_3)$

and  $v = (v_1, v_2, v_3)$  via the equations

$$\begin{aligned} d'_k(s) &= \left[ \sum_{i=1}^3 u_i(s) d_i(s) \right] \wedge d_k(s) \quad \text{for a.e. } s \in I, \quad k = 1, 2, 3, \\ \gamma'(s) &= \sum_{k=1}^3 v_k(s) d_k(s) \quad \text{for a.e. } s \in I, \\ \gamma(a) &= \gamma_0, \quad D(a) = D_0, \end{aligned} \tag{10}$$

where  $X_0^{p,q} := L^p(I, \mathbb{R}^3) \times L^q(I, \mathbb{R}^3) \times \mathbb{R}^3 \times SO(3)$ , which is a proper subset of the corresponding Banach space  $X^{p,q} := L^p(I, \mathbb{R}^3) \times L^q(I, \mathbb{R}^3) \times \mathbb{R}^3 \times \mathbb{R}^{3 \times 3}$ . The functions  $u_i$  and  $v_i$  may be identified as the components, in the moving frame  $\{d_i\}$ , of the Darboux vector for the frame field  $D(s)$  and the tangent vector for the curve  $\gamma(s)$ . Notice that  $u$  and  $v$  describe the shape of a framed curve whereas  $\gamma_0$  and  $D_0$  describe its spatial placement. The following result will be fundamental to our developments.

**Lemma 6.** *To each framed curve  $(\gamma, D) \in W^{1,q} \times W^{1,p}$ ,  $p, q \geq 1$ , we can associate a unique  $w = w(\gamma, D) \in X_0^{p,q}$  determined by (10). Conversely, to each  $w \in X_0^{p,q}$  we can associate a unique framed curve  $(\gamma, D) = (\gamma[w], D[w]) \in W^{1,q} \times W^{1,p}$  such that (10) holds.*

### 3.2. Interpreting the excluded volume constraint

There are generally two distinct tubes that can be associated with a closed framed curve  $(\gamma, D)$  and a constant  $\theta > 0$ . One tube is defined by the neighbourhood  $B_\theta(\Gamma(S_L))$  as considered in Section 2. Another tube is defined by  $p(\Omega_\theta)$ , where  $p : \Omega_\theta \rightarrow \mathbb{R}^3$  is the map

$$p(\sigma, \xi_1, \xi_2) = \gamma(\sigma) + \xi_1 d_1(\sigma) + \xi_2 d_2(\sigma) \tag{11}$$

and  $\Omega_\theta$  is the straight cylinder given by

$$\Omega_\theta := \{ (\sigma, \xi_1, \xi_2) \in \mathbb{R}^3 \mid \sigma \in [a, b), \quad \xi_1^2 + \xi_2^2 < \theta^2 \}.$$

The excluded volume constraint  $\Delta[\gamma] \geq \theta$  prevents the tube  $B_\theta(\Gamma(S_L))$  from self-intersecting. However, as a model for a physical object, it is the points of  $p(\Omega_\theta)$  that are naturally identified with material points, and the excluded volume constraint should guarantee the global injectivity of the mapping  $p : \Omega_\theta \rightarrow \mathbb{R}^3$ . Along these lines we have the following

**Lemma 7.** *Consider a closed framed curve  $(\gamma, D) \in W^{1,q} \times W^{1,p}$ ,  $p, q \geq 1$ , and let  $w = (u, v, \gamma_0, D_0) \in X_0^{p,q}$  be its shape and placement variables determined by (10). Suppose that  $\Delta[\gamma] > 0$  and  $v = (0, 0, v_3)$  with  $v_3 > 0$ . Then  $p : \Omega_\theta \rightarrow \mathbb{R}^3$  is globally injective iff  $\Delta[\gamma] \geq \theta > 0$ .*

The condition  $v = (0, 0, v_3)$  with  $v_3 > 0$  implies that the frame field  $D$  is adapted to  $\gamma$  in the sense that  $d_3(s)$  is (positively) parallel to  $\gamma'(s)$ . In this case,  $p(\Omega_\theta)$  may be identified with  $B_\theta(\Gamma(S_L))$  and the result follows from the regularity of  $B_\theta(\Gamma(S_L))$  as discussed in Section 2. Thus, when  $v = (0, 0, v_3)$  with  $v_3 > 0$ , the condition  $\Delta[\gamma] \geq \theta > 0$  provides an exact excluded volume constraint for the material tube  $p(\Omega_\theta)$ . When  $v$  is not of this form, the condition  $\Delta[\gamma] \geq \theta > 0$  is not an exact excluded volume constraint for  $p(\Omega_\theta)$ . Notice that  $p(\Omega_\theta)$  itself is not a uniform tube of radius  $\theta$  if  $v_1$  or  $v_2$  is non-zero.

### 3.3. Energy functionals and existence of minimizers

For framed curves  $(\gamma, D) = (\gamma[w], D[w])$  with  $w \in X_0^{p,q}$  we consider energy functionals of the form

$$E(\gamma[w], D[w]) = E(w) := \int_I W(u(s), v(s), s) ds \quad (12)$$

where  $W : \mathbb{R}^3 \times \mathbb{R}^3 \times I \rightarrow \mathbb{R} \cup \{\infty\}$  is a specified function. The basic question we shall address is the existence of framed curves  $(\gamma, D)$  that minimize  $E(w)$  subject to the excluded volume constraint  $\Delta[\gamma] \geq \theta > 0$  and other more typical side conditions, such as boundary conditions etc. In particular, we consider the problem of finding  $w_* \in C \subset X_0^{p,q}$  that satisfy

$$E(w_*) = \inf_{w \in C} E(w) \quad (13)$$

where  $C$  is a specified subset of  $X_0^{p,q}$ . Our main result is contained in the following

**Theorem 1.** *Let  $1 < p, q < \infty$  and suppose that*

- (W1)  $W(\cdot, \cdot, s)$  is continuous and convex for a.e.  $s \in I$ ,
- (W2)  $W(u, v, \cdot)$  is Lebesgue-measurable on  $I$  for all  $(u, v) \in \mathbb{R}^3 \times \mathbb{R}^3$ ,
- (W3) there are constants  $c_1, c_2 \geq 0$  and a function  $g \in L^1(I)$ , such that

$$W(u, v, s) \geq c_1|u|^p + c_2|v|^q + g(s)$$

for all  $(u, v) \in \mathbb{R}^3 \times \mathbb{R}^3$  and for a.e.  $s \in I$ .

Furthermore, assume that the set  $C \subset X_0^{p,q}$  is nonempty and weakly closed in  $X^{p,q}$  and that there is some constant  $c \geq 0$  such that  $|\gamma_0| \leq c$  for all  $(u, v, \gamma_0, D_0) \in C$ . Then there is a minimizer  $w_* \in C$  of (13) if one of the following conditions holds:

- (i)  $c_1, c_2 > 0$ ,
- (ii)  $c_1 > 0$ , and there is some  $\hat{v} \in \mathbb{R}^3$  such that  $v \equiv \hat{v}$  for all  $w = (u, v, \gamma_0, D_0) \in C$ ,
- (iii)  $c_2 > 0$  and there is some  $\hat{u} \in \mathbb{R}^3$  such that  $u \equiv \hat{u}$  for all  $w = (u, v, \gamma_0, D_0) \in C$ .

Assumptions (W1)-(W3) are standard for direct methods in the calculus of variations, and are met by a wide class of functions  $W$  that arise in applications. Thus, the above result reduces the existence problem to proving the weak closedness in  $X^{p,q}$  of the subset  $C \subset X_0^{p,q} \subset X^{p,q}$ . Here  $C$  represents those framed curves that satisfy the constraint  $\Delta[\gamma] \geq \theta > 0$  along with any other prescribed side conditions. We remark that this general existence result remains valid when a potential energy with at most linear growth is added to the energy functional  $E(w)$ .

### 3.4. Typical side conditions and weak closedness

Here we examine the weak closedness of typical side conditions that enter into the subset  $C$  of Theorem 1. Our main result in this direction is:

**Lemma 8.** *Let  $1 < p, q < \infty$  and consider a sequence  $\{w_n\} \subset X_0^{p,q}$  that converges weakly to  $w \in X^{p,q}$ , i.e.,  $w_n \rightharpoonup w$  in  $X^{p,q}$ . Then  $w \in X_0^{p,q}$  and*

$$D_n \rightarrow D \text{ in } C^0(\bar{I}, \mathbb{R}^{3 \times 3}), \quad \gamma_n \rightarrow \gamma \text{ in } C^0(\bar{I}, \mathbb{R}^3), \quad (14)$$

$$D_n \rightharpoonup D \text{ in } W^{1,p}(I, \mathbb{R}^{3 \times 3}), \quad \gamma_n \rightharpoonup \gamma \text{ in } W^{1,q}(I, \mathbb{R}^3), \quad (15)$$

where  $\gamma_n := \gamma[w_n]$ ,  $\gamma := \gamma[w]$ ,  $D_n := D[w_n]$ ,  $D := D[w]$ .

Thus, if a sequence of shape and placement variables  $w_n$  converges weakly in  $X^{p,q}$ , then the corresponding sequence of framed curves  $(\gamma_n, D_n)$  converges uniformly in  $C^0 \times C^0$ , and also weakly in  $W^{1,q} \times W^{1,p}$ .

We can now provide two prototypes of weakly closed sets that will be useful in our applications.

**Lemma 9.** *Let  $K(s) \subset \mathbb{R}^3 \times \mathbb{R}^3$  be a closed convex set for a.e.  $s \in I$  and let  $F : C^0(\bar{I}, \mathbb{R}^3) \times C^0(\bar{I}, \mathbb{R}^{3 \times 3}) \rightarrow \mathbb{R}$  be a continuous mapping. Then the sets*

$$(i) \quad C_1 := \{ (u, v, \gamma_0, D_0) \in X^{p,q} \mid (u(s), v(s)) \in K(s) \text{ for a.e. } s \in I \}$$

$$(ii) \quad C_2 := \{ w \in X_0^{p,q} \mid F(\gamma[w], D[w]) = 0 \}$$

are weakly closed in  $X^{p,q}$  ( $p, q > 1$ ).

The sets  $C_1$  and  $C_2$  are typical in applications involving elastic rods and strings as will be considered in Sections 4 and 5. Sets of the type  $C_1$  may be considered within the context of rods to ensure that contiguous cross-sections do not locally intersect each other and that orientation is locally preserved under deformation (see [1, Ch. VIII.6]). Sets of type  $C_2$  may be considered to prescribe pointwise conditions on both rods and strings, e.g., boundary conditions for  $\gamma$  and  $D$ . For example, we will consider framed curves where  $\gamma$  is closed and the frames  $D(a)$  and  $D(b)$  differ by a prescribed rotation. Notice that the above result remains valid if the equality in the definition of  $C_2$  is replaced by an inequality. Sets of this type arise in problems with rigid obstacles, where the material tube  $p(\Omega_\theta)$  is constrained to lie in a closed region of  $\mathbb{R}^3$ , and in problems with unilateral boundary conditions. Such obstacle problems for Cosserat rods are studied in [25],[26].

Fixing the endpoint conditions for the frame  $D$ , for example specifying  $D(a) = D(b) = D_0$ , does not entirely determine the total amount of twist or link. In fact,

any framed curve  $(\gamma, D)$  whose frame  $D$  turns an integer multiple of  $2\pi$  about the curve  $\gamma$  satisfies the above boundary condition. In order to identify link classes of framed curves we make the following

**Definition 3.** Two continuous mappings  $D_1, D_2 : [a, b] \rightarrow SO(3)$  with  $D_1(a) = D_2(a)$  and  $D_1(b) = D_2(b)$  are called homotopic, denoted  $D_1 \sim D_2$ , if there is a continuous mapping  $\Psi : [a, b] \times [0, 1] \rightarrow SO(3)$ , such that

$$\begin{aligned} \Psi(\cdot, 0) &= D_1(\cdot) \quad \text{and} \quad \Psi(\cdot, 1) = D_2(\cdot) \quad \text{on} \quad [a, b], \\ \Psi(a, \cdot) &= D_1(a) \quad \text{and} \quad \Psi(b, \cdot) = D_1(b) \quad \text{on} \quad [0, 1]. \end{aligned}$$

Roughly speaking, two frame fields  $D_1$  and  $D_2$  are homotopic if for a given curve  $\gamma$ , the framed curves  $(\gamma, D_1)$  and  $(\gamma, D_2)$  generate ribbons with the same link. The next result states that the set of frame fields in any fixed homotopy class define weakly closed subsets.

**Lemma 10.** Let  $\{w_n\} \subset X_0^{p,q}$  with  $w_n \rightarrow w$  in  $X^{p,q}$  ( $p, q > 1$ ) and assume that

$$D_n := D[w_n] \sim D[w_1], \quad \forall n \in \mathbb{N}. \quad (16)$$

Then  $w \in X_0^{p,q}$  and  $D := D[w] \sim D[w_1]$ .

Thus, for rods and ribbons one can expect to find elastic energy minimizers in each link class. The construction of the homotopy map between  $D$  and  $D_1$  is based on the fact that elements close to the identity in  $SO(3)$  can be represented by rotation vectors.

## 4. Applications to elastic rods

### 4.1. Rod theory

In this section we outline the special Cosserat theory which describes the behaviour of elastic rods that can undergo large deformations in space by suffering flexure, torsion, extension and shear. For a more comprehensive presentation see, for example, Antman [1, Ch. VIII].

**4.1.1. Kinematics** We suppose that each configuration of an elastic rod can be modelled by a framed curve  $(\gamma, D) \in W^{1,1} \times W^{1,1}$  together with a map  $p : \Omega_\theta \rightarrow \mathbb{R}^3$  as defined in Section 3. In particular, we identify the material rod with the tube  $p(\Omega_\theta)$ . Under this identification the curve  $\gamma(\sigma)$  describes the rod centreline and the frame field  $D(\sigma)$  describes the orientation of the rod cross-sections. The cross-section attached to a point  $\gamma(\sigma)$  on the centreline is spanned by  $\{d_1(\sigma), d_2(\sigma)\}$  and is parameterized by  $(\xi_1, \xi_2)$ . Thus, the particular form of  $\Omega_\theta$  given in Section 3 models a rod with circular cross-sections of radius  $\theta$ . Notice that cross-sections are not necessarily always orthogonal to the centreline  $\gamma$  (which means that the rod can be sheared), and that  $\sigma$  is not necessarily the arclength parameter for  $\gamma$  (which means that the rod can be stretched or compressed).

By Lemma 6, a framed curve  $(\gamma, D) \in W^{1,1} \times W^{1,1}$  can be uniquely identified with a set of shape and placement variables  $(u, v, \gamma_0, D_0) \in X_0^{1,1}$ . Energy functionals for rods can naturally be expressed in terms of the functions  $u = (u_1, u_2, u_3)$

and  $v = (v_1, v_2, v_3)$ , which are typically referred to as *strains* within the context of rod theory. Recall that  $u_i$  and  $v_i$  are the components, in the moving frame  $\{d_i\}$ , of the Darboux vector for the frame field  $D(s)$  and the tangent vector for the curve  $\gamma(s)$ .

We denote a relaxed, or stress-free, *reference configuration* by  $(\hat{\gamma}, \hat{D})$  or  $(\hat{u}, \hat{v}, \gamma_0, D_0)$ , where the functions  $(\hat{u}, \hat{v})$  are prescribed material parameters. There is little loss of generality in assuming, by convention, that  $\sigma$  is actually the arclength parameter for this reference centreline  $\hat{\gamma}$ , and moreover that cross-sections in this reference configuration are orthogonal to  $\hat{\gamma}$ , so that  $\hat{v} := (0, 0, 1)$ . Nevertheless notice that  $\hat{\gamma}$  need not be a straight line, because  $\hat{u}$  need not be zero.

It is reasonable to demand that the map  $p : \Omega_\theta \rightarrow \mathbb{R}^3$  describing a material rod be globally injective. Indeed, this is the essence of the self-contact or excluded volume constraint studied in this article. Necessary and sufficient conditions for global injectivity are given in Lemma 7 for a particular class of deformations. It is also reasonable to demand that the map  $p$  preserve orientation in the sense that

$$\det \left[ \frac{\partial p(\sigma, \xi_1, \xi_2)}{\partial (\sigma, \xi_1, \xi_2)} \right] > 0 \quad \text{for a.e. } (\sigma, \xi_1, \xi_2) \in \Omega_\theta, \quad (17)$$

which actually guarantees that  $p$  is locally (but not globally) injective. Because of the specific form of our domain  $\Omega_\theta$ , we deduce that (17) is equivalent to the following set of conditions on the strains:

$$v_3 > 0 \quad \text{and} \quad v_3 \geq \theta \sqrt{u_1^2 + u_2^2} \quad \text{a.e. on } I \quad (18)$$

(see Antman [1, Ch. VIII.6] for related conditions pertaining to more general domains). Below we discuss how these local conditions are related to the conditions in Lemma 7. Notice that (18) is often replaced by the single necessary condition

$$v_3 > 0 \quad \text{a.e. on } I. \quad (19)$$

**4.1.2. Constitutive models** We consider elastic rods whose material response can be described by a *stored energy density* function  $W$ , depending on  $(u, v, \sigma)$ , that is convex in  $(u, v)$  and which satisfies certain growth conditions as discussed in Section 3. The *total elastic energy* of the rod is given by

$$E(u, v) := \int_I W(u(\sigma), v(\sigma), \sigma) d\sigma.$$

An explicit dependence on  $\sigma$  in the energy density  $W$  occurs naturally in the case of inhomogeneous elastic rods, where material properties may vary from one cross-section to another.

The special case where  $W$  is a (shifted) quadratic in  $(u, v)$  plays an important role in various applications:

$$W(u, v, \sigma) = \left\langle A(\sigma) \begin{pmatrix} u - \hat{u} \\ v - \hat{v} \end{pmatrix}, \begin{pmatrix} u - \hat{u} \\ v - \hat{v} \end{pmatrix} \right\rangle, \quad (20)$$

where  $A : I \rightarrow \mathbb{R}^{6 \times 6}$  is a Lebesgue measurable function such that  $A(\sigma)$  is symmetric, positive definite for a.e.  $\sigma \in I$ , and  $(\hat{u}(\sigma), \hat{v}(\sigma))$  are the reference strains defined above.

The particular case of *unshearable* rods is defined by the material constraint  $v := (\hat{v}_1, \hat{v}_2, v_3) := (0, 0, v_3)$ , i.e. the first two components of  $v$  are required to always take their reference values. Thus the stored energy density  $W$  no longer depends upon  $v_1$  and  $v_2$ . Notice that the constraint  $v := (0, 0, v_3)$  together with (10) implies  $\gamma' = v_3 d_3$ , and that  $\gamma''$  generally does not exist even in the weak sense for  $v_3 \in L^1$ . However, when the conditions in (18) are satisfied, we find that the corresponding arclength parameterization  $\Gamma$  possesses the weak derivative  $\Gamma'' = (u_2 d_1 - u_1 d_2)/v_3$ , which implies that the curvature  $\kappa$  of  $\gamma$  is given by

$$\kappa = |\Gamma''| = \frac{\sqrt{u_1^2 + u_2^2}}{v_3} \quad (21)$$

(see Section 6.3 for details). Hence, for unshearable rods, the conditions in (18) may be written as

$$v_3 > 0 \quad \text{and} \quad \rho \geq \theta \quad \text{a.e. on } I \quad (22)$$

where  $\rho = 1/\kappa$  is the local radius of curvature of  $\gamma$ . Moreover, we find that  $\Gamma \in W^{2,\infty}$  since the second inequality in (22) implies that  $\kappa \leq \theta^{-1}$ . Notice the relation between the conditions in (22), which are equivalent to preservation of orientation and guarantee local injectivity, and the conditions in Lemma 7, which guarantee global injectivity. Preservation of orientation requires that the local radius of curvature be bounded below by the cross-sectional radius  $\theta$ , whereas global injectivity requires the stronger condition that the global radius of curvature be bounded below by  $\theta$ .

Unshearable, *inextensible* rods are a further specialization. They are defined by the material constraint  $v := \hat{v} := (0, 0, 1)$ , which by (10) yields

$$\gamma' = d_3 \quad \text{and} \quad \kappa = |\gamma''| = \sqrt{u_1^2 + u_2^2}.$$

Thus, both  $\gamma$  and  $\Gamma$  are arclength parameterizations in this case. The first identity above implies that  $\gamma \in W^{2,1}(I, \mathbb{R}^3)$ . Furthermore, when the conditions in (18) are satisfied, the second identity above implies that  $\gamma \in W^{2,\infty}(I, \mathbb{R}^3)$ .

#### 4.2. Existence of minimizers

Here we establish the existence of rod configurations that minimize a prescribed elastic energy subject to a self-contact or excluded volume constraint. We consider three distinct classes of rod models: unshearable, inextensible models, general models in which shear and extension are allowed, and unshearable, extensible models. Motivated by Lemmas 3 and 7, we employ a lower bound on the global radius of curvature as a model for the excluded volume constraint. This approach is in contrast to those pursued in [10], [22], [31], where various integral energies are introduced as repulsive potentials, and in [13], [30].



**4.2.1. Unshearable, inextensible models** A configuration  $(\gamma[w], D[w])$  of an unshearable, inextensible rod is uniquely described by an element  $w = (u, v, \gamma_0, D_0) \in X_0^{p,q}$  where the function  $v$  is constrained to take the value  $(0, 0, 1)$ . Thus, this class of rods is described by the set

$$X_0^p := \{w = (u, v, \gamma_0, D_0) \in X_0^{p,q} \mid v = (0, 0, 1), \gamma_0 = 0, D_0 = \text{Id}\}$$

where, without loss of generality, we fix  $\gamma_0$  and  $D_0$  to eliminate rigid translations and rotations. Notice that the choice of  $q$  is immaterial since the function  $v \equiv (0, 0, 1)$  is in  $L^q$  for any  $q \in (1, \infty)$ .

The stored energy density  $W$  for unshearable, inextensible rods reduces to the form  $W(u, \sigma)$ . We assume that  $W(\cdot, \sigma)$  is continuous and convex for a.e.  $\sigma \in I$ , that  $W(u, \cdot)$  is Lebesgue measurable on  $I$  for all  $u$ , and that

$$W(u, \sigma) \geq c_1 |u|^p + g(\sigma) \text{ for all } u \in \mathbb{R}^3, \text{ for a.e. } \sigma \in I, \quad (23)$$

where  $p \in (1, \infty)$ ,  $c_1 > 0$ , and  $g \in L^1(I)$ .

The basic problem we consider is the existence of minimizers for the total elastic energy functional

$$E(w) = E(u) = \int_I W(u(\sigma), \sigma) d\sigma \rightarrow \text{Min!}, \quad w \in X_0^p \quad (24)$$

subject to the following side conditions on  $(\gamma[w], D[w])$ :

$$\gamma[w](b) = \gamma_0, \quad D[w](b) = D_1, \quad (25)$$

$$\Delta[\gamma[w]] \geq \theta, \quad (26)$$

$$\gamma[w](\bar{I}) \simeq k, \quad (27)$$

$$D[w] \sim Q. \quad (28)$$

Here  $D_1 \in SO(3)$  is a given frame which coincides with  $D_0$  in its last column,  $\theta > 0$  is a constant that represents the cross-sectional radius of the rod,  $k$  is a continuous closed curve in  $\mathbb{R}^3$  that represents a given knot class, and  $Q : \bar{I} \rightarrow SO(3)$  with  $Q(a) = D_0$ ,  $Q(b) = D_1$  is a continuous map that represents a given link class (cf. Def. 2 and 3). The conditions in (25), together with the assumption on  $D_1$ , ensure that  $d_3[w](b) = d_3[w](a)$ , and that  $d_1[w](b)$  and  $d_1[w](a)$  differ by a given angle. Moreover, these conditions ensure that  $\gamma[w]$  is closed in the  $C^1$ -sense since  $\gamma'[w](\sigma) = d_3[w](\sigma)$  by the constraint on  $v$ .

Thus, we seek energy minimizers for non-self-intersecting, unshearable and inextensible rods of a prescribed knot and link type where the frames  $D[w](a)$  and  $D[w](b)$  differ by a prescribed rotation. Our main result in this direction is:

**Theorem 2.** *Let  $1 < p < \infty$  and assume that (23) holds. Suppose that there is an element  $\tilde{w} \in X_0^p$  satisfying (25)-(28). Then the minimization problem (24)-(28) has a solution  $w \in X_0^p$ , whose corresponding framed curve  $(\gamma[w], D[w]) \in W^{2,p}(I, \mathbb{R}^3) \times W^{1,p}(I, \mathbb{R}^{3 \times 3})$  has a centreline with an arclength parameterization  $\Gamma \in C^{1,1}$ .*

This result establishes the existence of energy minimizers subject to a geometrically exact excluded volume constraint. The exactness of (26) as a model for excluded volume follows from Lemma 7 and the condition on  $v$ . An important assumption in the theorem is the existence of a configuration that satisfies all the imposed side conditions; in particular, the conditions in (26) and (27). For given  $\theta$  and  $k$ , these conditions can be satisfied by rods of sufficiently large length. According to the remarks following Theorem 1, the above existence result remains valid when a potential energy with at most linear growth is added to the total elastic energy. Thus, for example, body forces that do not depend on the deformed shape of the rod, such as a uniform gravitational field, can also be included. (See [25] for related problems in which gravitational forces are considered.)

The classic energy involving the integral of the squared curvature (see e.g. [19],[20],[30]), or in our notation

$$E = \int_{\gamma} \kappa^2 ds,$$

can also be considered. This energy can be viewed as a simple model of an unframed, elastic, closed curve. (Note that for such unframed curves a prescribed link type has no obvious meaning.) The weak closure results of Lemma 4 and Lemma 5 allow us to conclude the existence of a minimizer of each prescribed knot type when our excluded volume constraint is enforced and the length of the curve is fixed. More precisely, we can consider curves  $\gamma \in W^{2,2}(I, \mathbb{R}^3)$  subject to the constraints  $|\gamma'(s)| = 1$  on  $\bar{I}$ ,  $\gamma(b) = \gamma(a) = 0$ ,  $\gamma'(a) = \gamma'(b) = e$ ,  $\Delta[\gamma] \geq \theta > 0$ , and  $\gamma(\bar{I}) \simeq k$ , where  $e$  is a given unit vector, and  $k$  represents a given knot type. Since the constraints are closed under weak convergence, and since (up to a constant factor) the integral of the squared curvature dominates the  $W^{2,2}$  norm  $\|\gamma\|$  on the admissible set, standard direct methods can be applied.

**4.2.2. General models** A configuration  $(\gamma[w], D[w])$  of a general shearable and extensible rod is uniquely described by an element  $w = (u, v, \gamma_0, D_0) \in X_0^{p,q}$ . We fix  $\gamma_0$  and  $D_0$  to eliminate rigid translations and rotations as before and we consider the class of rods described by the set

$$\tilde{X}_0^{p,q} := \{w = (u, v, \gamma_0, D_0) \in X_0^{p,q} \mid \gamma_0 = 0, D_0 = \text{Id}\}, \quad p, q \in (1, \infty).$$

We assume that the stored energy density  $W$  satisfies conditions (W1)-(W3) of Section 3 with  $c_1, c_2 > 0$ .

The basic problem is the existence of minimizers for the total elastic energy functional

$$E(w) := \int_I W(u(\sigma), v(\sigma), \sigma) d\sigma \longrightarrow \text{Min!}, \quad w \in \tilde{X}_0^{p,q} \quad (29)$$

subject to the following side conditions on  $(\gamma[w], D[w])$ :

$$\gamma[w](b) = \gamma_0, \quad D[w](b) = D_1, \quad (30)$$

$$\Delta[\gamma[w]] \geq \theta, \quad (31)$$

$$\gamma[w](\bar{I}) \simeq k, \quad (32)$$

$$D[w] \sim Q \quad (33)$$

where  $D_1$ ,  $\theta$ ,  $k$ , and  $Q$  are as defined in the previous problem. In the case of a general rod model the second equation in (30) ensures that  $d_3[w](a) = d_3[w](b)$ , but it does not imply that the tangents of the curve  $\gamma[w]$  are equal at the end points.

Our main result concerning the above problem is:

**Theorem 3.** *Let  $1 < p, q < \infty$ , let (W1)–(W3) be satisfied, and assume that there is some admissible  $\tilde{w} \in \tilde{X}_0^{p,q}$  respecting (30)–(33). Then the minimization problem (29)–(33) has a solution  $w \in \tilde{X}_0^{p,q}$ , whose corresponding framed curve  $(\gamma[w], D[w]) \in W^{1,q}(I, \mathbb{R}^3) \times W^{1,p}(I, \mathbb{R}^{3 \times 3})$  has a centreline with an arclength parameterization  $\Gamma \in C^{1,1}$ .*

This result establishes the existence of energy minimizers for general rod models subject to the constraint (31). However, in this general case, condition (31) is merely an approximate model for excluded volume as discussed in Section 3. As before, the existence result remains valid when a potential energy with at most linear growth is added to the total elastic energy.

**4.2.3. Unshearable, extensible models** Theorem 3 also applies in the case of an unshearable, extensible rod defined by  $v = (0, 0, v_3)$  (see Section 4.1) provided that we appropriately modify the hypothesis (W3). Specifically, the growth condition in (W3) should be satisfied for all  $(u, v_3) \in \mathbb{R}^3 \times \mathbb{R}$  instead of  $(u, v) \in \mathbb{R}^3 \times \mathbb{R}^3$ . This case can be interpreted as an intermediate one between the general case considered immediately above, and the unshearable, inextensible one considered earlier.

For the unshearable, extensible case the condition in (31) is an exact model for excluded volume provided that  $v_3 > 0$  (by Lemma 7). However,  $v_3 > 0$  is not a weakly closed condition in the spirit of Lemma 9, and configurations that satisfy (31) may not necessarily satisfy  $v_3 > 0$ . In fact, since the global radius of curvature cannot exceed the local radius of curvature, we deduce from (21) that (31) implies only the weaker inequality

$$v_3 \geq \theta \sqrt{u_1^2 + u_2^2} \quad \text{a.e. on } I \quad (34)$$

in this case of unshearable rods. Thus  $v_3 = 0$  is possible for some subset of  $I$ , but only on straight parts of the rod in accordance with (34). Consequently, an unshearable rod may fail to be globally injective on such parts. On the other hand, mechanically realistic energy densities should blow up on regions of large compression, i.e.,

$$W(u, v, s) \rightarrow \infty \quad \text{as } v_3 - \theta \sqrt{u_1^2 + u_2^2} \rightarrow 0 \quad (35)$$

(cf. Antman [1, Ch. VII.5, VIII]). In the case that this condition holds, we find that  $v_3 = 0$  is possible only on a subset of  $I$  with measure zero. Thus (31) together with (35) would ensure the global injectivity of an unshearable, extensible rod since arcs connecting two points on the centreline curve with different parameters have positive length. Notice that energy densities with property (35) satisfy conditions (W1)–(W3) and are covered by our existence theory.

## 5. Application to ideal knots

Here we establish the existence of curves of a prescribed knot type that minimize the arclength functional subject to a lower bound on the global radius of curvature. By Lemma 3, this lower bound provides a geometrically exact model for the self-contact or excluded volume constraint imposed on the curve by a tubular neighbourhood of fixed radius. The basic problem we consider is that of minimizing the functional

$$L(\gamma) = \int_I |\gamma'(\sigma)| d\sigma \rightarrow \text{Min!}, \quad \gamma \in W^{1,q}, \quad q \in (1, \infty), \quad (36)$$

subject to the conditions

$$\gamma(b) = \gamma(a), \quad \Delta[\gamma] \geq \theta \quad \text{and} \quad \gamma(\bar{I}) \simeq \tilde{\gamma}(\bar{I}). \quad (37)$$

Here  $\theta > 0$  is a constant and  $\tilde{\gamma} \in W^{1,q}$  is a continuous closed curve that represents the prescribed knot type and satisfies  $\Delta[\tilde{\gamma}] \geq \theta$ .

A solution  $\gamma$  of the above problem is called an *ideal knot* in the sense of [2], [16] and [21]. In other words, an ideal knot is a non-self-intersecting tube of fixed radius  $\theta > 0$  and prescribed knot type with a centreline curve  $\gamma$  of minimal length. Here we establish an existence result for ideal knots which shows that their centreline curves are always continuously differentiable. In fact, these curves have arclength parameterizations of class  $C^{1,1}$ , which means that their unit tangent vector fields are Lipschitz continuous.

To employ the general existence result in Section 3, we merely identify a curve  $\gamma \in W^{1,q}$  with a framed curve  $(\gamma, D) \in W^{1,q} \times W^{1,p}$  where  $D(s) \equiv \tilde{D}$ . Here  $\tilde{D} \in SO(3)$  is an arbitrary fixed frame which plays no role in our developments. Without loss of generality, we fix the initial point  $\gamma(a) = \gamma_0$  to eliminate rigid translations. Thus, for the ideal knot problem we consider framed curves described by the set

$$X_0^q := \{w = (u, v, \gamma_0, D_0) \in X_0^{p,q} \mid u = (0, 0, 0), \gamma_0 = 0, D_0 = \tilde{D}\},$$

and we seek minimizers of the functional

$$E(w) := \int_I |v(\sigma)| d\sigma \rightarrow \text{Min!}, \quad w = (u, v, \gamma_0, D_0) \in X_0^q$$

subject to the conditions

$$\gamma[w](b) = \gamma_0, \quad \Delta[\gamma[w]] \geq \theta \quad \text{and} \quad \gamma[w](\bar{I}) \simeq \tilde{\gamma}(\bar{I}). \quad (38)$$

In the above form it seems that the ideal knot problem can be treated by Theorem 1 and our investigations about weakly closed sets. However, the energy to be minimized here has merely linear growth and does not satisfy (W3) for  $q > 1$ . Nevertheless by showing that the minimization of  $\int_I |v|^q d\sigma$  ( $q > 1$ ) also provides a curve of minimal length, we are able to circumvent this difficulty and obtain the following

**Theorem 4.** *For  $q \in (1, \infty)$  the minimization problem defined by (36) and (37) has a solution  $\gamma_*$ . This curve has an arclength parameterization  $\Gamma_* \in C^{1,1}$ .*

This result establishes the existence of ideal knots and shows that their centreline curves have arclength parameterizations of class  $C^{1,1}$ . Similar existence results have been obtained by Kusner and co-workers [17] using ideas related to global radius of curvature. In addition, Cantarella et al. [3] have proved that an ideal or tight configuration of an unknotted 3-component link is achieved by centrelines made up from arcs of circles joined with straight line segments, i.e. a centreline that is  $C^{1,1}$  and also piecewise smooth, but not  $C^2$  overall. Similarly, numerical data presented in [12] suggest that ideal configurations of some true (but composite) knots are also not  $C^2$ . Thus there is some evidence supporting the conjecture that the regularity established in our existence result above may be quite sharp.

## 6. Proofs

In this section we provide proofs for the results described in Sections 2 to 5. We use the same notation as in the corresponding sections.

### 6.1. Proofs for Section 2

*Proof of Lemma 1.* For the first implication we assume  $L > 0$  and that the pair  $s, t \in S_L$  ( $s \neq t$ ) defines a double point of  $\gamma$  (there can be no double points if  $L = 0$ ). Then, by definition of  $\rho_G[\gamma]$  and  $R(x, y, z)$ , we have

$$\begin{aligned} \rho_G[\gamma](s) &= \inf \{ R(\Gamma(s), \Gamma(\sigma), \Gamma(\tau)) \mid \sigma, \tau \in S_L \setminus \{s\}, \sigma \neq \tau \} \\ &\leq \inf \{ R(\Gamma(s), \Gamma(t), \Gamma(\tau)) \mid \tau \in S_L \setminus \{s, t\} \} \\ &= \inf \{ |\Gamma(s) - \Gamma(t)|/2 \mid \tau \in S_L \setminus \{s, t\} \} \\ &= 0 \end{aligned}$$

and similarly for  $\rho_G[\gamma](t)$ . Thus, if  $\gamma$  is non-simple, then necessarily  $\Delta[\gamma] = 0$ , and the second implication follows.  $\square$

*Proof of Lemma 2.* 1. Consider a connected subarc  $A_1 := \Gamma([\sigma_0, \sigma_1])$  with fixed endpoints  $P_0 := \Gamma(\sigma_0)$  and  $P_1 := \Gamma(\sigma_1)$ , and suppose that  $\text{diam } A_1 < 2\theta$  and  $|P_1 - P_0| < \theta/2$ , which is possible by choosing  $|\sigma_1 - \sigma_0|$  sufficiently small. Let  $l_1$  be the lens-shaped intersection of all open balls of radius  $\theta$  containing  $P_0$  and  $P_1$  on their boundaries, i.e.,

$$l_1 := \bigcap_{z \in C(P_0, P_1)} B_\theta(z),$$

where  $C(P_0, P_1) := \{z \in \mathbb{R}^3 \mid |z - P_0| = |z - P_1| = \theta\}$ . We claim that

$$A_1 \subset \overline{l_1}. \quad (39)$$

To see this, suppose for contradiction that  $A_1 \not\subset \overline{l_1}$  and consider the set

$$\Xi := \bigcup_{z \in C(P_0, P_1)} B_\theta(z). \quad (40)$$

Then, using the facts that  $\gamma$  is simple (by Lemma 1),  $\text{diam } A_1 < 2\theta$  and  $|P_1 - P_0| < \theta/2$ , we deduce that there must be a point  $\bar{P} \in (A_1 \cap \Xi) \setminus \bar{l}_1$ . Moreover, we find that

$$R(P_0, P_1, \bar{P}) = \frac{|P_1 - P_0|}{2 \sin \bar{\alpha}} < \theta, \quad \text{where} \quad \bar{\alpha} := \angle(P_0 - \bar{P}, P_1 - \bar{P}). \quad (41)$$

Since this contradicts the lower bound  $\Delta[\gamma] \geq \theta$  we must have  $A_1 \subset \bar{l}_1$  as claimed.

Notice that there is indeed a point  $\bar{P} \in (A_1 \cap \Xi) \setminus \bar{l}_1$ . Otherwise, we would have  $\text{diam } A_1 \geq 2\theta$ , because any curve in  $\mathbb{R}^3 \setminus \Xi$  connecting  $P_0$  and  $P_1$  must have diameter at least as large as the great circle on  $\partial B_\theta(z)$  connecting  $P_0$  and  $P_1$  outside of  $l_1$  for any of the balls  $B_\theta(z)$  that generate  $\Xi$ . Moreover, since  $|P_1 - P_0| < \theta/2$ , the portion of such a great circle has diameter  $2\theta$ .

The result in (41) may be seen by considering the intersection of  $\Xi$  with the plane containing the three non-collinear points  $P_0, P_1$  and  $\bar{P}$ . This intersection may be described by two overlapping planar disks  $D_\theta(z_1)$  and  $D_\theta(z_2)$  of radius  $\theta$ , where  $\partial D_\theta(z_1) \cap \partial D_\theta(z_2) = \{P_0, P_1\}$ , and we may assume without loss of generality that  $\bar{P} \in D_\theta(z_1) \setminus D_\theta(z_2)$ . From elementary geometry we recall that, for any  $\xi \in \partial D_\theta(z_1) \setminus \{P_0, P_1\}$ , we have  $\theta = |P_1 - P_0| / (2 \sin \beta)$  where  $\beta := \angle(P_0 - \xi, P_1 - \xi)$ . To establish (41), we first suppose that  $\bar{\alpha} \in (0, \pi/2)$ . In this case we may choose  $\xi \in \partial D_\theta(z_1) \setminus D_\theta(z_2)$  such that  $\beta \in (0, \bar{\alpha})$ , i.e.,  $\sin \beta < \sin \bar{\alpha}$ , which implies (41). If we suppose that  $\bar{\alpha} \in [\pi/2, \pi)$ , then we may choose  $\xi \in \partial D_\theta(z_1) \cap D_\theta(z_2)$  such that  $\beta \in (\bar{\alpha}, \pi)$ , i.e.,  $\sin \beta < \sin \bar{\alpha}$ , which also implies (41).

2. Given  $\sigma_0, \sigma_1 \in S_L$  as above, we next consider a sequence  $\sigma_n \downarrow \sigma_0$  ( $n \geq 1$ ). We introduce  $P_n := \Gamma(\sigma_n)$ ,  $A_n := \Gamma([\sigma_0, \sigma_n])$  and the lens-shaped region  $l_n$  defined by  $P_0, P_n$  and  $\theta > 0$  as before. Moreover, for each  $n \geq 1$ , we introduce the tangent cone  $T_n$  of  $l_n$  in  $P_0$  as

$$T_n := \{x \in \mathbb{R}^3 \mid x = \lambda(q - P_0), \quad \lambda \geq 0, \quad q \in \bar{l}_n\}.$$

Since  $|P_n - P_0| < \theta/2$  and  $\text{diam } A_n < 2\theta$  we may use the same argument as in step 1 to conclude

$$A_n \subset \bar{l}_n, \quad \forall n \in \mathbb{N}. \quad (42)$$

Furthermore, by straightforward geometrical arguments we also find

$$l_{n+1} \subset l_n \quad \text{and} \quad T_{n+1} \subset T_n, \quad \forall n \in \mathbb{N}. \quad (43)$$

3. Let  $\alpha_n$  be the opening angle of the cone  $T_n$ . Since  $0 < |P_n - P_0| < \theta/2$  and

$$\sin(\alpha_n/2) = \frac{|P_n - P_0|}{2\theta} \quad (44)$$

we deduce  $\alpha_n \in (0, \pi/2)$ . Moreover, since  $|P_n - P_0| \rightarrow 0$  we deduce  $\alpha_n \rightarrow 0$  as  $n \rightarrow \infty$ .

4. For each  $n \geq 1$  we introduce a unit vector

$$t_n := (P_n - P_0) / |P_n - P_0| \in S^2,$$

which is well-defined since  $\sigma_n \downarrow \sigma_0$  and  $|P_n - P_0| > 0$ . By definition of the cone  $T_n$  we have  $t_n \in T_n$ , and since  $T_m \subset T_n$  ( $m \geq n$ ) and the opening angles satisfy  $\alpha_n \rightarrow 0$ , we deduce that  $\{t_n\}_{n \in \mathbb{N}} \subset S^2$  is a Cauchy sequence. Therefore we find a vector

$$t_R(\sigma_0) := \lim_{n \rightarrow \infty} \frac{\Gamma(\sigma_n) - \Gamma(\sigma_0)}{|\Gamma(\sigma_n) - \Gamma(\sigma_0)|} \in S^2.$$

Notice that  $t_R(\sigma_0)$  does not depend on the choice of sequence  $\sigma_n \downarrow \sigma_0$ . In fact, assuming that a different sequence  $\sigma'_n \downarrow \sigma_0$  leads to a different unit vector  $t'_R(\sigma_0) \neq t_R(\sigma_0)$ , we arrive at a contradiction. In particular, the mixed sequence  $\{\sigma''_n\} := \{\sigma_1, \sigma'_1, \sigma_2, \sigma'_2, \dots\}$  would lead to a Cauchy sequence of unit vectors with no unique limit. Thus we must have  $t'_R(\sigma_0) = t_R(\sigma_0)$ .

5. Given any point  $\sigma_0 \in S_L$  and two sequences  $\sigma_n \downarrow \sigma_0$  and  $\tau_k \uparrow \sigma_0$  we have two well-defined unit tangent vectors at  $\Gamma(\sigma_0)$ ; namely,  $t_R(\sigma_0)$  defined as above and

$$t_L(\sigma_0) := \lim_{k \rightarrow \infty} \frac{\Gamma(\sigma_0) - \Gamma(\tau_k)}{|\Gamma(\sigma_0) - \Gamma(\tau_k)|} \in S^2.$$

We claim that  $t_R(\sigma_0) = t_L(\sigma_0)$ . To see this, assume for contradiction that  $t_R(\sigma_0) \neq t_L(\sigma_0)$ . Consider the lens-shaped regions

$$l_n^R := \bigcap_{z \in C(P_0, \Gamma(\sigma_n))} B_\theta(z) \quad \text{and} \quad l_k^L := \bigcap_{z \in C(P_0, \Gamma(\tau_k))} B_\theta(z)$$

and the unit vectors

$$t_k := (\Gamma(\tau_k) - \Gamma(\sigma_0)) / |\Gamma(\tau_k) - \Gamma(\sigma_0)|$$

$$t_n := (\Gamma(\sigma_n) - \Gamma(\sigma_0)) / |\Gamma(\sigma_n) - \Gamma(\sigma_0)|.$$

By the same arguments as in step 1 we deduce that  $\Gamma([\tau_k, \sigma_0]) \cap l_n^R = \emptyset$  and  $\Gamma([\sigma_0, \sigma_n]) \cap l_k^L = \emptyset$  for all sufficiently large  $n, k \in \mathbb{N}$ . Thus the angle  $\vartheta \in [0, \pi]$  between  $t_R(\sigma_0)$  and  $-t_L(\sigma_0)$  satisfies  $0 < \vartheta < \pi$ . Moreover, since

$$\lim_{k, n \rightarrow \infty} \angle(t_k, t_n) = \vartheta$$

and

$$\lim_{k \rightarrow \infty} \Gamma(\tau_k) = \lim_{n \rightarrow \infty} \Gamma(\sigma_n) = \Gamma(\sigma_0)$$

we deduce that

$$\lim_{k, n \rightarrow \infty} R(\Gamma(\tau_k), \Gamma(\sigma_n), \Gamma(\sigma_0)) = \lim_{k, n \rightarrow \infty} \frac{|\Gamma(\tau_k) - \Gamma(\sigma_n)|}{2 \sin \angle(t_k, t_n)} = 0,$$

which contradicts the lower bound  $\Delta[\gamma] \geq \theta > 0$ . Thus we must have  $t_R(\sigma_0) = t_L(\sigma_0)$  as claimed.

6. If  $\sigma_0$  is a parameter where  $\Gamma$  is differentiable, then  $\Gamma'(\sigma_0) = t_R(\sigma_0) = t_L(\sigma_0)$ . This follows from the fact that, if  $\Gamma$  is differentiable at  $\sigma_0$ , then  $|\Gamma'(\sigma_0)| = 1$  and

$$\Gamma(\sigma_n) - \Gamma(\sigma_0) = \Gamma'(\sigma_0)(\sigma_n - \sigma_0) + o(|\sigma_n - \sigma_0|)$$

for any sequence  $\sigma_n \downarrow \sigma_0$ . The result follows since

$$\frac{\Gamma(\sigma_n) - \Gamma(\sigma_0)}{|\Gamma(\sigma_n) - \Gamma(\sigma_0)|} = \frac{\Gamma'(\sigma_0)(\sigma_n - \sigma_0) + o(|\sigma_n - \sigma_0|)}{|\sigma_n - \sigma_0|} \cdot \left[ 1 - \frac{o(|\sigma_n - \sigma_0|)}{|\sigma_n - \sigma_0|} \right]$$

and  $o(|\sigma_n - \sigma_0|)/|\sigma_n - \sigma_0| \rightarrow 0$  as  $|\sigma_n - \sigma_0| \rightarrow 0$ .

7. If  $\Gamma$  is differentiable at  $\sigma_1, \sigma_2 \in S_L$ , then

$$|\Gamma'(\sigma_1) - \Gamma'(\sigma_2)| \leq |\sigma_1 - \sigma_2|/\theta.$$

To establish this result, we consider first the case when  $|\Gamma(\sigma_1) - \Gamma(\sigma_2)| < \theta/2$ . In this case we have  $\Gamma'(\sigma_1) \in T_1$ , and by symmetry  $\Gamma'(\sigma_2) \in T_1$ , where  $T_1$  is the tangent cone of  $l_1$  in  $\Gamma(\sigma_1)$  with opening angle  $\alpha_1 \in (0, \pi/2)$ . Using the fact that

$$\sin(\alpha_1/2) = |\Gamma(\sigma_1) - \Gamma(\sigma_2)|/2\theta$$

together with the law of cosines we find

$$\begin{aligned} |\Gamma'(\sigma_1) - \Gamma'(\sigma_2)| &\leq \sqrt{2 - 2\cos\alpha_1} \\ &= |\Gamma(\sigma_1) - \Gamma(\sigma_2)|/\theta \leq |\sigma_1 - \sigma_2|/\theta, \end{aligned} \tag{45}$$

as claimed. In the case when  $|\Gamma(\sigma_1) - \Gamma(\sigma_2)| \geq \theta/2$  the result is still true. In particular, the arc  $[\sigma_1, \sigma_2] \subset S_L$  may be divided into subarcs  $[\tau_i, \tau_{i+1}] \subset S_L$  ( $i = 1, \dots, m$ ) such that  $\tau_i$  are points of differentiability (which is possible since  $\Gamma$  is Lipschitz continuous and hence differentiable almost everywhere),  $\sigma_1 = \tau_1$ ,  $\sigma_2 = \tau_{m+1}$  and  $|\Gamma(\tau_i) - \Gamma(\tau_{i+1})| < \theta/2$ . Applying (45) to the subarcs  $[\tau_i, \tau_{i+1}]$  and summing yields the required result.

8. We can now show that  $\Gamma \in C^{1,1}(\tilde{S}_L, \mathbb{R}^3)$  and that  $\Gamma'$  has Lipschitz constant  $1/\theta$ . To begin, we consider first the subset  $\tilde{S}_L$  of  $S_L$  where  $\Gamma$  is differentiable. Since  $\tilde{S}_L$  is dense in  $S_L$  and by (45) the map  $\Gamma' : \tilde{S}_L \rightarrow \mathbb{R}^3$  is uniformly continuous, we deduce that there is a unique uniformly continuous extension  $V : S_L \rightarrow \mathbb{R}^3$ . In particular,  $V \in C^{0,1}(\tilde{S}_L, \mathbb{R}^3)$  with Lipschitz constant  $1/\theta$ . To see that this implies  $\Gamma \in C^{1,1}(S_L, \mathbb{R}^3)$ , let  $\sigma_0 \in S_L$  be given and note that since  $\Gamma \in C^{0,1}(S_L, \mathbb{R}^3)$  is absolutely continuous we have

$$\Gamma(\sigma_n) - \Gamma(\sigma_0) = \int_{\sigma_0}^{\sigma_n} \Gamma'(\tau) d\tau = \int_{\sigma_0}^{\sigma_n} V(\tau) d\tau$$

which implies

$$\frac{\Gamma(\sigma_n) - \Gamma(\sigma_0)}{\sigma_n - \sigma_0} = \frac{1}{\sigma_n - \sigma_0} \int_{\sigma_0}^{\sigma_n} V(\tau) d\tau$$

for any  $\sigma_n \neq \sigma_0$ . Since  $V \in C^{0,1}(\tilde{S}_L, \mathbb{R}^3)$  the limit  $\sigma_n \rightarrow \sigma_0$  is well-defined, i.e.,  $\Gamma'(\sigma_0)$  exists and

$$\Gamma'(\sigma_0) = V(\sigma_0), \quad \forall \sigma_0 \in S_L.$$

Thus  $\Gamma' \in C^{0,1}(S_L, \mathbb{R}^3)$  with Lipschitz constant  $1/\theta$ .  $\square$



*Proof of Lemma 3.* 1. For any fixed  $s_0 \in S_L$  and  $\theta > 0$  let  $s_n \downarrow s_0$ ,  $P_n := \Gamma(s_n)$ ,  $P_0 := \Gamma(s_0)$  and

$$C_n := C(P_0, P_n) := \{z \in \mathbb{R}^3 \mid |z - P_0| = |z - P_n| = \theta\}.$$

Notice that  $C_n$  is the circle of radius  $\rho_n := \sqrt{\theta^2 - |P_n - P_0|^2/4}$  centred at  $y_n := (P_n + P_0)/2$  and perpendicular to the unit vector  $(P_n - P_0)/|P_n - P_0|$ . We claim that

$$\text{dist}_H(C_n, C(s_0, \theta)) \rightarrow 0 \quad \text{as } n \rightarrow \infty, \quad (46)$$

where  $C(s_0, \theta)$  is the circle defined in the statement of the lemma and  $\text{dist}_H(A, B)$  denotes the Hausdorff distance [9, p. 183] between two subsets  $A, B$  of  $\mathbb{R}^3$ . To establish this result, we note first that  $\rho_n \rightarrow \theta$  and  $y_n \rightarrow P_0$ . Moreover, since  $\Delta[\gamma] > 0$ , we have by Lemma 2 that  $(P_n - P_0)/|P_n - P_0| \rightarrow \Gamma'(s_0)$ . Thus  $C_n$  converges to a circle of radius  $\theta$  with centre  $P_0$  in the plane perpendicular to  $\Gamma'(s_0)$ . Since these properties completely characterize  $C(s_0, \theta)$  the result follows.

2. The first claim in item (i) is that if  $\Delta[\gamma] \geq \theta > 0$ , then  $\Gamma(S_L) \cap M(s_0, \theta) = \emptyset$  for all  $s_0 \in S_L$ . To establish this, we consider the sets

$$\Xi_n := \bigcup_{z \in C_n} B_\theta(z)$$

as in the proof of Lemma 2. We assume for contradiction that there is a point  $\bar{P} \in \Gamma(S_L) \cap M(s_0, \theta)$ , which implies  $\text{dist}(\bar{P}, C(s_0, \theta)) < \theta$ . For  $n \in \mathbb{N}$  sufficiently large, we deduce from (46) that  $\text{dist}(\bar{P}, C_n) < \theta$ , which implies  $\bar{P} \in \Xi_n$ , and moreover we have  $|\bar{P} - P_0| > |P_n - P_0|$ . These observations lead to the result  $\bar{P} \in \Xi_n \setminus \bar{l}_n$ , where

$$l_n := \bigcap_{z \in C_n} B_\theta(z).$$

By exactly the same arguments as in the proof of Lemma 2, we arrive at a statement of the form (41) with  $P_1$  replaced by  $P_n$ . Since this contradicts the lower bound  $\Delta[\gamma] \geq \theta$  the first claim in item (i) must be true.

3. The second claim in item (i) is that if  $\Gamma(S_L) \cap M(s_0, \theta) = \emptyset$  for all  $s_0 \in S_L$ , then  $\Delta[\gamma] \geq \theta$ . To establish this result, we assume for contradiction that  $0 < \Delta[\gamma] < \theta$  and we consider minimizing sequences  $s_n, \sigma_n, \tau_n \in S_L$  ( $s_n, \sigma_n, \tau_n$  mutually distinct for each  $n$ ) that achieve  $\Delta[\gamma]$ , i.e.,

$$\Delta[\gamma] = \lim_{n \rightarrow \infty} R(\Gamma(s_n), \Gamma(\sigma_n), \Gamma(\tau_n)).$$

Here  $R_n := R(\Gamma(s_n), \Gamma(\sigma_n), \Gamma(\tau_n))$  is the radius of the unique circle  $H_n$  defined by the three distinct points  $\Gamma(s_n)$ ,  $\Gamma(\sigma_n)$  and  $\Gamma(\tau_n)$ . (Recall that  $\Gamma$  is simple by Lemma 1 and has a Lipschitz continuous tangent field by Lemma 2 since  $\Delta[\gamma] > 0$ .) Since  $S_L$  is compact we may assume that  $s_n \rightarrow \bar{s}$ ,  $\sigma_n \rightarrow \bar{\sigma}$  and  $\tau_n \rightarrow \bar{\tau}$ , and without loss of generality, we have only three kinds of minimizing sequences: (a)  $\bar{s}, \bar{\sigma}, \bar{\tau}$  distinct, (b)  $\bar{s} \neq \bar{\sigma} = \bar{\tau}$  or (c)  $\bar{s} = \bar{\sigma} = \bar{\tau}$ . We claim that sequences of type (a) need not be considered, and those of type (b) and (c) lead to the required contradiction.

To see that sequences of type (a) may be excluded from consideration, we suppose that  $\Delta[\gamma]$  is achieved by distinct parameters  $\bar{s}$ ,  $\bar{\sigma}$  and  $\bar{\tau}$ , which correspond to three distinct points on  $\Gamma$ . Let  $\bar{H}$  denote the unique circle defined by these points and  $\bar{\Phi}$  the unique sphere that contains  $\bar{H}$  as a great circle. Unless the curve  $\Gamma$  is tangent to  $\bar{\Phi}$  at one of these points, we obtain an immediate contradiction, for otherwise we may shrink  $\bar{\Phi}$  and find three other distinct points that define a circle of radius smaller than  $\Delta[\gamma]$ . Assuming the tangency is at  $\Gamma(\bar{\sigma})$ , the circle through  $\Gamma(\bar{s})$  and tangent to  $\Gamma$  at  $\Gamma(\bar{\sigma})$  is on  $\bar{\Phi}$ , and hence has radius less than or equal to the great circle radius. Since this circle may be obtained as the limit of a sequence of type (b), we conclude that  $\Delta[\gamma]$  can never exclusively be achieved by a sequence of type (a).

If  $\Delta[\gamma] < \theta$  is achieved by a sequence of type (b), then there is a circle of radius  $\delta = \Delta[\gamma]$  that is tangent to  $\Gamma$  at  $\Gamma(\bar{\sigma})$  and contains  $\Gamma(\bar{s}) \neq \Gamma(\bar{\sigma})$ . Thus  $\Gamma(\bar{s}) \in \overline{M(\bar{\sigma}, \delta)} \setminus \{\Gamma(\bar{\sigma})\} \subset M(\bar{\sigma}, \theta)$ , which contradicts the hypothesis that  $\Gamma(S_L) \cap M(s_0, \theta) = \emptyset$  for all  $s_0 \in S_L$ .

If  $\Delta[\gamma] < \theta$  is achieved by a sequence of type (c), we also arrive at a contradiction. To see this, let  $p_n$  denote the centre of the circle  $H_n$  and without loss of generality assume  $s_n < \sigma_n < \tau_n$ . Thus

$$|\Gamma(s_n) - p_n| = |\Gamma(\sigma_n) - p_n| = |\Gamma(\tau_n) - p_n| = R_n$$

and  $R_n \rightarrow \delta < \theta$  where  $\delta = \Delta[\gamma]$ . By applying the Mean Value Theorem to the differentiable function  $f(s) = |\Gamma(s) - p_n|^2$ ,  $s \in [s_n, \sigma_n]$ , we deduce that there exists  $s_{-,n} \in (s_n, \sigma_n)$  such that  $\Gamma(s_{-,n}) - p_n$  is perpendicular to  $\Gamma'(s_{-,n})$ . Similarly, there exists  $s_{+,n} \in (\sigma_n, \tau_n)$  such that  $\Gamma(s_{+,n}) - p_n$  is perpendicular to  $\Gamma'(s_{+,n})$ . Following the same arguments as in the proof of Lemma 2 we must have  $\Gamma(s_{-,n}) \in \overline{l_{-,n}}$  and  $\Gamma(s_{+,n}) \in \overline{l_{+,n}}$  for  $n$  sufficiently large. Here  $l_{-,n}$  is the lens-shaped region defined by  $\Gamma(s_n)$ ,  $\Gamma(\sigma_n)$  and  $\delta > 0$ , and  $l_{+,n}$  defined by  $\Gamma(\sigma_n)$ ,  $\Gamma(\tau_n)$  and  $\delta > 0$ , as in Lemma 2. Since  $\text{diam}(l_{\pm,n}) \rightarrow 0$  and  $R_n \rightarrow \delta < \theta$  it follows that  $\delta_{\pm,n} := |\Gamma(s_{\pm,n}) - p_n| < \theta$  for  $n$  sufficiently large, and we may assume that  $\delta_{-,n} \leq \delta_{+,n}$ . This implies  $\Gamma(s_{-,n}) \in \overline{M(s_{+,n}, \delta_{+,n})} \setminus \{\Gamma(s_{+,n})\} \subset M(s_{+,n}, \theta)$ , which contradicts the hypothesis that  $\Gamma(S_L) \cap M(s_0, \theta) = \emptyset$  for all  $s_0 \in S_L$ . Thus we must have  $\Delta[\gamma] \geq \theta$  as claimed.

4. To establish the claim in item (ii) we assume  $\Delta[\gamma] \geq \theta$  and we consider any two points  $P_1 = \Gamma(s_1)$  and  $P_2 = \Gamma(s_2)$  ( $s_1, s_2 \in S_L$ ) that realize the diameter, i.e.,  $d := \text{diam } \Gamma(S_L) = |P_1 - P_2|$ . Then the function  $f_1(\tau) := |P_1 - \Gamma(\tau)|$  has a local maximum at  $s_2$ , and  $f_2(\tau) := |P_2 - \Gamma(\tau)|$  at  $s_1$ . Since  $\Gamma \in C^{1,1}(S_L, \mathbb{R}^3)$  we deduce that the tangent vectors  $\Gamma'(s_1)$  and  $\Gamma'(s_2)$  must be perpendicular to the chord  $\Gamma(s_1) - \Gamma(s_2)$ . Assuming  $d < 2\theta$  we arrive at a contradiction to item (i), since then  $\Gamma(s_1) \in M(s_2, \theta)$ . Thus we must have  $d \geq 2\theta$  as claimed.

5. The first claim in item (iii) is that if  $\Delta[\gamma] \geq \theta > 0$ , then the tubular neighbourhood  $B_\theta(\Gamma(S_L))$  is regular as defined in Section 2.1. To show that the closest-point projection map  $\Pi_\Gamma$  is well-defined for  $x \in B_\theta(\Gamma(S_L))$ , we note that if  $\text{dist}(x, \Gamma(S_L)) = 0$ , then  $x = \Pi_\Gamma(x)$  is well-defined since  $\gamma$  is simple by Lemma 1. If  $0 < \text{dist}(x, \Gamma(S_L)) < \theta$ , then there is at least one point  $s \in S_L$  such that  $|x - \Gamma(s)| = \text{dist}(x, \Gamma(S_L))$  since  $\Gamma(S_L)$  is a compact set. For any such  $s$  the differentiable function  $f(t) := |x - \Gamma(t)|^2$  has the property  $f(t) \geq f(s) := \delta^2$

for all  $t \in S_L$  where  $\delta < \theta$ . Thus  $0 = f'(s) = 2\langle x - \Gamma(s), \Gamma'(s) \rangle$ . If there were another point  $\sigma \in S_L$  with  $f(\sigma) = f(s)$  ( $s \neq \sigma$ ) then

$$\Gamma(\sigma) \in \partial B_\delta(x) \setminus \{\Gamma(s)\} \subset B_\theta(y) \subset M(s, \theta)$$

where  $y := \Gamma(s) + \theta(x - \Gamma(s))/|x - \Gamma(s)|$ , which contradicts item (i). Hence  $\Pi_\Gamma : B_\theta(\Gamma(S_L)) \rightarrow \Gamma(S_L)$  given by  $\Pi_\Gamma(x) := \Gamma(s(x))$  for  $x \in B_\theta(\Gamma(S_L))$  is well-defined. Assuming for contradiction that  $\Pi_\Gamma$  is not continuous, we could find a sequence  $x_n \rightarrow x \in B_\theta(\Gamma(S_L))$  and a constant  $c > 0$  with  $|\Pi_\Gamma(x_n) - \Pi_\Gamma(x)| \geq c$ . Since  $\Gamma(S_L)$  is compact, we may assume that  $\Pi_\Gamma(x_n) \rightarrow p \in \Gamma(S_L)$  with  $|p - \Pi_\Gamma(x)| \geq c$ . Using the continuity of the distance function  $\text{dist}(\cdot, \Gamma(S_L))$  and the uniqueness of  $s(x)$  we obtain

$$\begin{aligned} \text{dist}(x, \Gamma(S_L)) &= |x - \Pi_\Gamma(x)| < |x - p| = \lim_{n \rightarrow \infty} |x_n - \Pi_\Gamma(x_n)| \\ &= \lim_{n \rightarrow \infty} \text{dist}(x_n, \Gamma(S_L)) = \text{dist}(x, \Gamma(S_L)), \end{aligned}$$

which is a contradiction. Thus  $\Pi_\Gamma$  is also continuous and the regularity of  $B_\theta(\Gamma(S_L))$  is established.

6. The second claim in item (iii) is that if  $B_\theta(\Gamma(S_L))$  is regular, then  $\Delta[\gamma] \geq \theta > 0$ . To establish this claim, we assume  $B_\theta(\Gamma(S_L))$  is regular which, by definition, implies that  $\gamma$  is simple. We assume for contradiction that  $\Delta[\gamma] < \theta$ , which implies there is a point  $s_0 \in S_L$  such that  $\rho_G[\gamma](s_0) < \theta$ . Then, by Definition 1, there exist distinct points  $s_1, s_2 \in S_L$  different from  $s_0$  such that  $0 < \rho_G[\gamma](s_0) \leq \delta < \theta$  where  $\delta = R(\Gamma(s_0), \Gamma(s_1), \Gamma(s_2))$ . Moreover, since  $\gamma$  is simple, the points  $\Gamma(s_0)$ ,  $\Gamma(s_1)$  and  $\Gamma(s_2)$  are distinct. These points define a unique circle  $C$  of radius  $\delta$ , and we denote the centre of  $C$  by  $p$ . Without loss of generality we assume  $0 = s_0 < s_1 < s_2 < L$  and we consider the disjoint, open subarcs of  $S_L$  defined by  $D_0 = (s_0, s_1)$ ,  $E_1 = (s_1, s_2)$  and  $E_2 = (s_2, s_0)$ .

Since  $|p - \Gamma(s_i)| = \delta$  ( $i = 0, 1, 2$ ) we have  $\text{dist}(p, \Gamma(S_L)) \leq \delta < \theta$  which implies  $p \in B_\theta(\Gamma(S_L))$ . Moreover, we must have the strict inequality  $\text{dist}(p, \Gamma(S_L)) < \delta$  since by hypothesis there is a unique  $s(p) \in S_L$  such that  $\text{dist}(p, \Gamma(S_L)) = |p - \Gamma(s(p))|$ . Thus  $s(p) \neq s_i$  ( $i = 0, 1, 2$ ) and we may assume  $s(p) \in D_0$ .

We next consider the subarc  $D_1 = E_1 \cup \{s_2\} \cup E_2$  so that  $S_L = D_0 \cup D_1 \cup \{s_0, s_1\}$ , and we consider the line segment between  $p$  and  $\Gamma(s_2)$ , i.e.,

$$x(\alpha) = (1 - \alpha)p + \alpha\Gamma(s_2), \quad \alpha \in [0, 1].$$

This segment has the properties that  $x(0) = p$ ,  $x(1) = \Gamma(s_2)$ ,

$$|x(\alpha) - \Gamma(s_2)| < |x(\alpha) - \Gamma(s_i)|, \quad 0 < \alpha \leq 1 \quad (i = 0, 1)$$

and  $x(\alpha) \in B_\theta(\Gamma(S_L))$  for  $0 \leq \alpha \leq 1$ . To obtain the required contradiction, notice that

$$\begin{aligned} \text{dist}(x(\alpha), \Gamma(S_L)) &\leq |x(\alpha) - \Gamma(s_2)| \\ &< |x(\alpha) - \Gamma(s_i)| \quad 0 < \alpha \leq 1 \quad (i = 0, 1), \end{aligned}$$

which implies  $\Pi_\Gamma(x(\alpha)) \neq \Gamma(s_i)$  for  $0 < \alpha \leq 1$  ( $i = 0, 1$ ). However,  $\Pi_\Gamma(x(0)) = \Gamma(s(p)) \in \Gamma(D_0)$  and  $\Pi_\Gamma(x(1)) = \Gamma(s_2) \in \Gamma(D_1)$ . Thus the image of the line segment  $x(\alpha)$  under the map  $\Pi_\Gamma$  is disconnected. Since this contradicts the hypothesis that  $B_\theta(\Gamma(S_L))$  is regular we must have  $\Delta[\gamma] \geq \theta$  as claimed.

7. To establish the claim in item (iv) we assume that  $B_\theta(\Gamma(S_L))$  is regular. Then for each  $x \in B_\theta(\Gamma(S_L))$  there is a unique  $s = s(x) \in S_L$  such that  $|x - \Gamma(s)| < \theta$  and  $\langle x - \Gamma(s), \Gamma'(s) \rangle = 0$ . Notice that for each point  $x$  in a given normal disk  $D_\theta(s_0) := D_\theta(\Gamma(s_0), \Gamma'(s_0))$  the point  $s_0$  has these properties, which implies  $s(x) = s_0$  for all  $x \in D_\theta(s_0)$ . Thus  $\Pi_\Gamma(D_\theta(s_0)) = \Gamma(s_0)$ . Assuming for contradiction that there is a point  $y \in B_\theta(\Gamma(S_L)) \setminus D_\theta(s_0)$  such that  $\Pi_\Gamma(y) = \Gamma(s_0)$ , we must have  $\langle y - \Gamma(s_0), \Gamma'(s_0) \rangle = 0$ , which implies  $y \in \overline{D_\mu(s_0)} \setminus D_\theta(s_0)$  for some  $\mu \geq \theta$ . However, for such a point we would have  $\text{dist}(y, \Gamma(S_L)) \geq \theta$ , which is a contradiction. The claim follows.  $\square$

*Proof of Lemma 4.* 1. The Sobolev embedding  $W^{1,q}(I, \mathbb{R}^3) \hookrightarrow C^{0,1-1/q}(\bar{I}, \mathbb{R}^3)$  implies uniform convergence

$$\gamma_n \rightarrow \gamma \quad \text{in} \quad C^0(\bar{I}, \mathbb{R}^3). \quad (47)$$

Thus the limit curve  $\gamma$  is closed. Because of Lemma 3 and (47) we have  $\text{diam}(\Gamma(S_L)) \geq 2\theta$ , hence  $L > 0$  and  $\gamma$  is not a single point.

2. The limit curve  $\gamma$  is simple. If this were not the case, we could find  $s_1, s_3 \in S_L$  ( $s_1 \neq s_3$ ) such that  $\Gamma(s_1) = \Gamma(s_3)$ , where we may assume without loss of generality that  $0 = s_1 < s_3 < L$ . Let  $D$  denote the open subarc of  $S_L$  defined by  $(s_1, s_3)$  of length  $|s_3 - s_1|$  and let  $E$  denote the complementary open subarc of length  $L - |s_3 - s_1|$ . Since the curves defined by restricting  $\Gamma$  to  $D$  and  $E$  each have positive length and hence positive diameter, we can find a point  $s_2 \in D$  and a point  $s_4 \in E$  such that  $\Gamma(s_2) \neq \Gamma(s_4)$ , with each of these points distinct from  $\Gamma(s_1)$ . These two points may be found by considering the intersections of  $\Gamma(D)$  and  $\Gamma(E)$  with two spheres of different diameter centred at  $\Gamma(s_1)$ .

Assume without loss of generality that  $0 = s_1 < s_2 < s_3 < s_4 < L$ , let  $\delta := \min\{|\Gamma(s_1) - \Gamma(s_2)|, |\Gamma(s_1) - \Gamma(s_4)|, \theta\}$  and let  $a = t_1 < t_2 < t_3 < t_4 < b$  be parameters such that  $\gamma(t_i) = \Gamma(s_i)$  ( $i = 1, \dots, 4$ ). Moreover, let  $\sigma_i \in S_{L_n}$  be the arclength parameters for  $t_i$  on  $\gamma_n$ , i.e.,  $\Gamma_n(\sigma_i) = \gamma_n(t_i)$  and  $0 = \sigma_1 < \sigma_2 < \sigma_3 < \sigma_4 < L_n$ . Since each curve  $\gamma_n$  satisfies the hypotheses of Lemma 3 we notice first that  $\Pi_{\Gamma_n}$  is continuous on  $B_\theta(\Gamma_n(S_{L_n}))$ . Moreover, from (47) we deduce that there exists an  $N$  such that  $|\gamma_n(t_i) - \gamma(t_i)| < \delta/8$  for all  $n \geq N$  ( $i = 1, \dots, 4$ ).

We next consider the line segment

$$x(\alpha) = \alpha \Gamma_n(\sigma_1) + (1 - \alpha) \Gamma_n(\sigma_3), \quad \alpha \in [0, 1].$$

This segment has the property that  $\text{dist}(x(\alpha), \Gamma_n(S_{L_n})) \leq \delta/4$ , which implies  $x(\alpha) \in B_\theta(\Gamma_n(S_{L_n}))$ , for all  $\alpha \in [0, 1]$  and all  $n \geq N$ . Thus we clearly have the strict inequality

$$|x(\alpha) - \Pi_{\Gamma_n}(x(\alpha))| < 3\delta/8, \quad \forall \alpha \in [0, 1], \quad \forall n \geq N.$$

Since for each  $n \geq N$  we have  $\Pi_{\Gamma_n}(x(0)) = \Gamma_n(\sigma_3)$  and  $\Pi_{\Gamma_n}(x(1)) = \Gamma_n(\sigma_1)$ , but

$$|\Gamma_n(\sigma_i) - x(\alpha)| \geq \delta/2, \quad \forall \alpha \in [0, 1], \quad (i = 2, 4),$$

we conclude that the image of the line segment  $x(\alpha)$  under the continuous map  $\Pi_{\Gamma_n}$  cannot be connected. Since this contradicts the continuity of  $\Pi_{\Gamma_n}$  the curve  $\gamma$  must be simple as claimed.

3. The limit curve  $\gamma$  satisfies the lower bound  $\Delta[\gamma] \geq \theta$ . To establish this claim, we assume for contradiction that there is a point  $s_0 \in S_L$  such that  $\rho_G[\gamma](s_0) < \theta$ . Then, by Definition 1 and the fact that  $\gamma$  is simple, there exist distinct points  $s_1, s_2 \in S_L$  different from  $s_0$  such that

$$R(\Gamma(s_0), \Gamma(s_1), \Gamma(s_2)) = \frac{|\Gamma(s_2) - \Gamma(s_0)|}{2 \sin \alpha} < \theta \quad (48)$$

where  $\alpha := \angle(\Gamma(s_0) - \Gamma(s_1), \Gamma(s_2) - \Gamma(s_1)) \in (0, \pi)$ . By (47), we can find three distinct points  $\Gamma_n(\sigma_i)$  that converge to  $\Gamma(s_i)$  ( $i = 0, 1, 2$ ). For sufficiently large  $n$  we thus have

$$R(\Gamma_n(\sigma_0), \Gamma_n(\sigma_1), \Gamma_n(\sigma_2)) = \frac{|\Gamma_n(\sigma_2) - \Gamma_n(\sigma_0)|}{2 \sin \alpha_n} < \theta$$

where  $\alpha_n := \angle(\Gamma_n(\sigma_0) - \Gamma_n(\sigma_1), \Gamma_n(\sigma_2) - \Gamma_n(\sigma_1)) \in (0, \pi)$ . Since this contradicts the hypothesis  $\Delta[\gamma_n] \geq \theta$  we must have  $\Delta[\gamma] \geq \theta$  as claimed.  $\square$

*Proof of Lemma 5.* By equation (47) we may consider  $n \in \mathbb{N}$  so large that  $\|\gamma_n - \gamma\|_{C^0} < \theta/2$ , in particular  $\gamma(\bar{I}) \subset B_\theta(\Gamma_n(S_{L_n}))$ . It suffices to show that the projection  $\Pi_{\Gamma_n}|_\Gamma : \Gamma \rightarrow \Gamma_n$  is a bijective mapping for  $n$  sufficiently large. In fact, then we can argue as follows: For  $z := \Gamma_n(\sigma)$  and  $z' := \Gamma'_n(\sigma)$  there is exactly one point  $p(z) \in \Gamma(S_L)$  such that  $z = \Pi_{\Gamma_n}(p(z))$ , i.e.,  $p(z) = (\Pi_{\Gamma_n}|_\Gamma)^{-1}(z)$ . Hence we can look at the planar open disks  $D_{\theta/2}(z, z')$  and  $D_{\theta/2}(p(z), z')$  of radius  $\theta/2$  centred at  $z \in \Gamma_n(S_{L_n})$  and  $p(z) \in \Gamma(S_L)$  respectively, perpendicular to  $z'$  and define the open neighbourhoods

$$N_n := \bigcup_{z \in \Gamma_n(S_{L_n})} D_{\theta/2}(z, z') \quad \text{and} \\ \tilde{N}_n := \bigcup_{z \in \Gamma_n(S_{L_n})} D_{\theta/2}(p(z), z').$$

By Lemma 3 we readily see that  $N_n$  is just the open  $\theta/2$ -neighbourhood of  $\Gamma_n(S_{L_n})$  and by (49) below  $\tilde{N}_n$  is an open neighbourhood of  $\Gamma(S_L)$  at least for large  $n \in \mathbb{N}$ . In fact, we can use the same argument as the one at the end of the proof showing that the set  $J_n$  considered there is open for  $n$  sufficiently large.

The desired isotopy  $\gamma(\bar{I}) \simeq \gamma_n(\bar{I}) \simeq \gamma_1(\bar{I})$  for  $n$  sufficiently large is furnished by the following mapping  $\Phi : \tilde{N}_n \times [0, 1] \rightarrow \mathbb{R}^3$  defined as

$$\Phi(x, \tau) := x + \tau [\Pi_{\Gamma_n}(x) - (\Pi_{\Gamma_n}|_\Gamma)^{-1}(\Pi_{\Gamma_n}(x))] \quad \text{for } x \in \tilde{N}_n, \tau \in [0, 1].$$

In fact,  $\Phi$  is continuous with  $\Phi(x, 0) = x$  for all  $x \in \tilde{N}_n$ ,  $\Phi(\tilde{N}_n, 1) = N_n$ , since  $\Phi(\cdot, 1)$  is just the translation of the planar disk  $D_{\theta/2}(p(z), z')$  onto  $D_{\theta/2}(z, z')$  for each  $z \in \Gamma_n(S_{L_n})$ . Moreover, for all  $p \in \Gamma(S_L)$

$$\Phi(p, 1) = p + \Pi_{\Gamma_n}(p) - (\Pi_{\Gamma_n|_{\Gamma}})^{-1}(\Pi_{\Gamma_n}(p)) = p + \Pi_{\Gamma_n}(p) - p = \Pi_{\Gamma_n}(p),$$

hence  $\Phi(\Gamma(S_L), 1) \subset \Gamma_n(S_{L_n})$ . We even get equality, since  $\Pi_{\Gamma_n|_{\Gamma}}$  is surjective. The continuous inverse  $\Phi^{-1}(\cdot, \tau)$  of  $\Phi(\cdot, \tau)$  is given by

$$\Phi^{-1}(\xi, \tau) := \xi - \tau [\Pi_{\Gamma_n}(\xi) - (\Pi_{\Gamma_n|_{\Gamma}})^{-1}(\Pi_{\Gamma_n}(\xi))] \text{ for } \xi \in N_n, \tau \in [0, 1],$$

since for  $\xi \in D_{\theta/2}(z, z')$  one has by Lemma 3

$$\Pi_{\Gamma_n}(\xi) = \Pi_{\Gamma_n}(\xi - \tau [\Pi_{\Gamma_n}(\xi) - (\Pi_{\Gamma_n|_{\Gamma}})^{-1}(\Pi_{\Gamma_n}(\xi))]) = z,$$

which implies  $\Phi(\Phi^{-1}(\xi, \tau), \tau) = \xi$ . This way we obtain  $\gamma(\bar{I}) \simeq \gamma_n(\bar{I})$  for  $n$  sufficiently large and by assumption (i) also  $\gamma(\bar{I}) \simeq \gamma_1(\bar{I})$ .

It remains to show that  $\Pi_{\Gamma_n|_{\Gamma}}$  is bijective for  $n$  sufficiently large. We first claim that for  $s \in S_L$

$$\lim_{n \rightarrow \infty} |\langle \Gamma'(s), \Gamma'_n(\sigma_n) \rangle| = 1, \quad (49)$$

where  $\sigma_n \in S_{L_n}$  is the unique parameter such that  $\Pi_{\Gamma_n}(\Gamma(s)) = \Gamma_n(\sigma_n)$ . Assuming (49) is not true we can find some  $\delta > 0$  such that for all  $n_0 \in \mathbb{N}$  there is  $n \geq n_0$  such that

$$|\langle \Gamma'(s), \Gamma'_n(\sigma_n(s)) \rangle| \leq 1 - \delta. \quad (50)$$

Taking subsequences if necessary we can assume that

$$|\Gamma_n(\sigma_n(s)) - \Gamma(s)| = \text{dist}(\Gamma(s), \Gamma_n) \leq \|\gamma - \gamma_n\|_{C^0(\bar{I}, \mathbb{R}^3)} \leq 1/n. \quad (51)$$

Let  $C_n := C(\sigma_n(s), \theta)$  be the planar circle of radius  $\theta > 0$  centred at  $\Gamma_n(\sigma_n(s))$  perpendicular to  $\Gamma'_n(\sigma_n(s))$  as introduced in Lemma 3 (i). For some  $\epsilon \in (0, \theta)$  to be specified later we look at the set

$$M_n := M(\sigma_n(s), \theta - \epsilon) := \bigcup_{z \in C_n} B_{\theta - \epsilon}(z),$$

and observe that

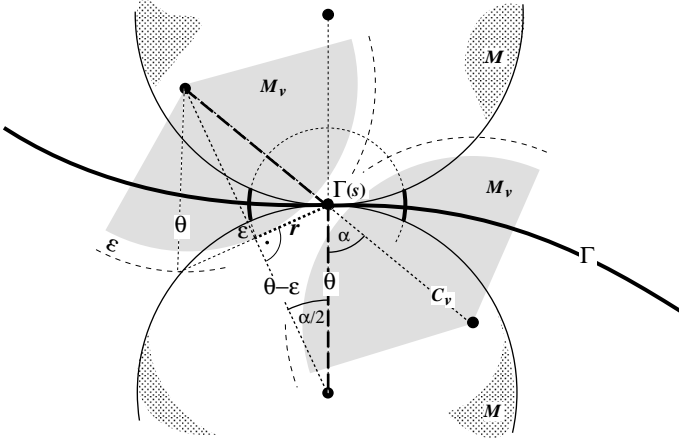
$$M_n \cap B_\epsilon(\Gamma_n) = \emptyset, \quad (52)$$

since  $M(\sigma_n(s), \theta) \cap \Gamma_n(S_{L_n}) = \emptyset$  by Lemma 3 (i) applied to  $\gamma_n \in \mathcal{G}$ . Furthermore the corresponding set  $M := M(s, \theta)$  for  $\Gamma$  at  $\Gamma(s)$  satisfies

$$M \cap \Gamma(S_L) = \emptyset. \quad (53)$$

But (50) implies that  $\Gamma'_n(\sigma_n(s)) \rightarrow v \in S^2$  for  $n \rightarrow \infty$  with

$$|\langle \Gamma'(s), v \rangle| \leq 1 - \delta \quad (54)$$



**Fig. 2.** Two-dimensional illustration of the set  $\partial B_r(\Gamma(s)) - M \subset M_v$ .

for some further subsequence. Together with (51) this implies

$$\text{dist}_H(C_n, C_v) \longrightarrow 0 \text{ for } n \rightarrow \infty, \quad (55)$$

where  $C_v$  is the planar circle of radius  $\theta$  centred at  $\Gamma(s)$  perpendicular to  $v$  and where  $\text{dist}_H(\cdot, \cdot)$  is the Hausdorff distance as in the previous proof.

An elementary geometric argument shows that for  $\alpha := \arccos(1 - \delta) \in (0, \pi/2]$ ,  $r := \theta \sin(\alpha/2)$ ,  $\epsilon := \theta(1 - \cos(\alpha/2))$  and the set

$$M_v := \bigcup_{z \in C_v} B_{\theta - \epsilon}(z)$$

the relation  $(\partial B_r(\Gamma(s)) - M) \subset M_v$ , holds, i.e.,  $\text{dist}(y, C_v) < \theta - \epsilon$  for all  $y \in \partial B_r(\Gamma(s)) - M$ . Now from (55) we infer

$$\text{dist}(y, C_n) < \theta - \epsilon \text{ for all } y \in \partial B_r(\Gamma(s)) - M \text{ for } n \text{ sufficiently large.} \quad (56)$$

Since  $\gamma$  has no double points (see Lemma 4 and 1) and is a closed continuous curve with  $\text{diam}(\gamma(\bar{I})) \geq 2\theta$  (Lemma 3 (ii)), it must intersect  $\partial B_r - M$  by (53), say in  $\Gamma(\tilde{s})$  for some  $\tilde{s} \in S_L$ . This leads to a contradiction, since (51) implies  $\Gamma(\tilde{s}) \in B_\epsilon(\Gamma_n)$  for  $n$  sufficiently large, but on the other hand by (56)  $\Gamma(\tilde{s}) \in M_n$ , i.e.  $\Gamma(\tilde{s}) \notin B_\epsilon(\Gamma_n)$  by (52). Hence (49) is proved.

Now we can show that  $\Pi_{\Gamma_n}|_\Gamma$  is injective for sufficiently large  $n$ . Otherwise there exist infinitely many distinct integers  $m \in \mathbb{N}$  and pairs of distinct parameters  $s_{1m} \neq s_{2m}$  in  $S_L$  such that

$$\Pi_{\Gamma_m}(\Gamma(s_{1m})) = \Gamma_m(\sigma_m(s_{1m})) = \Gamma_m(\sigma_m(s_{2m})) = \Pi_{\Gamma_m}(\Gamma(s_{2m})).$$

Consequently, if  $m$  is chosen large enough,

$$\begin{aligned} |\Gamma(s_{1m}) - \Gamma(s_{2m})| &\leq |\Gamma(s_{1m}) - \Pi_{\Gamma_m}(\Gamma(s_{1m}))| + |\Pi_{\Gamma_m}(\Gamma(s_{2m})) - \Gamma(s_{2m})| \\ &\leq 2\|\gamma - \gamma_m\| \leq 2/m. \end{aligned} \quad (57)$$

In addition, we have by the proof of Lemma 3 (iii)

$$\Gamma(s_{1m}) - \Gamma(s_{2m}) \perp \Gamma'_m(\sigma_m(s_{1m})). \quad (58)$$

A simple geometric observation using (49), (57), (58) now shows that  $\Gamma(s_{2m}) \in M(s_{1m}, \theta)$  for  $m$  sufficiently large, contradicting Lemma 3 (i), which is applicable to  $\Gamma$  by Lemma 4.

Finally we are going to prove that  $\Pi_{\Gamma_n}|_{\Gamma}$  is surjective. We consider the set  $J_n := \{\sigma \in S_{L_n} \mid \Gamma_n(\sigma) \in \Pi_{\Gamma_n}(\Gamma(S_L))\}$  and claim that  $J_n = S_{L_n}$  for  $n$  large enough. Since both  $\Gamma(S_L)$  and  $\Gamma_n(S_{L_n})$  are compact, there is at least one pair of points  $(x, x_n) \in \Gamma(S_L) \times \Gamma_n(S_{L_n})$  such that  $x_n = \Pi_{\Gamma_n}(x)$ , hence  $J_n \neq \emptyset$ .

$J_n$  is also closed, because for a convergent sequence  $\sigma_i \rightarrow \sigma, \sigma_i \in J_n$  we have a sequence  $s_i \in S_L$  with  $\Gamma_n(\sigma_i) = \Pi_{\Gamma_n}(\Gamma(s_i))$ . For a subsequence one has  $s_i \rightarrow s \in S_L$ , hence by continuity we arrive at  $\Gamma_n(\sigma) = \Pi_{\Gamma_n}(\Gamma(s))$ , i.e.  $\sigma \in J_n$ . In order to show that  $J_n$  is open, we observe by Lemma 3 (iv) that we can rewrite  $J_n$  as

$$J_n = \{\sigma \in S_{L_n} \mid \Gamma_n(\sigma) = \Pi_{\Gamma_n}(\Gamma \cap D_\theta(\Gamma_n(\sigma), \Gamma'_n(\sigma)))\},$$

where  $D_\theta(\Gamma_n(\sigma), \Gamma'_n(\sigma))$  denotes the planar disk of radius  $\theta$  perpendicular to  $\Gamma'_n(\sigma)$  centred at  $\Gamma_n(\sigma)$ . Now (49) implies that, for  $n$  sufficiently large,  $\Gamma$  intersects  $D_\theta(\Gamma_n(\sigma), \Gamma'_n(\sigma))$  transversely. Consequently, we have  $D_\theta(\Gamma_n(\bar{\sigma}), \Gamma'_n(\bar{\sigma})) \cap \Gamma(S_L) \neq \emptyset$  for all  $\bar{\sigma} \in S_{L_n}$  with  $|\sigma - \bar{\sigma}|$  sufficiently small and  $n$  sufficiently large, since  $\Gamma'_n$  is Lipschitz continuous. Hence  $J_n$  is open, which finishes the proof that  $J_n = S_{L_n}$ , i.e.  $\Pi_{\Gamma_n}|_{\Gamma}$  is surjective for  $n$  sufficiently large.  $\square$

## 6.2. Proofs for Section 3

*Proof of Lemma 6.* To each framed curved  $(\gamma, D) \in W^{1,q} \times W^{1,p}$  we can associate a unique  $w = w(\gamma, D) \in X_0^{p,q}$  given by (10) as follows. The first equation in (10) is obtained by differentiating the map  $s \mapsto D(s)D(s_0)^{-1}$  at  $s = s_0$  and observing that the tangent space to the manifold  $SO(3) \subset \mathbb{R}^{3 \times 3}$  at the identity is the set of skew matrices [14, II, Ch.17]. The second equation in (10) is just the representation of  $\gamma'(s)$  in the frame  $D(s)$ . Solving these two equations for  $u$  and  $v$  leads to the result

$$u_i = \frac{1}{2} \sum_{j,k=1}^3 \varepsilon_{ijk} \langle d'_j, d_k \rangle \quad \text{and} \quad v_i = \langle \gamma', d_i \rangle \quad (i = 1, 2, 3).$$

Here  $\varepsilon_{ijk} = \langle e_i, e_j \wedge e_k \rangle$  is the permutation symbol where  $e_i$  is the standard basis for  $\mathbb{R}^3$ . Conversely, given  $w = (u, v, \gamma_0, D_0) \in X_0^{p,q}$ , the initial value problem (10) for the frame field has a unique absolutely continuous solution  $D = (d_1|d_2|d_3) \in$



$W^{1,p}(I, \mathbb{R}^{3 \times 3})$ , see e.g., [15, p. 193] or [33, vol.II, p. 1043]. In addition, since  $D(s)$  is continuous and

$$\frac{d}{ds} \langle d_k, d_l \rangle = \langle [\sum_{i=1}^3 u_i d_i] \wedge d_k, d_l \rangle + \langle d_k, [\sum_{i=1}^3 u_i d_i] \wedge d_l \rangle = 0 \quad \text{a.e. in } I,$$

we deduce that  $D(s) \in SO(3)$  for each  $s \in \bar{I}$ . Notice that standard existence results guarantee only a local solution for  $D(s)$ . However, since orthonormality implies boundedness, local solutions can be continued to all of  $[a, b]$ . Once  $D(s)$  is known, the initial value problem for  $\gamma$  may be solved by quadrature, namely

$$\gamma(s) = \gamma_0 + \sum_{k=1}^3 \int_a^s v_k(\tau) d_k(\tau) d\tau. \quad \square$$

*Proof of Lemma 7.* 1. Notice first that  $\gamma \in \mathcal{G}$  and  $\Delta[\gamma] > 0$ , hence  $\gamma$  possesses an arclength parameterization  $\Gamma \in C^{1,1}(S_L, \mathbb{R}^3)$  by Lemma 2. Moreover, since  $|\gamma'| = |v_3| > 0$ , there is a bijection between  $t \in [a, b]$  and  $s \in [0, L]$ . Notice also that, for each fixed  $t \in [a, b]$ , the map  $p(t, \cdot, \cdot)$  is injective and that the image of  $p(t, \cdot, \cdot)$  is the open disk  $D_\theta(\Gamma(s(t)), \Gamma'(s(t)))$  as considered in Lemma 3.

2. Our first claim is that if  $\Delta[\gamma] \geq \theta$ , then  $p : \Omega_\theta \rightarrow \mathbb{R}^3$  is globally injective. To see this, assume for contradiction that  $p$  does not have this property. Then there exists  $t_1, t_2 \in [a, b]$  ( $t_1 \neq t_2$ ), with corresponding arclength parameters  $s_1 \neq s_2$ , such that  $D_\theta(\Gamma(s_1), \Gamma'(s_1)) \cap D_\theta(\Gamma(s_2), \Gamma'(s_2)) \neq \emptyset$ . We denote by  $x$  any point in this intersection. Since  $\Delta[\gamma] \geq \theta$  we may apply Lemma 3 (iii) to conclude that the projection  $\Pi_\Gamma : B_\theta(\Gamma(S_L)) \rightarrow \Gamma(S_L)$  is single-valued, and apply Lemma 3 (iv) to conclude that  $\Pi_\Gamma(x) = \Gamma(s_1)$  and  $\Pi_\Gamma(x) = \Gamma(s_2)$ , which is a contradiction. Thus  $p : \Omega_\theta \rightarrow \mathbb{R}^3$  must be globally injective.

3. Our second claim is that if  $p : \Omega_\theta \rightarrow \mathbb{R}^3$  is globally injective, then  $\Delta[\gamma] \geq \theta$ . To see this, assume for contradiction that  $0 < \Delta[\gamma] < \theta$  and consider any  $\eta$  such that  $\Delta[\gamma] < \eta < \theta$ . Then by Lemma 3 (i) there is a parameter  $s_* \in S_L$  such that  $\Gamma(S_L) \cap M(s_*, \eta) \neq \emptyset$ . This implies there is a point  $z_* \in C(s_*, \eta) = \partial D_\eta(\Gamma(s_*), \Gamma'(s_*))$  such that  $\text{dist}(z_*, \Gamma(S_L)) < \eta$ . By compactness, there is a point  $\bar{s}$  such that  $\text{dist}(z_*, \Gamma(S_L)) = |z_* - \Gamma(\bar{s})|$ , and  $\bar{s} \neq s_*$  since  $|z_* - \Gamma(\bar{s})| < \eta$ . Moreover,  $\langle z_* - \Gamma(\bar{s}), \Gamma'(\bar{s}) \rangle = 0$ . Since  $\eta < \theta$  we have  $z_* \in D_\theta(\Gamma(\bar{s}), \Gamma'(\bar{s}))$  and also  $z_* \in D_\theta(\Gamma(s_*), \Gamma'(s_*))$ , which contradicts the global injectivity of  $p : \Omega_\theta \rightarrow \mathbb{R}^3$ . Thus  $\Delta[\gamma] \geq \theta$  as claimed.  $\square$

*Proof of Theorem 1.* Since  $C \neq \emptyset$  we may assume there is some  $\tilde{w} \in C$  with  $E(\tilde{w}) < \infty$ ; otherwise, any  $w \in C$  will satisfy (13) with infinite energy. Thus, any minimizing sequence  $\{w_n\}_{n \in \mathbb{N}} = \{(u_n, v_n, \gamma_{0,n}, D_{0,n})\}_{n \in \mathbb{N}} \subset C$  stays bounded in  $X^{p,q}$  since

$$\lim_{n \rightarrow \infty} E(w_n) = \inf_{w \in C} E(w) \leq E(\tilde{w}) < \infty.$$

To see this, notice that condition (W3) guarantees in all three cases (i)-(iii) that  $\|u_n\|_{L^p}$  and  $\|v_n\|_{L^q}$  are uniformly bounded for all  $n \in \mathbb{N}$ . Moreover,  $SO(3)$  is compact in  $\mathbb{R}^{3 \times 3}$  and, by assumption,  $|\gamma_{0,n}| \leq c$  for all  $n \in \mathbb{N}$ .

Since  $\{w_n\}$  is bounded and the space  $X^{p,q}$  ( $p, q > 1$ ) is reflexive, there is a weakly convergent subsequence  $w_{n_k} \rightharpoonup w_* \in X^{p,q}$ . In particular, we have  $(u_{n_k}, v_{n_k}) \rightharpoonup (u_*, v_*) \in L^p(I, \mathbb{R}^3) \times L^q(I, \mathbb{R}^3)$  and  $(\gamma_{0,n_k}, D_{0,n_k}) \rightarrow (\gamma_{0,*}, D_{0,*}) \in \mathbb{R}^3 \times SO(3)$  as  $k \rightarrow \infty$ . Moreover,  $w_* \in C$  because  $C$  is weakly closed. Since conditions (W1)-(W3) imply that  $E$  is weakly lower-semicontinuous on  $X^{p,q}$  (see, e.g., [5, Thm. 3.4, p. 74]), we deduce  $E(w_*) = \inf_{w \in C} E(w)$ . Thus  $E$  attains a global minimum at the point  $w_* \in C$ .  $\square$

*Proof of Lemma 8.* 1. Given  $1 < p, q < \infty$  and  $\{w_n\} \subset X_0^{p,q}$  we are assuming  $w_n \rightharpoonup w$  in  $X^{p,q}$  where  $w_n = (u_n, v_n, \gamma_{0,n}, D_{0,n})$  and  $w = (u, v, \gamma_0, D_0)$ . Notice first that, since  $D_{0,n} \in SO(3) \subset \mathbb{R}^{3 \times 3}$  and  $D_{0,n} \rightarrow D_0$  we have  $D \in SO(3)$ . This implies that  $w \in X_0^{p,q}$  as claimed.

2. In (14) we claim that weak convergence of the shape and placement variables  $w_n$  implies convergence in  $C^0$  of the framed curves  $(\gamma_n, D_n)$ . To establish this result, we note first that  $u_n \rightharpoonup u$  in  $L^p(I, \mathbb{R}^3)$  implies there is a constant  $c > 0$  such that  $\|u_n\|_{L^p} \leq c < \infty$  for all  $n \in \mathbb{N}$ . Let  $d_{1,n}$  denote the first column of  $D_n$ ,  $d_1$  the first column of  $D$ , and consider any  $t_1 \in (a, b)$  such that  $|t_1 - a| \leq (3c)^{-p^*}$  where  $1/p^* + 1/p = 1$ . Then, by continuity, there is a  $\sigma_n \in [a, t_1]$  such that

$$|d_{1,n}(\sigma_n) - d_1(\sigma_n)| = \max_{\tau \in [a, t_1]} |d_{1,n}(\tau) - d_1(\tau)|, \quad (59)$$

and by compactness we can find a subsequence (keeping the index  $n$  for convenience)  $\sigma_n \rightarrow \sigma \in [a, t_1]$ . From (59) and an integrated version of (10) we obtain

$$\begin{aligned} \|d_{1,n} - d_1\|_{C^0([a, t_1], \mathbb{R}^3)} &= |d_{1,n}(\sigma_n) - d_1(\sigma_n)| \\ &= \left| d_{1,n}^0 + \int_a^{\sigma_n} \left[ \sum_{i=2}^3 u_{i,n}(\tau) d_{i,n}(\tau) \right] \wedge d_{1,n}(\tau) d\tau \right. \\ &\quad \left. - d_1^0 - \int_a^{\sigma_n} \left[ \sum_{i=2}^3 u_i(\tau) d_i(\tau) \right] \wedge d_1(\tau) d\tau \right| \end{aligned}$$

where  $d_{1,n}^0$  denotes the first column of  $D_{0,n}$  and so on. Expanding the vector products, rearranging terms and applying the triangle inequality leads to

$$\begin{aligned} \|d_{1,n} - d_1\|_{C^0([a, t_1], \mathbb{R}^3)} &\leq |d_{1,n}^0 - d_1^0| \\ &\quad + \left| \int_a^{\sigma_n} \{ [u_{3,n}(\tau) - u_3(\tau)] d_2(\tau) + [u_2(\tau) - u_{2,n}(\tau)] d_3(\tau) \} d\tau \right| \\ &\quad + \left| \int_a^{\sigma_n} \{ u_{3,n}(\tau) [d_{2,n}(\tau) - d_2(\tau)] + u_{2,n}(\tau) [d_3(\tau) - d_{3,n}(\tau)] \} d\tau \right|. \end{aligned}$$

Since  $u_n$  is bounded in  $L^p$  this implies

$$\begin{aligned} & \|d_{1,n} - d_1\|_{C^0([a,t_1],\mathbb{R}^3)} \leq |d_{1,n}^0 - d_1^0| \\ & + \left| \int_a^b \{[u_{3,n}(\tau) - u_3(\tau)]d_2(\tau) + [u_2(\tau) - u_{2,n}(\tau)]d_3(\tau)\} \chi_{[a,\sigma_n]}(\tau) d\tau \right| \\ & + |\sigma_n - a|^{1/p^*} \|u_n\|_{L^p} \sum_{i=2}^3 \|d_{i,n} - d_i\|_{C^0([a,t_1],\mathbb{R}^3)}, \end{aligned}$$

and by choice of  $t_1$  and  $\sigma_n$  we obtain

$$\begin{aligned} & \|d_{1,n} - d_1\|_{C^0([a,t_1],\mathbb{R}^3)} \leq |d_{1,n}^0 - d_1^0| \\ & + \left| \int_a^b \{[u_{3,n}(\tau) - u_3(\tau)]d_2(\tau) + [u_2(\tau) - u_{2,n}(\tau)]d_3(\tau)\} \chi_{[a,\sigma_n]}(\tau) d\tau \right| \\ & + \frac{1}{3} \sum_{i=2}^3 \|d_{i,n} - d_i\|_{C^0([a,t_1],\mathbb{R}^3)} \end{aligned} \quad (60)$$

where  $\chi_{[a,\sigma_n]}$  is the characteristic function for the interval  $[a, \sigma_n]$ . By Lebesgue's theorem of dominated convergence we have

$$d_2 \chi_{[a,\sigma_n]} \rightarrow d_2 \chi_{[a,\sigma]} \quad \text{and} \quad d_3 \chi_{[a,\sigma_n]} \rightarrow d_3 \chi_{[a,\sigma]} \quad \text{in} \quad L^{p^*}(I, \mathbb{R}^3).$$

Using this result, together with the facts that  $u_n \rightharpoonup u$  in  $L^p$  and  $d_{1,n}^0 \rightarrow d_1^0$ , we deduce from (60) that for any  $\epsilon > 0$  there is an  $N$  such that

$$\|d_{1,n} - d_1\|_{C^0([a,t_1],\mathbb{R}^3)} \leq \frac{1}{3} \sum_{i=2}^3 \|d_{i,n} - d_i\|_{C^0([a,t_1],\mathbb{R}^3)} + \epsilon/9, \quad \forall n \geq N.$$

Taking further subsequences, we can deduce analogous inequalities for  $\|d_{i,n} - d_i\|_{C^0([a,t_1],\mathbb{R}^3)}$  ( $i = 2, 3$ ), which after summation gives

$$\sum_{i=1}^3 \|d_{i,n} - d_i\|_{C^0([a,t_1],\mathbb{R}^3)} \leq \frac{2}{3} \sum_{i=1}^3 \|d_{i,n} - d_i\|_{C^0([a,t_1],\mathbb{R}^3)} + \epsilon/3$$

and consequently

$$\sum_{i=1}^3 \|d_{i,n} - d_i\|_{C^0([a,t_1],\mathbb{R}^3)} \leq \epsilon, \quad \forall n \geq N. \quad (61)$$

This implies convergence on the subinterval  $[a, t_1]$ . However, we can then consider any  $t_2 > t_1$  such that  $|t_2 - t_1| \leq (3c)^{-p^*}$ , and using  $d_{i,n}(t_1)$  instead of  $d_{i,n}^0$  and so on, we can obtain an estimate analogous to (61) on  $[t_1, t_2]$ . Hence, after finitely many steps, we cover the interval  $\bar{I} = [a, b]$  and obtain  $D_n \rightarrow D$  in  $C^0(\bar{I}, \mathbb{R}^{3 \times 3})$  for some subsequence.

Continuing with the subsequence of  $(\gamma_n, D_n)$  found above, we can find for each  $n$  a parameter  $s_n \in [a, b]$  such that

$$|\gamma_n(s_n) - \gamma(s_n)| = \max_{\tau \in [a, b]} |\gamma_n(\tau) - \gamma(\tau)|. \quad (62)$$

By compactness, we can extract a further subsequence (again indicated by  $n$ ) such that  $s_n \rightarrow s \in [a, b]$ . From (62) and an integrated version of (10) we obtain

$$\begin{aligned} \|\gamma_n - \gamma\|_{C^0(\bar{I}, \mathbb{R}^3)} &= |\gamma_n(s_n) - \gamma(s_n)| \\ &= \left| \gamma_{0,n} + \int_a^{s_n} \sum_{k=1}^3 v_{k,n}(\tau) d_{k,n}(\tau) d\tau - \gamma_0 - \int_a^{s_n} \sum_{k=1}^3 v_k(\tau) d_k(\tau) d\tau \right|. \end{aligned}$$

Rearranging terms, applying the triangle inequality and employing the characteristic function for  $[a, s_n]$  leads to

$$\begin{aligned} \|\gamma_n - \gamma\|_{C^0(\bar{I}, \mathbb{R}^3)} &\leq |\gamma_{0,n} - \gamma_0| \\ &+ \sum_{k=1}^3 \left| \int_a^b v_{k,n}(\tau) [d_{k,n}(\tau) - d_k(\tau)] \chi_{[a, s_n]} d\tau \right| \\ &+ \sum_{k=1}^3 \left| \int_a^b [v_{k,n}(\tau) - v_k(\tau)] d_k(\tau) \chi_{[a, s_n]} d\tau \right|, \end{aligned}$$

and since the subsequence  $D_n$  converges in  $C^0$  we obtain

$$\begin{aligned} \|\gamma_n - \gamma\|_{C^0(\bar{I}, \mathbb{R}^3)} &\leq |\gamma_{0,n} - \gamma_0| + \|D_n - D\|_{C^0(\bar{I}, \mathbb{R}^3 \times \mathbb{R}^3)} \|v_n\|_{L^1(I, \mathbb{R}^3)} \\ &+ \sum_{k=1}^3 \left| \int_a^b [v_{k,n}(\tau) - v_k(\tau)] d_k(\tau) \chi_{[a, s_n]} d\tau \right|. \end{aligned} \quad (63)$$

For each  $k = 1, 2, 3$  we have as before that

$$d_k \chi_{[a, s_n]} \rightarrow d_k \chi_{[a, s]} \quad \text{in } L^{q^*}(I, \mathbb{R}^3)$$

where  $1/q^* + 1/q = 1$ . Thus, we conclude that the right-hand side of (63) converges to zero as  $n \rightarrow \infty$ . Hence  $\gamma_n \rightarrow \gamma$  in  $C^0(\bar{I}, \mathbb{R}^3)$  for some subsequence. Since the previous arguments apply to any subsequence of  $\{w_n\}_{n \in \mathbb{N}} \subset X_0^{p,q}$ , and the same limits  $D$  and  $\gamma$  are obtained, the whole sequence must satisfy (14) as claimed.

3. In (15) we claim that weak convergence of the shape and placement variables  $w_n$  implies weak convergence in  $W^{1,q} \times W^{1,p}$  of the framed curves  $(\gamma_n, D_n)$ . To see this, we multiply (10) by an arbitrary element  $g \in L^{q^*}(I, \mathbb{R}^3)$  ( $1/q^* + 1/q = 1$ ) and integrate to obtain

$$\int_I \langle \gamma'_n(\tau), g(\tau) \rangle d\tau = \int_I \sum_{k=1}^3 v_{k,n}(\tau) \langle d_{k,n}(\tau), g(\tau) \rangle d\tau. \quad (64)$$

Since by (14) we have  $\langle d_{k,n}, g \rangle \rightarrow \langle d_k, g \rangle$  in  $L^{q^*}(I, \mathbb{R})$ , and by assumption we have  $v_{k,n} \rightharpoonup v_k$  in  $L^q(I, \mathbb{R})$  for  $k = 1, 2, 3$ , we obtain

$$\int_I \langle \gamma'_n(\tau), g(\tau) \rangle d\tau \rightarrow \int_I \langle \gamma'(\tau), g(\tau) \rangle d\tau, \quad \forall g \in L^{q^*}(I, \mathbb{R}^3).$$

This implies  $\gamma'_n \rightharpoonup \gamma'$  in  $L^q(I, \mathbb{R}^3)$ . Moreover, by (14), we also have  $\gamma_n \rightarrow \gamma$  in  $L^q(I, \mathbb{R}^3)$ . This readily implies that  $\gamma_n \rightharpoonup \gamma$  in  $W^{1,q}$  as claimed. By applying the same reasoning to  $D_n$  the result (15) is established.  $\square$

*Proof of Lemma 9.* To establish the result for  $C_1$ , we note first that a sequence  $\{w_n\}_{n \in \mathbb{N}} \subset C_1$  that converges strongly  $w_n \rightarrow w$  in  $X^{p,q}$  contains a subsequence  $\{w_{n_k}\}_{k \in \mathbb{N}} \subset C_1$  such that  $w_{n_k}(s) \rightarrow w(s)$  for a.e.  $s \in I$ . Since  $K(s)$  is closed for a.e.  $s \in I$ , we have  $w(s) \in K(s)$  for a.e.  $s \in I$ , which implies  $w \in C_1$ . Thus  $C_1$  is strongly closed. Furthermore,  $C_1$  is convex since  $K(s)$  is convex for a.e.  $s \in I$ . Thus  $C_1$  is also weakly closed [23, Thm 3.12] as claimed. The result for  $C_2$  follows directly from Lemma 8.  $\square$

*Proof of Lemma 10.* The elements  $Q \in SO(3)$  can be represented by a vector  $\xi(Q) \in \mathbb{R}^3$  where the direction of  $\xi(Q)$  describes the rotation axis and the length of  $\xi(Q)$  gives the rotation angle in  $[-\pi, \pi]$ . In a neighbourhood of the identity in  $SO(3)$ , the mapping  $Q \mapsto \xi(Q) \in \mathbb{R}^3$  is uniquely defined and continuous as well as the inversion  $\xi \mapsto Q(\xi) \in SO(3)$ . In particular, we have  $Q(\xi(Q)) = Q$ ,  $\xi(Id) = 0 \in \mathbb{R}^3$  and  $Q(0) = Id \in SO(3)$ . By Lemma 8, we have  $w \in X_0^{p,q}$  and  $D_n \rightarrow D$  in  $C^0$ , which implies  $D(a) = D_n(a)$  and  $D(b) = D_n(b)$  for all  $n \in \mathbb{N}$  since  $D_n \sim D_1$ . Furthermore, the continuity of  $A \mapsto A^{-1}$  in  $GL(3)$  (Cramer's Rule) implies that  $D(s)D_n(s)^{-1}$  is continuous in  $s$  and uniformly close to the identity for all  $n \in \mathbb{N}$  sufficiently large. With this in mind, we consider the homotopy map

$$\Psi(s, \tau) := Q(\tau \xi(D(s)D_n(s)^{-1}))D_n(s), \quad s \in [a, b], \quad \tau \in [0, 1].$$

Notice that  $\Psi(s, 0) = D_n(s)$  and  $\Psi(s, 1) = D(s)$  for all  $s \in [a, b]$ , and that  $\Psi : [a, b] \times [0, 1] \rightarrow SO(3)$  is continuous. Moreover, it is straightforward to show that  $\Psi(a, \tau) = D_n(a)$  and  $\Psi(b, \tau) = D_n(b)$  for all  $\tau \in [0, 1]$ . Hence,  $D \sim D_n$  for all  $n$  sufficiently large. Since  $D_n \sim D_1$  for all  $n \in \mathbb{N}$  we conclude that  $D \sim D_1$  as claimed.  $\square$

### 6.3. Proofs for Section 4

*Proof of Equation (21).* Since  $\gamma' = v_3 d_3$  for the unshearable extensible case, the arclength of  $\gamma$  is given by

$$[a, b] \ni t \mapsto s(t) := \int_a^t v_3(\tau) d\tau \in [0, L].$$

This map is strictly monotone by (18), hence invertible. Denoting the inverse function by  $\tau : [0, L] \rightarrow [a, b]$ , we form the composition  $\Gamma := \gamma \circ \tau : [0, L] \rightarrow \mathbb{R}^3$  and compute the derivatives

$$\begin{aligned}\Gamma'(s) &= \gamma'(\tau(s)) \frac{d}{ds} \tau(s) = v_3(\tau(s)) d_3(\tau(s)) \frac{1}{v_3(\tau(s))} = d_3(\tau(s)) \\ \Gamma''(s) &= d'_3(\tau(s)) \frac{d}{ds} \tau(s) = d'_3(\tau(s)) \frac{1}{v_3(\tau(s))}.\end{aligned}$$

From (10) we deduce  $d'_3 = -u_1 d_2 + u_2 d_1$ , which proves the formulas for  $\Gamma''$  and the curvature  $\kappa$  given in (21).  $\square$

*Proof of Theorem 2.* Let  $C$  be the subset of elements  $w \in X_0^p \subset X^{p,q}$ ,  $q \in (1, \infty)$ , that satisfy conditions (25)-(28), which by assumption is non-empty. We claim that  $C$  is weakly closed. To see this, notice that Lemma 9 (ii) applies to condition (25), Lemma 8 and Lemma 4 apply to condition (26), Lemma 5 applies to condition (27) and Lemma 10 applies to condition (28), which establishes the claim. The existence result now follows from Theorem 1 (ii), which is applicable since conditions (W1)-(W3) are satisfied with  $c_2 = 0$  and  $\gamma_0 = 0$ . The regularity statement follows from Lemma 2 by (26) and from  $\gamma'[w] = d_3[w] \in W^{1,p}(I, \mathbb{R}^3)$ .  $\square$

*Proof of Theorem 3.* The result follows from Theorem 1 (i) and arguments similar to those used in the proof of Theorem 2.  $\square$

#### 6.4. Proof of Theorem 4

Let  $C$  be the subset of elements  $w \in X_0^q \subset X^{p,q}$  that satisfy the conditions in (38). Notice that  $C$  is non-empty by assumption ( $\tilde{w} = w[\tilde{\gamma}]$  is in this set), and by Lemmas 9 (ii), 4 and 5, it is also weakly closed. Moreover, for any  $1 < q < \infty$ , notice that the modified energy

$$E_q(w) := \int_a^b |v(\sigma)|^q d\sigma$$

has a minimizer  $w_* \in C$ . This follows from Theorem 1 (iii).

We claim that  $w_*$  also minimizes the desired energy  $E(w)$ . To see this, consider any  $w_1 \in C$ , let  $\gamma_1 = \gamma[w_1]$  be the corresponding curve with arclength parameterization  $\Gamma_1$  and define an auxiliary curve

$$\gamma_2(\tau) := \Gamma_1(L_1(\tau - a)/(b - a)), \quad \tau \in [a, b],$$

where  $L_1 := \int_a^b |\gamma'_1(\sigma)| d\sigma = E(w_1)$ . Notice that  $L_1 < \infty$  since  $\gamma'_1 \in L^q$ ,

$$\left| \frac{d}{d\tau} \gamma_2(\tau) \right| \equiv \frac{L_1}{b - a} = \frac{E(w_1)}{b - a}$$

and that  $w_2 = w[\gamma_2]$  is also in  $C$ . Using the definitions of  $E$  and  $E_q$ , together with Hölder's inequality, we have

$$\begin{aligned} [E(w_*)]^q &:= \left[ \int_a^b |\gamma'_*(\tau)| \, d\tau \right]^q \\ &\leq (b-a)^{q-1} \int_a^b |\gamma'_*(\tau)|^q \, d\tau =: (b-a)^{q-1} E_q(w_*). \end{aligned}$$

Moreover, since  $w_*$  is a minimizer of  $E_q$  and  $|\gamma'_2| = E(w_1)/(b-a)$  is constant, we obtain

$$[E(w_*)]^q \leq (b-a)^{q-1} E_q(w_*) \leq (b-a)^{q-1} E_q(w_2) = [E(w_1)]^q.$$

Since this inequality holds for arbitrary  $w_1 \in C$  we conclude that  $w_* \in C$  is a minimizer of  $E$  as claimed. The regularity statement that  $\Gamma_* \in C^{1,1}(S_{L_*}, \mathbb{R}^3)$  follows from Lemma 2.  $\square$

*Acknowledgements.* It is a pleasure to thank A. Goriely, A. Stasiak and M.J. Tilby for making the image data for Fig. 1a and 1b available, and T. Ilmanen for his insightful comments. The following generous support is gratefully acknowledged: OG the US and Swiss National Science Foundations, JHM the Swiss National Science Foundation, FS and HvdM, the Sonderforschungsbereich 256 at the University of Bonn, and the Max-Planck Institute for Mathematics in the Sciences in Leipzig.

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**Note added in proof:** A different analytical approach to enforcing global injectivity is presented in: F. Schuricht, Global injectivity and topological constraints for spatial nonlinearly elastic rods, *MPI for Mathematics in the Sciences*, Leipzig, Preprint 1, 2001.