

On rectifiable curves with L^p -bounds on global curvature: self-avoidance, regularity, and minimizing knots

Paweł Strzelecki · Heiko von der Mosel

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Abstract We discuss the analytic properties of curves γ whose global curvature function $\rho_G[\gamma]^{-1}$ is p -integrable. It turns out that the L^p -norm $\mathcal{U}_p(\gamma) := \|\rho_G[\gamma]^{-1}\|_{L^p}$ is an appropriate model for a self-avoidance energy interpolating between “soft” knot energies in form of singular repulsive potentials and “hard” self-obstacles, such as a lower bound on the global radius of curvature introduced by Gonzalez and Maddocks. We show in particular that for all $p > 1$ finite \mathcal{U}_p -energy is necessary and sufficient for $W^{2,p}$ -regularity and embeddedness of the curve. Moreover, compactness and lower-semicontinuity theorems lead to the existence of \mathcal{U}_p -minimizing curves in given isotopy classes. There are obvious extensions to other variational problems for curves and nonlinearly elastic rods, where one can introduce a bound on \mathcal{U}_p to preclude self-intersections.

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1 Introduction

A central issue in the mathematical modeling of physical strands, such as rope, string or wire, or—on a much smaller length scale—polymers and proteins, is the enforcement of self-avoidance in order to guarantee that the geometric objects are embedded. Standard continuum models incorporating self-avoidance are usually based on pairwise repulsive, and therefore singular, potentials, which require some sort of regularization [17], [11], [13], [44], [28], [5], [37]. Typical examples are *knot energies* introduced by

P. Strzelecki
Instytut Matematyki, Uniwersytet Warszawski, ul. Banacha 2, 02-097 Warsaw, Poland
e-mail: pawelst@mimuw.edu.pl

H. von der Mosel (✉)
Institut für Mathematik, RWTH Aachen, Templergraben 55, 52062 Aachen, Germany
e-mail: heiko@instmath.rwth-aachen.de

O’Hara [36] in the search of optimal knot representatives as energy minimizers within a given knot class. The basic idea is to integrate twice an inverse power of the Euclidean distance over a closed curve $\gamma : S^1 \rightarrow \mathbb{R}^3$ to account for the mutual repulsion of every pair of distinct points on the curve. Without any regularization one would obtain the singular double integral

$$\int_{S^1} \int_{S^1} \frac{1}{|\gamma(s) - \gamma(t)|^p} ds dt, \quad p \geq 2, \tag{1.1}$$

which is infinite for *any* continuous curve due to the effect that $\gamma(s) \rightarrow \gamma(t)$ as $s \rightarrow t$. There are several ways to remove this divergence, for instance, by subtracting some equally divergent terms, or by a multiplicative factor with a suitable decay as $s \rightarrow t$. This variety of possible regularizations, on the other hand, reflects the physically undesirable lack of an intrinsic length scale on which repulsive interaction between neighbouring points on the curve is cut off. Moreover, the mathematical analysis of such singular integrals is quite complicated, only for O’Hara’s energy (1.1) for $p = 2$ a satisfactory existence and regularity theory for minimizing knots is developed [16], [27], see also [39]. Linear combinations of self-avoidance energies of type (1.1) with curvature dependent elastic energies were investigated in [36], [50]. Higher-dimensional analogues of (1.1) for surfaces or general submanifolds in \mathbb{R}^n were suggested by Kusner and Sullivan [29], but no existence or regularity result seems to be known.

In contrast to the approach using “soft” repulsive potentials without any inherent length scale for the thickness of the curves, one can prescribe a “hard” steric constraint. One may think of a tubular neighborhood of a fixed radius with the curve as its centerline as a so-called *excluded volume constraint*, or various other self-obstacle conditions, to impose a positive thickness of the curve [6], [12], [30], [34], [51], [14], [15]. In that context the *global radius of curvature* introduced by Gonzalez and Maddocks [20] turned out to be both a mathematically precise and analytically tractable notion to tackle energy minimization problems in nonlinear elasticity and knot theory for curves and rods with a given thickness [22], [8], [19]. Instead of the Euclidean distance as interaction function for two points as in (1.1), one considers here the circumcircle radius $R(\cdot, \cdot, \cdot)$ as a function of *three* points on the curve. Then the thickness constraint is given by a prescribed positive lower bound on this specific *multipoint function* R if one varies among all possible triplets of distinct points along the curve.

To be more precise, let $S_L := \mathbb{R}/L\mathbb{Z}$, $L > 0$, denote the circle with perimeter L , and denote by $\Gamma : S_L \rightarrow \mathbb{R}^3$ the arclength parametrization of a closed rectifiable curve $\gamma : S^1 \rightarrow \mathbb{R}^3$. Then the *global radius of curvature function* $\rho_G[\gamma] : S_L \rightarrow \mathbb{R}$ is defined as

$$\rho_G[\gamma](s) := \inf_{\substack{\sigma, \tau \in S_L \setminus \{s\} \\ \sigma \neq \tau}} R(\Gamma(s), \Gamma(\sigma), \Gamma(\tau)), \quad s \in S_L, \tag{1.2}$$

and the *global radius of curvature* $\Delta[\gamma]$ of γ is given by

$$\Delta[\gamma] := \inf_{s \in S_L} \rho_G[\gamma](s). \tag{1.3}$$

To impose a positive thickness $\theta > 0$ for the curve γ one requires the inequality

$$\Delta[\gamma] \geq \theta. \tag{1.4}$$

The analytic properties of R , ρ_G , $\Delta[\cdot]$, and several related multi-point functions are well investigated [20], [21], [45], [41], [18]; (see [47], [48] for surfaces). Due to the nonsmooth character of $\Delta[\cdot]$, however, the regularity theory for (a priori nonsmooth) maximizers of (1.3), or minimizers of other variational problems constrained by (1.4), turned out to be quite challenging, see [42], [43], [7], [14]. Moreover, the numerical treatment of such nonsmooth constraints with gradient methods seems rather complicated, at present we are only aware of recent work by Cantarella et al. [9] on a numerical gradient flow.

Banavar et al. [3] suggested to integrate over multi-point functions mainly to avoid the natural singularities of the repulsive potentials, so that no regularization is required. In fact, for a smooth simple closed curve $\Gamma : S_L \rightarrow \mathbb{R}^3$ the circumcircle radius $R(\Gamma(s), \Gamma(\sigma), \Gamma(\tau))$ tends to the classical local radius of curvature and not to zero as $\sigma, \tau \rightarrow s$. Therefore, the multiple integral

$$\int_{S_L} \int_{S_L} \int_{S_L} \frac{1}{R^p(\Gamma(s), \Gamma(\sigma), \Gamma(\tau))} ds d\sigma d\tau \tag{1.5}$$

is finite. Numerical investigations by Banavar and co-workers using this concept lead to considerable progress in the protein science [4], [2], [35], but there are apparently only very few analytical contributions regarding (1.5). For $p = 2$ this energy functional is called the *total Menger curvature*, and Léger [32] could show with sophisticated measure-theoretic tools that one-dimensional Borel sets with bounded total Menger curvature are 1-rectifiable, i.e. these sets are essentially contained in a union of Lipschitz graphs; for $p \neq 2$ see [33], and for a more general setting in metric spaces see [25], [26]. However, we are unaware of any existence or regularity result for energy minimizing curves for (1.5).

As a first step towards a deeper analytic understanding of (1.5) we are going to investigate a closely related self-avoidance energy blending the concept of global radius of curvature and integration, as was already proposed by Gonzalez and Maddocks in [20, p. 4772]. Namely, we look at the L^p -norm of $1/\rho_G$, that is,

$$\mathcal{U}_p(\gamma) := \left(\int_{S_L} \frac{1}{\rho_G[\gamma](s)^p} ds \right)^{1/p}, \quad p \geq 1, \tag{1.6}$$

whose limit $p \rightarrow \infty$ is the global radius of curvature $\Delta[\gamma]$. One may view \mathcal{U}_p as an intermediate “semi-soft” energy interpolating between the “soft” repulsive potentials of type (1.1) and the “hard” self-obstacle condition given by (1.4). In fact we can imagine that an upper bound on \mathcal{U}_p reflects some kind of inseparable but flexible jelly surrounding the curve, that allows close approach of two different strands only for the cost of larger thickness at other places. The exponent p can then be interpreted as a parameter measuring the resistance of the jelly.

In Lemma 1 we show that any closed curve with finite \mathcal{U}_p -energy is embedded, so \mathcal{U}_p penalizes self-intersections. Moreover, we prove in Theorem 1 that Γ is contained in the Sobolev space $W^{2,p}(S_L, \mathbb{R}^3)$, i.e., has generalized second derivatives in $L^p(S_L, \mathbb{R}^3)$, which implies for $p > 1$ that Γ has a Hölder continuous derivative. Here, the corresponding pointwise estimate

$$|\Gamma''(s)| \leq \frac{1}{\rho_G[\gamma](s)} \quad \text{for a.e. } s \in S_L,$$

replaces the global $C^{1,1}$ -estimate $|\Gamma''| \leq 1/\Delta[\gamma]$ for curves with $\Delta[\gamma] > 0$, see [22, Lemma 2]. For the proof of Theorem 1 we combine a geometric local oscillation estimate for the derivative Γ' (Lemma 2) with an analytical subdivision argument in Lemma 3 inspired by the clever methods developed by Hajłasz for his metric characterization of Sobolev spaces [23], [24]. Conversely, one may ask which closed curves γ have finite \mathcal{U}_p -energy. It turns out that for $p > 1$ every simple curve γ with a $W^{2,p}$ -regular arclength parametrization has in fact finite energy $\mathcal{U}_p(\gamma)$. Hence \mathcal{U}_p characterizes simple $W^{2,p}$ -regular loops, just as positive thickness $\Delta[\cdot]$ did in the $C^{1,1}$ -setting (see [41, Theorem 1 (iii)]). The proof of Theorem 2 rests on the Hardy–Littlewood maximal theorem, since there is an intricate relation between $1/\rho_G[\gamma]$ and the maximal function of $|\Gamma''|$. The assumption $p > 1$ in Theorem 2 is essential: for $p = 1$ we provide an example of a simple curve $\Gamma \in W^{2,1}$ with infinite \mathcal{U}_1 energy.

A general energy estimate for \mathcal{U}_p from below (Lemma 7) shows that circles uniquely minimize \mathcal{U}_p among all closed curves of fixed length. A corresponding uniqueness result for O’Hara’s energy (1.1) was proven by Abrams et al. in [1]. Lemma 7 also serves as a starting point for our discussion on sequences of closed curves with finite \mathcal{U}_p -energy. We present two compactness and lower-semicontinuity results, Theorem 3 for curves with fixed length, and Theorem 4 for curves with a uniform bound on their lengths. As a variational application we prove the existence of \mathcal{U}_p -minimizing knots in a given isotopy class (Theorem 5). Clearly, our results on sequences with uniformly bounded energy, Theorems 3 and 4, are strong enough to prove various other existence theorems for curves or nonlinearly elastic rods, where a uniform upper bound on \mathcal{U}_p as a side constraint ensures that the competing objects are embedded. In fact, the general existence theory for nonlinearly elastic rods with positive thickness of [22] carries over if one replaces inequality (1.4) there by

$$\mathcal{U}_p(\gamma) \leq c. \tag{1.7}$$

This L^p -bound imposed on the global curvature is less restrictive than the L^∞ -bound (1.4). In fact, for $p > 1$ one can construct $W^{2,p}$ regular loops—i.e., closed curves with finite \mathcal{U}_p -energy according to Theorem 2—with unbounded global curvature. In Lemma A.1 of the Appendix we show that the arclength parametrization of the graph of any $W^{2,p}$ -function is again of class $W^{2,p}$. Extending such a graph by suitable straight segments and circular arcs yields a closed $W^{2,p}$ -regular loop to which Theorem 2 applies.¹

We should point out that—in contrast to (1.3)—in order to evaluate $\mathcal{U}_p(\gamma)$ numerically only a one-dimensional minimization is necessary by means of the following identity (proven for C^2 -curves in [20, p. 4770]):

$$\rho_G[\gamma](s) = \rho_{pt}[\gamma](s) := \inf_{\sigma \in S_L \setminus \{s\}} pt(s, \sigma), \tag{1.8}$$

which, in fact, is valid for all points $s \in S_L$ such that $\Gamma''(s)$ exists, cf. Lemma 5. Here $pt(s, \sigma)$ is defined as the radius of the (unique) circle through $\Gamma(s)$ and tangent to Γ at $\Gamma(\sigma)$. (As before, $\Gamma : S_L \rightarrow \mathbb{R}^3$ denotes the arclength parametrization of γ .) A numerical computation of \mathcal{U}_p -minimizing curves with, e.g., simulated annealing techniques would be an interesting addition to the remarkable computations by Carlen,

¹ Another explicit geometric construction of a loop with finite \mathcal{U}_p -energy but with unbounded global curvature—a direct construction which works also for $p = 1$ and does not rely on Theorem 2—can be found in the appendix of our preprint [49].

Laurie, Maddocks, and Smutny [10], [45] of *ideal knots*, which, by definition, maximize thickness $\Delta[\cdot]$ under a uniform length bound. In fact, the relation between ideal knots, minimizers of repulsive potentials, and \mathcal{U}_p -minimizing knots remains to be investigated, at present only one result relating the first two seems to be available [38]. In addition, we have no result yet about higher regularity for \mathcal{U}_p -minimizing curves or critical points. The proof of higher regularity for minimizers of O Hara’s energy (1.1) for $p = 2$ relies heavily on the invariance of this particular potential under Möbius transformations in \mathbb{R}^3 [16], [27], a property which is not shared by the \mathcal{U}_p -energy. For ideal knots, i.e., the $C^{1,1}$ -regular maximizers of global curvature $\Delta[\cdot]$, on the other hand, the numerical results of [10], [45] seem to suggest that local curvature may jump, but analytically the regularity properties are far from being well understood.

2 Embeddedness and regularity of γ

Throughout the paper we assume that

$$\gamma : S^1 \rightarrow \mathbb{R}^3$$

is a closed, rectifiable and continuous curve of positive length $L > 0$. Its arclength parametrization

$$\Gamma : S_L \rightarrow \mathbb{R}^3$$

is automatically Lipschitz continuous, i.e., $\Gamma \in C^{0,1}(S_L, \mathbb{R}^3)$. For three parameters $s, \sigma, \tau \in S_L$ we define $R(\Gamma(s), \Gamma(\sigma), \Gamma(\tau))$ to be the radius of the smallest circle containing the points $\Gamma(s), \Gamma(\sigma)$, and $\Gamma(\tau)$. This radius coincides with the unique circumcircle radius if the points are not collinear. The global radius of curvature $\rho_G[\gamma](s)$ and the energy $\mathcal{U}_p(\gamma)$ are, throughout the paper, defined by (1.2) and (1.6), respectively.

Let us begin with the observation that curves with finite energy $\mathcal{U}_p, p \geq 1$, are embedded:

Lemma 1 *If $\mathcal{U}_p(\gamma) < \infty$ for some $p \geq 1$, then γ is simple.*

Proof By Hölder’s inequality $\mathcal{U}_1(\gamma)$ is finite whenever $\mathcal{U}_p(\gamma) < \infty$ for some $p > 1$. Thus it suffices to prove the lemma for $p = 1$.

Assume that γ is not simple, i.e., there are two distinct arclength parameters $s_0, t_0 \in S_L$, such that the arclength parametrization $\Gamma \in C^{0,1}(S_L, \mathbb{R}^3)$ of γ satisfies $\Gamma(s_0) = \Gamma(t_0)$. We can assume w.l.o.g. that $s_0 = 0$. For $s \neq 0$ consider a circle through the points $\Gamma(0)$ and $\Gamma(s)$ with diameter $|\Gamma(0) - \Gamma(s)|$. By assumption this circle contains also the point $\Gamma(t_0)$. Thus

$$\rho_G[\gamma](s) \leq R(\Gamma(s), \Gamma(0), \Gamma(t_0)) = \frac{|\Gamma(s) - \Gamma(0)|}{2} \leq \frac{|s|}{2},$$

hence $1/\rho_G[\gamma]$ is not integrable, which is a contradiction. □

The following example suggests that curves with finite \mathcal{U}_p -energy might possess tangents everywhere.

Example If γ has a corner at some point, then $\mathcal{U}_p(\gamma) = \infty$ for each $p \geq 1$. To see this, consider e.g. the square

$$\Gamma(s) = \begin{cases} (-1 - s, -1, 0) & \text{for } s \in [-2, -1], \\ (0, s, 0) & \text{for } s \in (-1, 0], \\ (s, 0, 0) & \text{for } s \in (0, 1], \\ (1, 1 - s, 0) & \text{for } s \in (1, 2]. \end{cases}$$

Taking into account circles in the xy -plane that are tangent to both sides of the right angle of γ at $(0, 0, 0)$, one easily sees that

$$\varrho_G[\gamma](s) \leq |s|, \quad s \in [-1, 1]$$

and therefore

$$\mathcal{U}_p(\gamma) \geq \int_{-1}^1 \left(\frac{1}{\varrho_G[\gamma](s)} \right)^p ds$$

diverges for every $p \geq 1$.

By [41, Theorem 1 (ii)], we know that if

$$\varrho_G[\gamma](s) > 0 \quad \text{for some } s \in S_L,$$

then γ has a geometric tangent $T(s)$ at $\Gamma(s)$, and with the arclength parametrization $\Gamma : S_L \rightarrow \mathbb{R}^3$ one computes this tangent as

$$T(s) = \lim_{\sigma \rightarrow s^+} \frac{\Gamma(\sigma) - \Gamma(s)}{|\Gamma(\sigma) - \Gamma(s)|} = \lim_{\tau \rightarrow s^-} \frac{\Gamma(s) - \Gamma(\tau)}{|\Gamma(s) - \Gamma(\tau)|}.$$

Moreover, $T(s) = \Gamma'(s)$ if Γ' exists at s . Now, if $\mathcal{U}_p(\gamma) < \infty$, then $\varrho_G[\gamma]$ must be positive almost everywhere. Thus, finiteness of \mathcal{U}_p yields $T(s) = \Gamma'(s)$ a.e. on S_L .

For our regularity investigations we start with a local estimate for the oscillation of Γ' .

Lemma 2 *Let $\mathcal{U}_p(\gamma) < \infty$ for some $p \geq 1$ and suppose that $\Gamma'(s_0)$ exists at $s_0 \in S_L$ and that $\varrho_G[\gamma](s_0) =: \varrho > 0$. Then*

$$\text{for all } s \in B_{\varrho/2}(s_0) := (s_0 - \varrho/2, s_0 + \varrho/2)$$

such that $\Gamma'(s)$ exists we can estimate

$$|\Gamma'(s_0) - \Gamma'(s)| \leq \frac{|\Gamma(s_0) - \Gamma(s)|}{\varrho_G[\gamma](s_0)} \leq \frac{|s_0 - s|}{\varrho_G[\gamma](s_0)}. \tag{2.9}$$

Proof The proof rests on arguments similar to those in [22, pp. 49–52].

Step 1 For the arc $A := \Gamma((s_0, s)), s \in B_{\frac{3}{2}}(s_0)$, one has

$$\text{diam } A \leq \varrho, \tag{2.10}$$

since the arclength parametrization Γ satisfies

$$|\Gamma(\sigma) - \Gamma(\tau)| \leq |\sigma - \tau| \quad \text{for all } \sigma, \tau \in B_{\varrho/2}(s_0). \tag{2.11}$$

We claim that for the lens-shaped region

$$l := \bigcap_{z \in C_\rho(\Gamma(s_0), \Gamma(s))} B_\rho(z)$$

we have

$$A \subset \bar{l}, \tag{2.12}$$

where we used the notation

$$C_\rho(P, Q) := \{z \in \mathbb{R}^3 : |z - P| = |z - Q| = \rho\}.$$

Indeed, assuming contrariwise that (2.12) does not hold we could infer

$$A \cap \left[\bigcup_{z \in C_\rho(\Gamma(s_0), \Gamma(s))} B_\rho(z) \setminus \bar{l} \right] \neq \emptyset, \tag{2.13}$$

since otherwise the arc A with endpoints $\Gamma(s_0)$ and $\Gamma(s)$ would be contained in

$$\mathbb{R}^3 \setminus \bigcup_{z \in C_\rho(\Gamma(s_0), \Gamma(s))} B_\rho(z).$$

That in turn together with (2.11) for $\sigma := s_0$ and $\tau := s$ and the fact that γ is simple by Lemma 1 would imply that the diameter of A is at least as large as that of a great circle on one of the spheres $\partial B_\rho(z)$, $z \in C_\rho(\Gamma(s_0), \Gamma(s))$, i.e., $\text{diam } A \geq 2\rho$ contradicting (2.10).

Now, fix any point $\Gamma(t)$ in the nonempty intersection in (2.13). The intersection of

$$\bigcup_{z \in C_\rho(\Gamma(s_0), \Gamma(s))} B_\rho(z) \setminus \bar{l}$$

with the plane spanned by $\Gamma(s_0)$, $\Gamma(s)$ and $\Gamma(t)$ consists of two intersecting disks D_1 and D_2 , each of radius ρ , with $\partial D_1 \cap \partial D_2 = \{\Gamma(s_0), \Gamma(s)\}$. By symmetry, we can assume $\Gamma(t) \in D_1 \setminus \bar{D}_2$. Then, for $\beta := \arcsin(|\Gamma(s_0) - \Gamma(s)|/2\rho)$ we have, using the classical relation between central and inscribed angles in the circle ∂D_1 ,

$$\begin{aligned} \sphericalangle(\Gamma(s_0) - \xi, \Gamma(s) - \xi) &= \beta && \text{for all } \xi \in \partial D_1 \setminus \bar{D}_2, \\ \sphericalangle(\Gamma(s_0) - \xi, \Gamma(s) - \xi) &= \pi - \beta && \text{for all } \xi \in \partial D_1 \cap D_2, \end{aligned}$$

and clearly

$$\alpha(s_0, s, t) := \sphericalangle(\Gamma(s_0) - \Gamma(t), \Gamma(s) - \Gamma(t)) \in (\beta, \pi - \beta)$$

since $\Gamma(t) \in D_1 \setminus \bar{D}_2$. We would then have

$$R(\Gamma(s_0), \Gamma(s), \Gamma(t)) = \frac{|\Gamma(s_0) - \Gamma(s)|}{2 \sin \alpha(s_0, s, t)} < \frac{|\Gamma(s_0) - \Gamma(s)|}{2 \sin \beta} = \varrho_G[\gamma](s_0),$$

contradicting the definition of $\varrho_G[\gamma](s_0)$. Hence, (2.13) is absurd, which proves (2.12).

Step 2 Taking sequences $\{t_i\}, \{\tau_i\} \subset (s_0 - \varrho/2, s)$ with $t_i \rightarrow s_0^+$ and $\tau_i \rightarrow s^-$ as $i \rightarrow \infty$ we find

$$\begin{aligned} \lim_{i \rightarrow \infty} \frac{\Gamma(t_i) - \Gamma(s_0)}{|\Gamma(t_i) - \Gamma(s_0)|} &= T(s_0) = \Gamma'(s_0), \\ \lim_{i \rightarrow \infty} \frac{\Gamma(s) - \Gamma(\tau_i)}{|\Gamma(s) - \Gamma(\tau_i)|} &= T(s) = \Gamma'(s). \end{aligned}$$

On the other hand, (2.12) implies that for all $i \in \mathbb{N}$ the unit vectors

$$\frac{\Gamma(t_i) - \Gamma(s_0)}{|\Gamma(t_i) - \Gamma(s_0)|}, \quad \frac{\Gamma(s) - \Gamma(\tau_i)}{|\Gamma(s) - \Gamma(\tau_i)|},$$

and therefore also the limits $\Gamma'(s_0)$ and $\Gamma'(s)$, lie in the intersection $K_\varrho \cap \mathbb{S}^2$, where K_ϱ denotes the cone

$$K_\varrho := \{x \in \mathbb{R}^3 : x = \lambda(P - \Gamma(s_0)), \lambda \geq 0, P \in I\}$$

with opening angle $\alpha_\varrho \in (0, \pi)$ satisfying

$$\sin \frac{\alpha_\varrho}{2} = \frac{|\Gamma(s_0) - \Gamma(s)|}{2\varrho}.$$

Consequently,

$$|\Gamma'(s_0) - \Gamma'(s)| \leq \sqrt{2 - 2 \cos \alpha_\varrho} = \frac{|\Gamma(s_0) - \Gamma(s)|}{\varrho} \leq \frac{|s_0 - s|}{\varrho}.$$

□

The next lemma shows that Γ' belongs to the Sobolev space $W^{1,p}$ whenever the global curvature of γ is of class L^p . It is inspired by the metric characterizations of Sobolev spaces in [23] and [24]. In order to obtain an optimal constant, we do not use the results from these papers directly.

Lemma 3 *If $\mathcal{U}_p(\gamma) < \infty$ for some $p \geq 1$, then the arclength parametrization Γ of γ satisfies the inequality*

$$|\Gamma'(s) - \Gamma'(t)| \leq \int_s^t \frac{1}{\varrho_G[\gamma](\tau)} d\tau$$

for all $s, t \in S_L, s < t$. Thus, in particular, Γ' is absolutely continuous on S_L , Γ'' exists a.e. and satisfies

$$|\Gamma''(s)| \leq 1/\varrho_G[\gamma](s) \quad \text{for a.e. } s \in S_L. \tag{2.14}$$

Proof By Hölder’s inequality, $\mathcal{U}_1(\gamma)$ is finite whenever $\mathcal{U}_p(\gamma) < \infty$ for some $p > 1$. Thus, it is enough to prove the lemma for $p = 1$.

Let $D := \{s \in S_L \mid \Gamma'(s) \text{ exists}\}$. Fix $s < t$ such that $s, t \in D$. Let $s = t_0 < t_1 < t_2 < \dots < t_n = t$ where the partition points t_i are chosen in such a way that $\Gamma'(t_i)$ exists for all $i = 1, \dots, n - 1$, and moreover, such that the intervals $I_j = [t_{j-1}, t_j]$ satisfy

$$\frac{|t - s|}{2n} \leq |I_j| \leq \frac{2|t - s|}{n}, \quad j = 1, 2, \dots, n. \tag{2.15}$$

Choosing n sufficiently large, we can guarantee that

$$\int_{I_j} \frac{1}{\varrho_G[\gamma](\tau)} d\tau < \frac{1}{2}, \tag{2.16}$$

by the absolute continuity of the integral. Now, we pick for each j a point $s_{0,j} \in I_j$ such that

$$\frac{1}{\varrho_G[\gamma](s_{0,j})} \leq \int_{I_j} \frac{1}{\varrho_G[\gamma](\tau)} d\tau, \quad \text{and such that } \Gamma'(s_{0,j}) \text{ exists.} \tag{2.17}$$

Inequalities (2.15)–(2.17) yield

$$0 < |I_j| \leq \varrho_G[\gamma](s_{0,j}) \int_{I_j} \frac{1}{\varrho_G[\gamma](\tau)} d\tau < \frac{\varrho_G[\gamma](s_{0,j})}{2}.$$

Thus $\varrho_G[\gamma](s_{0,j})$ is sufficiently large to allow us to apply Lemma 2 and estimate $|\Gamma'(s_{0,j}) - \Gamma'(\sigma)|$ for every $\sigma \in I_j$ such that $\Gamma'(\sigma)$ exists. We write

$$\begin{aligned} |\Gamma'(s) - \Gamma'(t)| &\leq \sum_{j=1}^n |\Gamma'(t_{j-1}) - \Gamma'(t_j)| \\ &\leq \sum_{j=1}^n (|\Gamma'(t_{j-1}) - \Gamma'(s_{0,j})| + |\Gamma'(s_{0,j}) - \Gamma'(t_j)|) \\ &\stackrel{(2.9)}{\leq} \sum_{j=1}^n \frac{1}{\varrho_G[\gamma](s_{0,j})} (|t_{j-1} - s_{0,j}| + |s_{0,j} - t_j|) \\ &= \sum_{j=1}^n \frac{1}{\varrho_G[\gamma](s_{0,j})} |I_j| \\ &\stackrel{(2.17)}{\leq} \sum_{j=1}^n \int_{I_j} \frac{1}{\varrho_G[\gamma](\tau)} d\tau = \int_s^t \frac{1}{\varrho_G[\gamma](\tau)} d\tau. \end{aligned}$$

Due to the absolute continuity of the integral on the right-hand side this estimate is uniform and yields a unique uniformly continuous extension of Γ' from D to S_L . This extension—let us still denote it by Γ' —is then absolutely continuous. Hence Γ' has a generalized derivative Γ'' satisfying (2.14) and we have

$$\Gamma'(s) = \Gamma'(s_0) + \int_{s_0}^s \Gamma''(\tau) d\tau,$$

where $s_0 \in D$ is fixed and $s \in S_L$ is arbitrary. It is a simple elementary exercise to check that the extended function Γ' is in fact equal to the derivative of Γ on all of S_L , i.e., *a posteriori* we have $D = S_L$. This completes the proof. \square

Theorem 1 *Let $p \geq 1$. Assume that $\gamma \in C^0(I, \mathbb{R}^3)$ is a rectifiable closed curve with $\mathcal{U}_p(\gamma) < \infty$. Then the arclength parametrization Γ of γ satisfies the following conditions.*

- (i) Γ is 1–1, i.e., γ has no double points.
- (ii) $\Gamma \in W^{2,p}(S_L, \mathbb{R}^3)$ and $|\Gamma''| \leq 1/\varrho_G[\gamma]$ almost everywhere.
- (iii) Γ' is absolutely continuous and

$$|\Gamma'(s) - \Gamma'(t)| \leq \int_s^t \frac{1}{\varrho_G[\gamma](\tau)} d\tau \quad \text{for all } s < t.$$

- (iv) If $p > 1$, then Γ' is Hölder continuous and

$$|\Gamma'(s) - \Gamma'(t)| \leq \mathcal{U}_p(\gamma) |t - s|^\alpha, \quad \alpha := 1 - \frac{1}{p}.$$

Proof The first statement (i) is just a consequence of Lemma 1. Conditions (ii) and (iii) were proven in Lemma 3, and (iv) is a simple consequence of (iii) and the Hölder inequality. \square

The last theorem of this section shows that for $p > 1$ any embedded curve with a $W^{2,p}$ -regular arclength parametrization has finite \mathcal{U}_p -energy. Combined with the previous result this means that simple $W^{2,p}$ -loops are *characterized* by the fact that the global curvature function ρ_G^{-1} has finite L^p -norm if $p > 1$.

Theorem 2 *Assume that $p > 1$. Let γ be an embedded continuous closed and rectifiable curve of length L with arclength parametrization Γ of class $W^{2,p}(S_L, \mathbb{R}^3)$, then*

$$\mathcal{U}_p(\gamma) < \infty.$$

The assumption $p > 1$ is really crucial; see the example at the end of this section.

To prepare the proof of this result we are first going to prove two technical lemmas relating ρ_G and ρ_{pt} , the latter quantity was defined in (1.8). For the corresponding results in the context of C^2 -curves see [20], [21].

Lemma 4 *For any continuous, closed and rectifiable curve γ with arclength parametrization $\Gamma \in C^1(S_L, \mathbb{R}^3)$ one has*

$$\rho_{pt}[\gamma](s) \geq \rho_G[\gamma](s) \quad \text{for all } s \in S_L. \tag{2.18}$$

Proof For any $\sigma \in S_L \setminus \{s\}$ we obtain

$$\begin{aligned} pt(s, \sigma) &= \frac{|\Gamma(s) - \Gamma(\sigma)|^2}{2|(\Gamma(s) - \Gamma(\sigma)) \wedge \Gamma'(\sigma)|} \\ &= \lim_{\sigma \neq \tau \rightarrow \sigma} R(\Gamma(s), \Gamma(\sigma), \Gamma(\tau)) \geq \rho_G[\gamma](s), \end{aligned} \tag{2.19}$$

since

$$R(\Gamma(s), \Gamma(\sigma), \Gamma(\tau)) = \frac{|\Gamma(s) - \Gamma(\sigma)|}{2 \left| \frac{\Gamma(s) - \Gamma(\tau)}{|\Gamma(s) - \Gamma(\tau)|} \wedge \frac{\Gamma(\sigma) - \Gamma(\tau)}{|\Gamma(\sigma) - \Gamma(\tau)|} \right|} \quad \text{for } s \neq \sigma \neq \tau \neq s,$$

and since $|\Gamma'| \equiv 1$,

$$\frac{|\Gamma(\sigma) - \Gamma(\tau)|}{|\Gamma(\sigma) - \Gamma(\tau)|} = \frac{\Gamma'(\sigma)(\sigma - \tau) + o(|\sigma - \tau|)}{|\sigma - \tau|} \cdot \left[1 + \frac{o(|\sigma - \tau|)}{|\sigma - \tau|} \right] \xrightarrow{\tau \rightarrow \sigma} \pm \Gamma'(\sigma).$$

Taking the infimum in (2.19) over all $\sigma \in S_L \setminus \{s\}$ one arrives at (2.18). \square

Lemma 5 *Let $\Gamma \in W^{2,1}(S_L, \mathbb{R}^3)$ be the arclength parametrization of a simple closed curve γ , and assume that $s \in S_L$ is a Lebesgue point of Γ'' . Then*

$$\rho_G[\gamma](s) = \rho_{pt}[\gamma](s).$$

Proof Since $W^{2,1}(S_L, \mathbb{R}^3)$ embeds into $C^1(S_L, \mathbb{R}^3)$, Lemma 4 applies, so it suffices to show that

$$\rho_{pt}[\gamma](s) \leq \rho_G[\gamma](s) \quad \text{for all Lebesgue points } s \text{ of } \Gamma''.$$

We assume that $\rho_G[\gamma](s)$ is finite, otherwise there is nothing to prove. Let us distinguish between different situations of how the infimum in the definition (1.2) of ρ_G is attained.

Case I Assume

$$\rho_G[\gamma](s) = R(\Gamma(s), \Gamma(t), \Gamma(\sigma)) \quad \text{for } s \neq t \neq \sigma \neq s.$$

Then the corresponding circumcircle c touches Γ tangentially in $\Gamma(t)$ or $\Gamma(\sigma)$. Indeed, otherwise the intersection $\partial B_R \cap \Gamma$ – where ∂B_R is the sphere containing c as a great circle – would be transversal at $\Gamma(t)$ and $\Gamma(\sigma)$; then we could find a slightly smaller sphere $S_1 \subset \overline{B}_R$ such that $S_1 \cap \partial B_R = \{\Gamma(s)\}$ and S_1 intersects Γ transversally in two other distinct points $\Gamma(t_1)$ and $\Gamma(\sigma_1)$, close to $\Gamma(t)$ and $\Gamma(\sigma)$, respectively, with $t_1 \neq s \neq \sigma_1$. Hence,

$$\rho_G[\gamma](s) \leq R(\Gamma(s), \Gamma(t_1), \Gamma(\sigma_1)) < R = \rho_G[\gamma](s),$$

which is absurd.

So we have $\rho_G[\gamma](s) = pt(s, t)$, or $\rho_G[\gamma](s) = pt(s, \sigma)$. In any case we can take the infimum on the respective right-hand side to obtain

$$\rho_G[\gamma](s) \geq \rho_{pt}[\gamma](s).$$

Case II If

$$\rho_G[\gamma](s) = \lim_{\substack{t, \sigma \rightarrow \tau \\ \tau \neq s}} R(\Gamma(s), \Gamma(t), \Gamma(\sigma))$$

then $\rho_G[\gamma](s) = pt(s, \tau)$, which can be seen by the same computation as in the proof of Lemma 4. So again,

$$\rho_G[\gamma](s) \geq \rho_{pt}[\gamma](s).$$

Case III If

$$\rho_G[\gamma](s) = \lim_{\substack{\sigma \rightarrow s \\ t \rightarrow \tau \neq s}} R(\Gamma(s), \Gamma(t), \Gamma(\sigma)) = \lim_{\substack{\sigma \rightarrow s \\ t \rightarrow \tau \neq s}} R(\Gamma(t), \Gamma(s), \Gamma(\sigma))$$

then we find similarly as before

$$\rho_G[\gamma](s) = pt(\tau, s),$$

but we claim that the circle c realizing this point-tangent function is actually also tangent to the curve in the point $\Gamma(\tau)$, since otherwise we could proceed as in Case I and once again shrink the sphere for which c is an equatorial circle to obtain a contradiction against the definition of $\rho_G[\gamma](s)$. Hence

$$\rho_G[\gamma](s) = pt(s, \tau) \geq \rho_{pt}[\gamma](s).$$

Case IV If

$$\rho_G[\gamma](s) = \lim_{t, \sigma \rightarrow s} R(\Gamma(s), \Gamma(t), \Gamma(\sigma))$$

then we can apply [41, Lemma 7 (57)] setting $s_j := s$, $\tau_j := t$, $\sigma_j := \sigma$, (w.l.o.g. $s_j < \sigma_j < \tau_j$) to obtain

$$\rho_G[\gamma](s) = \frac{1}{|\Gamma''(s)|}.$$

According to the expansion [41, Lemma 7 (52)] we can argue that for $s \neq \sigma$

$$\begin{aligned}
 pt(s, \sigma) &= \lim_{s_3 \rightarrow \tau^+} R(\Gamma(s), \Gamma(\sigma), \Gamma(s_3)) \\
 &\stackrel{([41, (52)])}{=} \frac{|\Gamma'(\sigma) + \frac{1}{s-\sigma} \int_{\sigma}^s \int_{\sigma}^t \Gamma''(\omega) \, d\omega dt|^2}{2 \left| \Gamma'(\sigma) \wedge \frac{1}{\sigma-s} \int_0^1 \int_{\sigma-t(\sigma-s)}^{\sigma} \Gamma''(\omega) \, d\omega dt \right|}, \tag{2.20}
 \end{aligned}$$

where we used the identity $A \wedge A = 0$ for $A \in \mathbb{R}^3$ to simplify the denominator in the last line. Analyzing this expression we obtain

$$\lim_{\sigma \rightarrow s} pt(s, \sigma) = \frac{1}{|\Gamma''(s)|}, \tag{2.21}$$

which proves

$$\rho_{pt}[\gamma](s) \leq \frac{1}{|\Gamma''(s)|} = \rho_G[\gamma](s)$$

also in this last case. □

The last preparation for the proof of Theorem 2 consists in the following local estimate for the pt -function:

Lemma 6 *Let $p > 1$ and $\Gamma \in W^{2,p}(S_L, \mathbb{R}^3)$ be the arclength parametrization of an embedded closed continuous curve γ . Fix $q \in (1, p)$. Then, for every $s, \sigma \in S_L$ we have*

$$|\sigma - s| + pt(s, \sigma) \geq \frac{1}{2A(s)}, \tag{2.22}$$

where

$$A(s) := \left(M(M|\Gamma''|)^q(s) \right)^{1/q}$$

and Mf denotes the non-centered Hardy–Littlewood maximal function of f , i.e.,

$$Mf(t) = \sup_{B_r(u) \ni t} \frac{1}{2r} \int_{u-r}^{u+r} |f(\tau)| \, d\tau.$$

Remark 1. Since $p > p/q > 1$, we may apply the Hardy–Littlewood maximal theorem (see e.g. Stein’s monograph [46, Chap. 1]) twice, to obtain

$$M|\Gamma''| \in L^p, \quad (M|\Gamma''|)^q \in L^{p/q}, \quad M(M|\Gamma''|)^q \in L^{p/q}.$$

Thus, $A(\cdot)$ defined in the Lemma is of class L^p .

- For closed, embedded curves γ we certainly have $M|\Gamma''|(s) > 0$ for each s . Thus, $A(s) > 0$.

Proof of Lemma 6 Without loss of generality we can assume $s > \sigma$, $\Gamma(\sigma) = 0$, $\Gamma'(\sigma) = (1, 0, 0)$, and that the circle realizing $r := pt(s, \sigma)$ has its center at $(0, 0, r)$.

We now estimate, using Hölder’s inequality for the exponents q and $q' = q/(q - 1)$,

$$\begin{aligned}
 |\Gamma(s) - \Gamma(\sigma) - \Gamma'(\sigma)(s - \sigma)| &= \left| \int_{\sigma}^s (\Gamma'(\tau) - \Gamma'(\sigma)) d\tau \right| \\
 &= \left| \int_{\sigma}^s \int_{\sigma}^{\tau} \Gamma''(\omega) d\omega d\tau \right| \\
 &\leq \left| \int_{\sigma}^s (\tau - \sigma) M|\Gamma''|(\tau) d\tau \right| \\
 &\leq |s - \sigma|^{2-1/q} \left(\int_{\sigma}^s (M|\Gamma''|(\tau))^q d\tau \right)^{1/q} \\
 &\leq |s - \sigma|^2 A(s), \tag{2.23}
 \end{aligned}$$

and therefore (2.23) implies the estimates

$$|\Gamma^3(s)| \leq A(s)|\sigma - s|^2 \quad \text{and} \quad |\Gamma^1(s)| \geq |\sigma - s| - A(s)|\sigma - s|^2.$$

If $|\sigma - s| - A(s)|\sigma - s|^2 < 0$, then $|\sigma - s| > 1/A(s)$ and the lemma holds true. Otherwise, we obtain

$$\begin{aligned}
 r^2 &= |\Gamma(s) - (0, 0, r)|^2 \geq (\Gamma^1(s))^2 + (\Gamma^3(s) - r)^2 \\
 &\geq |\sigma - s|^2 - 2A(s)|\sigma - s|^3 - 2r|\Gamma^3(s)| + r^2 \\
 &\geq |\sigma - s|^2 \{1 - 2A(s)|\sigma - s| - 2rA(s)\} + r^2,
 \end{aligned}$$

which is only possible if the term in brackets is non-positive, i.e., if

$$r + |\sigma - s| \geq \frac{1}{2A(s)}. \quad \square$$

Now we can turn to the

Proof of Theorem 2 Fix a Lebesgue point $s \in S_L$ of Γ'' . We are going to estimate $pt(s, \sigma)$ from below by analyzing formula (2.20). Since

$$\left| \int_{\sigma}^t \Gamma''(\omega) d\omega \right| \leq |t - \sigma|^{1-1/p} \|\Gamma''\|_{L^p([\sigma, s], \mathbb{R}^3)} \quad \text{for all } t \in [\sigma, s],$$

we find that the numerator in (2.20) can be estimated from below by

$$1 - \frac{|\sigma - s|^{1-1/p}}{2 - 1/p} \|\Gamma''\|_{L^p([\sigma, s], \mathbb{R}^3)} \geq \frac{1}{2} \tag{2.24}$$

for $\sigma \in B_{\epsilon_1}(s)$, where the number $\epsilon_1 = \epsilon_1(p, \gamma)$ is chosen sufficiently small and does not depend on s .

From

$$\left| \int_{\sigma-t(\sigma-s)}^{\sigma} \Gamma''(\omega) d\omega \right| \leq (t|\sigma - s|)^{1-1/p} \|\Gamma''\|_{L^p([\sigma, s], \mathbb{R}^3)} \quad \text{for all } t \in [0, 1]$$

we deduce

$$\left| \frac{1}{\sigma - s} \int_0^1 \int_{\sigma-t(\sigma-s)}^\sigma \Gamma''(\omega) \, d\omega dt \right| \leq \frac{|\sigma - s|^{-1/p}}{2 - 1/p} \|\Gamma''\|_{L^p(S_L, \mathbb{R}^3)}.$$

Similarly, we estimate

$$\left| \int_0^1 \int_\sigma^{\sigma-t(\sigma-s)} \Gamma''(\omega) \, d\omega dt \right| \leq \frac{|\sigma - s|^{1-1/p}}{2 - 1/p} \|\Gamma''\|_{L^p(S_L, \mathbb{R}^3)},$$

so that an upper bound for the denominator in (2.20) is given by

$$\frac{2}{|\sigma - s|^{1/p}} \left[1 + |\sigma - s|^{1-1/p} \|\Gamma''\|_{L^p(S_L, \mathbb{R}^3)} \right] \frac{\|\Gamma''\|_{L^p(S_L, \mathbb{R}^3)}}{2 - 1/p} \leq \frac{c(p, \gamma)}{|\sigma - s|^{1/p}}$$

for some constant $c(p, \gamma)$ depending only on p and γ . This together with the lower bound (2.24) for the numerator leads to

$$pt(s, \sigma) \geq \frac{|\sigma - s|^{1/p}}{2c(p, \gamma)} \quad \text{for all } \sigma \in B_{\epsilon_1}(s). \tag{2.25}$$

Moreover, shrinking ϵ_1 if necessary, we can assume that

$$pt(s, \sigma) \geq \frac{|\sigma - s|^{1/p}}{2c(p, \gamma)} \geq |\sigma - s| \quad \text{for all } \sigma \in B_{\epsilon_1}(s). \tag{2.26}$$

Thus, by Lemma 6,

$$pt(s, \sigma) \geq \frac{1}{4A(s)} \quad \text{for all } \sigma \in B_{\epsilon_1}(s), \tag{2.27}$$

Notice that since γ is simple we obviously have

$$pt(s, \sigma) \geq \frac{|\Gamma(s) - \Gamma(\sigma)|}{2} \geq c_1 > 0 \quad \text{for all } \sigma \in S_L \setminus B_{\epsilon_1}(s) \tag{2.28}$$

for some positive constant c_1 depending only on γ .

Estimates (2.27) and (2.28) yield

$$\frac{1}{\rho_G[\gamma](s)} = \frac{1}{\rho_{pt}[\gamma](s)} \leq \max \left\{ \frac{1}{c_1}, 4A(s) \right\} \quad \text{for all } \sigma \in S_L.$$

Since $A \in L^p$, the Theorem follows. □

A counterexample to the statement of Theorem 2 for $p = 1$.

Set $x_0 = 1/e^3$ and define

$$\Phi(x) = \int_0^x \left(\log \frac{1}{t} \right)^{-1} dt, \quad x \in (0, x_0]. \tag{2.29}$$

Extend Φ to an even, continuous function on $[-x_0, x_0]$. It is clear that $\Phi'(0) = 0$ and Φ is of class C^1 . In fact, $\Phi \in C^\infty$ away from 0, and

$$\Phi''(x) = \left(|x| \log^2 \frac{1}{|x|} \right)^{-1}, \quad x \in [-x_0, x_0] \setminus \{0\}.$$

Since

$$\int_0^\delta \left(s \log^2 \frac{1}{s} \right)^{-1} ds = \left(\log \frac{1}{\delta} \right)^{-1},$$

we have also $\Phi \in W^{2,1}((-x_0, x_0))$.

Now, consider the graph of $\Phi : [-x_0, x_0] \rightarrow \mathbb{R}^2$. It follows from Lemma A.1 (see Appendix) that we can close this graph with a smooth arc to obtain a closed, convex C^1 curve $\gamma \subset \mathbb{R}^2$ whose arclength parametrization $\Gamma \in W^{2,1}$ is of class C^∞ except at $(0, 0) \in \mathbb{R}^2$.

We shall now show that the energy $\mathcal{U}_1(\gamma)$ is infinite. To this end, assume that the arclength parametrization of the graph of Φ is given by

$$t \mapsto (x(t), \Phi(x(t)))$$

where $t \mapsto x(t)$ is increasing and $t = 0$ corresponds to $x = 0$. Let us estimate the radius $\rho_G[\gamma](t)$ for small positive t . Consider the circle σ_t which is tangent to the graph of Φ at two points, $(\pm x(t), \Phi(x(t)))$. The center of σ_t is at $(0, \Phi(x(t)) + x(t)/\Phi'(x(t)))$. A computation shows that the radius $r(t)$ of σ_t is given by

$$r(t) = \frac{x(t)}{\Phi'(x(t))} \sqrt{1 + \Phi'(x(t))^2}.$$

Then, since x' is close to 1 and Φ' is bounded, one can obtain

$$r(t) \leq 2 \frac{x(t)}{\Phi'(x(t))} \leq Ct \log \frac{1}{t}.$$

Since $\rho_G[\gamma](t) \leq r(t)$, the last estimate gives

$$\mathcal{U}_1(\gamma) \geq \int_0^{t_0} \frac{dt}{\rho_G[\gamma](t)} \geq \int_0^{t_0} \frac{dt}{r(t)} \geq \frac{1}{C} \int_0^{t_0} \left(t \log \frac{1}{t} \right)^{-1} dt = +\infty. \tag{2.30}$$

3 Sequences of curves and existence of energy minimizing knots

We start with an energy estimate providing a lower bound for the \mathcal{U}_p -energy in terms of the length, which is obtained only for circles.

Lemma 7 *Let $p \geq 1$ and let γ be a closed rectifiable curve of positive length $\mathcal{L}(\gamma)$ with $\mathcal{U}_p(\gamma) < \infty$. Then*

$$\mathcal{U}_p(\gamma) \geq 2\pi \mathcal{L}(\gamma)^{(1/p)-1} \tag{3.1}$$

with equality if and only if γ is a circle of the same length.

Proof Set $L := \mathcal{L}(\gamma)$ and $U := \mathcal{U}_p(\gamma)$. We claim that there is an arclength parameter $s \in S_L$, such that

$$\rho_G[\gamma](s) \geq \frac{L^{1/p}}{U}. \tag{3.2}$$

Indeed, if we had

$$\rho_G[\gamma](\sigma) < \frac{L^{1/p}}{U} \quad \text{for all } \sigma \in S_L,$$

then we could estimate

$$U = \left(\int_{S_L} \frac{1}{\rho_G[\gamma](\sigma)^p} d\sigma \right)^{1/p} > \frac{U}{L^{1/p}} \cdot \mathcal{H}^1(S_L)^{1/p} = U,$$

which is absurd.

By (3.2), $\varrho_G[\gamma](s)$ is positive and therefore [41, Theorem 1 (iv)(a)] implies that

$$\Gamma(S_L) \cap M(s, \rho_G[\gamma](s)) = \emptyset,$$

where the set $M(s, \rho_G[\gamma](s))$ is the union of all open balls of radius $\rho_G[\gamma](s)$ tangent to γ at the point $\Gamma(s)$. (As before we used the notation Γ for the arclength parametrization of γ .) This implies that L is at least as large as the length of the shortest closed C^1 curve of positive length in $\mathbb{R}^3 \setminus M(s, \rho_G[\gamma](s))$ containing the point $\Gamma(s)$, which is a great circle on one of the balls with radius $\rho_G[\gamma](s)$ generating $M(s, \rho_G[\gamma](s))$, i.e. by (3.2),

$$L \geq 2\pi\rho_G[\gamma](s) \geq 2\pi \frac{L^{1/p}}{U}.$$

with equality if and only if γ is such a great circle. □

Remark As a consequence of Lemma 7 we note that (up to rotations and translations) circles are the unique minimizers of the energy \mathcal{U}_p among all closed curves of fixed length. The same is trivially true if one maximizes the global radius of curvature $\Delta[\gamma]$ without further topological restrictions, but also for minimizers of the repulsive knot energies of the type (1.1) only that the corresponding uniqueness proof of Abrams et al. is more involved, see [1].

Our existence proof for energy minimizers in nontrivial isotopy classes (Theorem 5) relies on the following compactness and lower-semicontinuity result.

Theorem 3 Fix $p > 1$ and let $\alpha = (p - 1)/p$. Assume that $\gamma_j, j = 1, 2, \dots$ are closed rectifiable curves of fixed length L with arclength parametrizations Γ_j defined on S_L .

If $\sup_j \mathcal{U}_p(\gamma_j) \leq K < \infty$ then there exists a simple curve $\Gamma \in C^{1,\alpha}(S_L, \mathbb{R}^3)$ with $|\Gamma'| \equiv 1$, such that, for a subsequence $j' \rightarrow \infty$, $\Gamma_{j'} \rightarrow \Gamma$ in C^1 and

$$\varrho_G[\Gamma](s) \geq \limsup_{j' \rightarrow \infty} \varrho_G[\gamma_{j'}](s) \quad \text{for each } s \in S_L. \tag{3.3}$$

Moreover, $\mathcal{U}_p(\Gamma) \leq \liminf_{j' \rightarrow \infty} \mathcal{U}_p(\gamma_{j'}) \leq K$.

Remark Notice that one cannot expect continuity of $\rho_G[\cdot](s)$ in the C^1 -topology: Consider e.g. the following arclength parametrizations of “elbow-curves” that were also mentioned in [8]:

$$\Gamma_i(s) := \begin{cases} (\cos s, \sin s, 0) & \text{for } s \in (-\frac{1}{i}, \frac{1}{i}) \\ (\cos \frac{1}{i}, \sin \frac{1}{i}, 0) + (s - i^{-1})(-\sin \frac{1}{i}, \cos \frac{1}{i}, 0) & \text{for } s \in [\frac{1}{i}, 1] \\ (\cos \frac{1}{i}, \sin(-\frac{1}{i}), 0) + (s + i^{-1})(\sin \frac{1}{i}, \cos \frac{1}{i}, 0) & \text{for } s \in [-1, -\frac{1}{i}], \end{cases}$$

which² converge in C^1 to a straight vertical line Γ of length 2 centered in $(1, 0, 0)$. Hence at $s = 0$ we obtain

$$\infty = \varrho_G[\Gamma](0) > \limsup_{i \rightarrow \infty} \varrho_G[\Gamma_i](0) = 1,$$

since $\varrho_G[\Gamma_i](0) = 1$ for all $i \in \mathbb{N}$.

Proof of Theorem 3 By Theorem 1 (iv), we have

$$|\Gamma'_j(s) - \Gamma'_j(t)| \leq K|s - t|^\alpha, \quad j = 1, 2, \dots \tag{3.4}$$

By the Arzela–Ascoli theorem we obtain a subsequence $\Gamma_j \rightarrow \Gamma$ (still denoted by the same index j) in the C^1 -topology. Passing to the limit $j \rightarrow \infty$ in (3.4) for this subsequence, we obtain $\Gamma \in C^{1,\alpha}(S_L, \mathbb{R}^3)$ with $|\Gamma'| \equiv 1$.

The crucial difficulty is to prove that Γ is simple. Again, as in the proof of Lemma 1, we argue by contradiction.

Assume that $\Gamma(s_0) = \Gamma(t)$ for some $t \neq s_0$. W.l.o.g. suppose that $s_0 = 0$, $\Gamma(0) = 0 \in \mathbb{R}^3$, and $\Gamma'(0) = (1, 0, 0)$. Thus, for some $d = d(K, \alpha) \in (0, |t|/8)$ we have

$$\Gamma(s) = (s + \rho_1(s), \rho_2(s), \rho_3(s)), \quad s \in (-d, d),$$

where $\rho_i(s) = o(s)$ as $s \rightarrow 0$ and $|\rho_i(s)| < |s|/12$ for all $s \in (-d, d)$. For each parameter $s \in (-d/3, 0)$ the sphere $\partial B_{r(s)}(0)$ of radius $r(s)$, where

$$\frac{3}{4}|s| < r(s) \equiv |\Gamma(s)| < \frac{4}{3}|s|,$$

contains $\Gamma(\tau)$ for at least four different values of the parameter τ . Namely,

$$\Gamma(\tau_1) \in \partial B_{r(s)}(0) \quad \text{for } \tau_1 = s \in (-d/3, 0), \tag{3.5}$$

$$\Gamma(\tau_2) \in \partial B_{r(s)}(0) \quad \text{for some } \tau_2 = \tau_2(s) \in (0, d),$$

and $\Gamma(\tau_3), \Gamma(\tau_4) \in \partial B_{r(s)}(0)$ for two other parameters $\tau_{3,4}$ in a neighbourhood of t . (Keep in mind that $\Gamma(t) = \Gamma(0)$.)

We now fix a number $N > 16$ such that

$$\frac{1}{4} \log N > KL^{(p-1)/p}. \tag{3.6}$$

Let $\varepsilon = d/3N$. Fix j so large that

$$\|\Gamma_j - \Gamma\|_\infty + \|\Gamma'_j - \Gamma'\|_\infty < \frac{\varepsilon}{100}. \tag{3.7}$$

We shall estimate $\varrho_G[\Gamma_j](s)$ from above on the interval $(-d/3, -\varepsilon)$. Using (3.5) and the triangle inequality, we check that

$$\begin{aligned} \Gamma_j(-\varepsilon) &\in B_{4\varepsilon}(0) \setminus B_{\varepsilon/4}(0), \\ \Gamma_j(-d/3) &\in B_{4d}(0) \setminus B_{d/4}(0), \end{aligned}$$

² These open curves could easily be closed by suitably large circular arcs, and we would still observe this local effect of discontinuity of $\varrho_G[\cdot](0)$.

and in general $\Gamma_j(s) \in B_{4s}(0) \setminus B_{s/4}(0)$ for all $s \in (-d/3, -\varepsilon)$. Now, for each $s \in (-d/3, -\varepsilon)$, the sphere $\partial B_{r_j(s)}(0)$, where $r_j(s) := |\Gamma_j(s)|$, contains the points $\Gamma_j(\tau)$ for three other values of the parameter τ . One of them is positive and belongs to $(0, d)$. Two more values of τ belong to a neighbourhood of t , as the equality $\Gamma(t) = \Gamma(0)$ combined with (3.7) yields $\Gamma_j(t) \in B_{\varepsilon/100}(0)$. Thus, invoking the definition of the global radius of curvature function, we have

$$\varrho_G[\gamma_j](s) \leq 4|s|, \quad -\frac{d}{3} < s < -\varepsilon.$$

Hence,

$$\begin{aligned} \left[\int_{S_L} \left(\frac{1}{\varrho_G[\gamma_j](\tau)} \right)^p d\tau \right]^{1/p} &\geq L^{(1-p)/p} \int_{S_L} \frac{1}{\varrho_G[\gamma_j](\tau)} d\tau \\ &\geq L^{(1-p)/p} \int_{-d/3}^{-\varepsilon} \frac{1}{4|s|} ds \\ &= \frac{1}{4} L^{(1-p)/p} (\log \frac{d}{3} - \log \varepsilon) \\ &= \frac{1}{4} L^{(1-p)/p} \log N > K \quad \text{by (3.6).} \end{aligned}$$

Thus, $\mathcal{U}_p(\gamma_j) > K$, a contradiction.

To finish the proof, we have to deal with the upper semicontinuity of ϱ_G .

Since γ is simple, we note that if

$$\varrho_G[\gamma_j](s) \geq \delta > 0 \quad \text{for infinitely many } j, \tag{3.8}$$

then

$$\varrho_G[\gamma](s) \geq \delta > 0.$$

since otherwise we would find two distinct parameters t, τ different from s such that

$$R(\Gamma(s), \Gamma(t), \Gamma(\tau)) < \delta.$$

By the C^1 -convergence we would then obtain

$$R(\Gamma_j(s), \Gamma_j(t), \Gamma_j(\tau)) < \delta \quad \text{for } j \gg 1$$

contradicting (3.8). Hence, if $\limsup_{j \rightarrow \infty} \varrho_G[\gamma_j](s) \geq \delta$, then $\varrho_G[\gamma](s) \geq \delta - \varepsilon$ for every $\varepsilon > 0$. Inequality (3.3) follows. Now, the estimate

$$\mathcal{U}_p(\Gamma) \leq \liminf_{j \rightarrow \infty} \mathcal{U}_p(\gamma_j) \leq K$$

follows from Fatou's lemma. □

We can weaken the hypothesis of fixed to bounded length in Theorem 3 to obtain

Theorem 4 *Suppose there exist constants K and L_0 with*

$$\frac{2\pi}{K} \leq L_0^{(p-1)/p} \tag{3.9}$$

such that the lengths $L_j := \mathcal{L}(\gamma_j)$ of closed rectifiable curves $\gamma_j, j \in \mathbb{N}$, with arclength parametrizations Γ_j defined on S_{L_j} satisfy

$$\sup_j L_j \leq L_0, \tag{3.10}$$

and such that

$$\sup_j \mathcal{U}_p(\gamma_j) \leq K. \tag{3.11}$$

Then there exists L with

$$\left(\frac{2\pi}{K}\right)^{p/(p-1)} \leq L \leq L_0, \tag{3.12}$$

a simple curve $\Gamma \in C^{1,\alpha}(S_L, \mathbb{R}^3)$ with $|\Gamma'| \equiv 1$, such that, for a subsequence $j' \rightarrow \infty$, the rescaled, arclength parametrized curves

$$\Gamma_{j'}^*(s) := \frac{L}{L_{j'}} \Gamma_{j'}(L_{j'} \cdot s/L), \quad s \in S_L, \tag{3.13}$$

and therefore also the unscaled but reparametrized curves

$$\Gamma_{j'} \circ (L_{j'}/L) : S_L \rightarrow \mathbb{R}^3,$$

converge to Γ in C^1 . Moreover,

$$\varrho_G[\Gamma](s) \geq \limsup_{j' \rightarrow \infty} \varrho_G[\Gamma_{j'}^*](s) = \limsup_{j' \rightarrow \infty} \varrho_G[\Gamma_{j'} \circ (L_{j'}/L)](s) \quad \text{for each } s \in S_L, \tag{3.14}$$

and

$$\mathcal{U}_p(\Gamma) \leq \liminf_{j' \rightarrow \infty} \mathcal{U}_p(\Gamma_{j'}^*) = \liminf_{j' \rightarrow \infty} \mathcal{U}_p(\Gamma_{j'} \circ (L_{j'}/L)) \leq K. \tag{3.15}$$

Proof Lemma 7 implies that

$$L_j \geq \left(\frac{2\pi}{\mathcal{U}_p(\gamma_j)}\right)^{p/(p-1)} \geq \left(\frac{2\pi}{K}\right)^{p/(p-1)} \quad \text{for all } j \in \mathbb{N},$$

which together with the consistency condition (3.9) implies the existence of a number L satisfying (3.12) and a subsequence $j' \rightarrow \infty$ such that

$$L_{j'} \rightarrow L \quad \text{as } j' \rightarrow \infty. \tag{3.16}$$

Now we look at the rescaled curves $\Gamma_{j'}^*$ as defined in (3.13). We observe that for the radius $R(\Gamma_{j'}^*(s), \Gamma_{j'}^*(t), \Gamma_{j'}^*(\sigma))$ of the smallest circle containing three points $\Gamma_{j'}^*(s), \Gamma_{j'}^*(t)$, and $\Gamma_{j'}^*(\sigma)$ for distinct arclength parameters s, t , and σ in S_L one has, by definition,

$$R(\Gamma_{j'}^*(s), \Gamma_{j'}^*(t), \Gamma_{j'}^*(\sigma)) = \frac{L}{L_{j'}} R(\Gamma_j(L_j \cdot s/L), \Gamma_j(L_j \cdot t/L), \Gamma_j(L_j \cdot \sigma/L))$$

and therefore

$$\rho_G[\Gamma_{j'}^*](s) = \frac{L}{L_{j'}} \rho_G[\Gamma_j \circ (L_{j'}/L)](s). \tag{3.17}$$

This together with the change of variables formula implies

$$\begin{aligned} \mathcal{U}_p(\Gamma_j^*) &= \left(\int_{S_L} \frac{1}{\rho_G[\Gamma_j^*](s)^p} ds \right)^{1/p} \\ &= \left(\frac{L_j}{L} \right)^{1-(1/p)} \left(\int_{S_{L_j}} \frac{1}{\rho_G[\gamma_j](t)^p} dt \right)^{1/p} \\ &= \left(\frac{L_j}{L} \right)^{1-(1/p)} \mathcal{U}_p(\gamma_j). \end{aligned}$$

In particular, by (3.10)–(3.12) we obtain

$$\mathcal{U}_p(\Gamma_j^*) \leq \left(\frac{L_0}{\left(\frac{2\pi}{K}\right)^{p/(p-1)}} \right)^{(p-1)/p} K = \frac{L_0^{1-1/p}}{2\pi} K^2 =: K^*,$$

and therefore by Theorem 1 (iv)

$$|(\Gamma_j^*)'(s) - (\Gamma_j^*)'(t)| \leq K^* |s - t|^\alpha \quad \text{for } \alpha := (p - 1)/p.$$

From now on we can proceed exactly as in the proof of Theorem 3 replacing Γ_j by Γ_j^* in the line of arguments following (3.4). Since $\Gamma_j^* \rightarrow \Gamma$ in $C^1([0, L], \mathbb{R}^3)$ we infer from (3.16) that

$$\Gamma_j \circ (L_j/L) = (L_j/L)\Gamma_j^* \rightarrow \Gamma \quad \text{in } C^1([0, L], \mathbb{R}^3) \quad \text{as } j' \rightarrow \infty.$$

Identity (3.17) together with (3.16) implies the equality in (3.14) and therefore also in (3.15). □

We recall the definition of knot or *isotopy classes* in \mathbb{R}^3 : Two continuous closed curves $\gamma_1, \gamma_2 \subset \mathbb{R}^3$ are isotopic, denoted as $\gamma_1 \simeq \gamma_2$, if there are open neighbourhoods N_1 of γ_1, N_2 of γ_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 $\Phi(\gamma_1, 1) = \gamma_2$.

We consider the variational problem of minimizing the \mathcal{U}_p -energy for $p > 1$ on curves of fixed length in a given isotopy class. That is, we look at

$$\mathcal{U}_p(\gamma) \longrightarrow \min$$

in the class

$$\mathcal{C}_{L,k} := \{\gamma \in C^0(S^1, \mathbb{R}^3) : \text{length}(\gamma) = L, \gamma \simeq k\},$$

where $L > 0$ is a given constant, and k is a given isotopy class.

Theorem 5 *Let $p > 1$. For any isotopy class k there exists an arclength parametrized curve $\Gamma \in W^{2,p}(S_L, \mathbb{R}^3)$, such that*

$$\mathcal{U}_p(\Gamma) = \inf_{\mathcal{C}_{L,k}} \mathcal{U}_p(\cdot).$$

Proof The class $\mathcal{C}_{L,k}$ is not empty since we can scale a smooth parametrization of k to have length L . For a minimal sequence $\{\gamma_i\}$ with

$$\mathcal{U}_p(\gamma_i) \longrightarrow \inf_{\mathcal{C}_{L,k}} \mathcal{U}_p(\cdot) < \infty \quad \text{as } i \rightarrow \infty$$

with arclength parametrizations $\Gamma_i \in C^{0,1}(S_L, \mathbb{R}^3)$ we can apply Theorem 3 to obtain a simple arclength parametrized limit curve $\Gamma \in C^1$, such that $\Gamma_i \rightarrow \Gamma$ in $C^1(S_L, \mathbb{R}^3)$ for an (equally labelled) subsequence. According to the stability of isotopy in the C^1 -topology (see e.g. [40]) we infer from $\Gamma_i \simeq k$ that also $\Gamma \simeq k$; hence $\Gamma \in \mathcal{C}_{L,k}$. Since, by Theorem 3, \mathcal{U}_p is lower-semicontinuous with respect to this type of convergence, we obtain

$$\inf_{\mathcal{C}_{L,k}} \mathcal{U}_p(\cdot) \leq \mathcal{U}_p(\Gamma) \leq \liminf_{i \rightarrow \infty} \mathcal{U}_p(\gamma_i) = \inf_{\mathcal{C}_{L,k}} \mathcal{U}_p(\cdot).$$

The $W^{2,p}$ -regularity for Γ follows from Theorem 1, Part (ii). □

Remark It is clear that one may also consider other variational problems with a uniform upper bound on \mathcal{U}_p as a side constraint ensuring self-avoidance of the competing curves. Either one fixes or bounds the length in addition, to apply Theorem 3 or Theorem 4, or it may be that the length is part of the total energy to be minimized. It may also happen that a uniform bound on the length follows automatically from minimizing a higher order, e.g., curvature dependent elastic energy when keeping one point of the curves fixed, cf. e.g. [31], [51]. In the light of this we can also deal with variational problems for nonlinearly elastic rods prescribing a uniform upper bound on \mathcal{U}_p for the rod centerlines ensuring a positive thickness of the rods, compare with [22] where the global radius of curvature $\Delta[\cdot]$ was used to prescribe a positive thickness.

Appendix

Lemma A.1 *Assume that $p \geq 1$ and $\Phi \in W^{2,p}(I)$, where $I = (x_0, x_1)$. Then the arclength parametrization Γ of the graph of Φ is of class $W^{2,p}(J, \mathbb{R}^2)$, where $J = (t_0, t_1)$ and*

$$|J| = t_1 - t_0 := \int_{x_0}^{x_1} \sqrt{1 + \Phi'(x)^2} \, dx.$$

Proof We have

$$\Gamma(t) = (x(t), \Phi(x(t))), \quad t \in (t_0, t_1), \tag{A.1}$$

where the map $(t_0, t_1) \ni t \mapsto x(t) \in (x_0, x_1)$ is given by the implicit formula

$$t = \int_{x_0}^{x(t)} \sqrt{1 + \Phi'(x)^2} \, dx. \tag{A.2}$$

By (A.2), $x(t)$ is monotonically increasing and the derivative $x'(t)$ is given by

$$\frac{1}{\sqrt{1 + \Phi'(x(t))^2}} = x'(t), \tag{A.3}$$

so that we have

$$0 < c_0 \leq x'(t) \leq 1,$$

where $c_0 := (1 + \|\Phi\|_{C^1}^2)^{-1/2}$. (In dimension 1, $W^{2,p}(I)$ is embedded into $C^1(\bar{I})$.)

Now, note that since $\Phi' \in W^{1,p}(I)$ and $x \in C^1(J)$, we have $\Phi' \circ x \in W^{1,1}_{loc}(J)$ (it is easy to see that $\Phi' \circ x$ is an absolutely continuous function on J , using the fundamental theorem of calculus and the monotonicity of x). Therefore, by (A.3), x' is also of class $W^{1,1}_{loc}$. Thus, we can compute

$$x''(t) = -\frac{\Phi'(x(t))\Phi''(x(t))}{(1 + \Phi'(x(t))^2)^2}.$$

Since $W^{2,p}(I) \subset C^1(\bar{I})$, we obtain $|x''(t)| \leq C|\Phi''(x(t))|$. Thus,

$$\Gamma''(t) = (x''(t), \Phi''(x(t))x'(t)^2 + \Phi'(x(t))x''(t))$$

satisfies

$$\int_{t_0}^{t_1} |\Gamma''(t)|^p dt \leq C \int_{t_0}^{t_1} |\Phi''(x(t))|^p dt \leq C \cdot c_0^{-1} \int_{x_0}^{x_1} |\Phi''(x)|^p dx < \infty.$$

This completes the proof of Lemma A.1. □

Using this lemma, we can construct closed, $W^{2,p}$ -regular loops in the x - y -plane from graphs of $W^{2,p}$ -functions. Here is a sketch of such a construction. Take $\Phi \in W^{2,p}((x_0, x_1))$. Then, Φ' has a finite limit at x_0 and x_1 . Take the tangents to the graph of Φ at $P_0 = (x_0, \Phi(x_0))$ and $P_1 = (x_1, \Phi(x_1))$.

We follow the tangential ray emanating from the graph of Φ at P_0 up to the point Q_0 where it hits the line $\{y = \sup \Phi\}$ or $\{y = \inf \Phi\}$ depending on the sign of $\Phi'(x_0)$. In the same way we obtain a point Q_1 on the tangent ray starting in P_1 .

If these tangent rays are parallel we identify their common direction with the unit vector $T \in S^1 \subset \mathbb{R}^2$ (such that $(Q_1 - Q_0) \cdot T > 0$) and translate the segment $\{Q_0 + s((Q_1 - Q_0) \cdot T)T, s \in [0, 1]\}$ in a direction perpendicular to T to obtain a segment R_0R_1 parallel to T which does not intersect the graph of Φ any more. Then we can find two unique semi-circles C_0 and C_1 connecting R_0 with Q_0 and R_1 with Q_1 , respectively, such that the union

$$\text{Graph } \Phi \cup P_0Q_0 \cup C_0 \cup R_0R_1 \cup C_1 \cup Q_1P_1$$

forms a simple $W^{2,p}$ -regular loop, since it is globally C^1 and piecewise (at least) $W^{2,p}$.

If the tangent lines containing P_0Q_0 and P_1Q_1 intersect in a point $S \in \mathbb{R}^2$, and if, say, $|SQ_0| \geq |SQ_1|$ then we extend the segment P_1Q_1 to find a point \tilde{Q}_1 collinear with P_1 and Q_1 and with $|P_1\tilde{Q}_1| \geq |P_1Q_1|$ and $|SQ_0| = |S\tilde{Q}_1|$. Then we take the unique circular arc C connecting Q_0 and \tilde{Q}_1 which is tangent to P_0Q_0 in Q_0 and to $P_1\tilde{Q}_1$ in \tilde{Q}_1 . Again, the union

$$\text{Graph } \Phi \cup P_0Q_0 \cup C \cup \tilde{Q}_1P_1$$

yields a simple $W^{2,p}$ -regular loop.

If we choose Φ so that the curvature of the graph blows up at one point, then so does $1/\varrho_G[\gamma]$ for the resulting loop γ .

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