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Modeling repulsive forces on fibres via knot energies

by

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Abstract
Modeling of repulsive forces is essential to the understanding of certain bio-physical processes, especially for the motion of DNA molecules. These kinds of phenomena seem to be driven by some sort of “energy” which especially prevents the molecules from strongly bending and forming self-intersections.
Inspired by a physical toy model, numerous functionals have been defined during the past twenty-five years that aim at modeling self-avoidance. The general idea is to produce “detangled” curves having particularly large distances between distant strands.
In this survey we present several families of these so-called *knot energies*. It turns out that they are quite similar from an analytical viewpoint. We focus on proving self-avoidance and existence of minimizers in every knot class. For a suitable subfamily of these energies we show how to prove that these minimizers are even infinitely differentiable.

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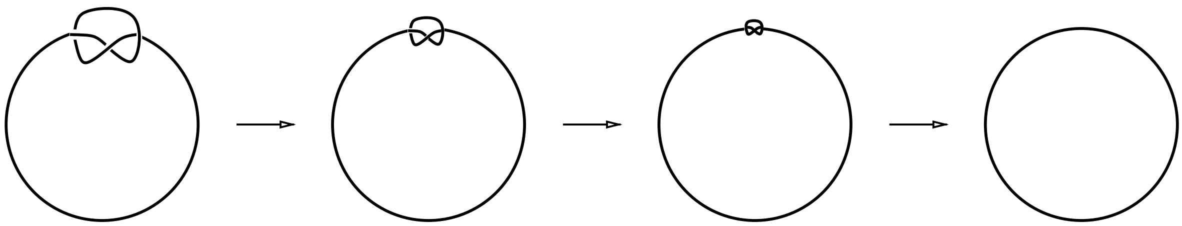

Fig 1. The pull-tight phenomenon.

1. Introduction

Self-repelling forces play an important rôle in nature, e.g. for the behaviour of protein foldings [19] and the motion of knotted DNA structures in electrophoresis gels [12]. For instance, in order to access the information stored in the DNA, specific topological and geometrical transformations have to be applied by the corresponding enzymes. Therefore, the topological shape of DNA molecules has an important impact in this process [28]. In fact, one is led to speculate that these kinds of phenomena are driven by some "energy" [20] which is of course difficult to determine. Especially, such an energy should prevent the molecule from strongly bending and forming self-intersections.

Inspired by a physical toy model, several functionals appeared in the literature during the past twenty-five years that aim at modeling self-avoidance. The original idea tracing back to Fukuhara [15] was to consider the deformation of a thin fibre charged with electrons lying in a viscous liquid. Assuming that this fibre is infinitesimally thin, it may be regarded as a curve

$$\gamma : [0,1] \to \mathbb{R}^n$$

where, in general, $n = 3$. We will restrict to closed curves, so the points 0 and 1 can be identified and the preimage becomes the quotient space $\mathbb{R}/\mathbb{Z}$, i.e., the curve is a 1-periodic mapping $\mathbb{R} \to \mathbb{R}^n$. Heuristically, the electrostatic energy acts as a repulsive potential, so the interaction of two given points $\gamma(u)$ and $\gamma(v)$ can be written as

$$\frac{1}{|\gamma(u) - \gamma(v)|^\alpha}$$

for some $\alpha > 0$ which has to be chosen in an appropriate way. If we are not in an equilibrium, the electrostatic energy is turned into kinetic energy which will result in some deformation of the curve. As the electrons lead to self-avoidance, we expect the curve to "detangle", resulting in a shape having particular large distances between different strands.

In this spirit, the basic idea in constructing self-repelling forces is to penalize distant points of the curve having a small Euclidean distance. We particularly aim at maintaining the *knot type* or, synonymously, *knot class*, which defines an equivalence relation among all embedded closed curves. Roughly speaking, two given knots belong to the same knot class if one can continuously be deformed into the other without self-intersections or pulling-tight of small knotted arcs as indicated in Figure 1. A precise definition can be found, e.g., in [10].

The motivation to restrict to closed curves is mainly due to convenience. In this case the topological shape of a closed embedded curve is essentially determined by its knot type while there is no satisfactory notion of "knottedness" of open curves. Of course, one could adopt the definition of "knot type contained in a ball" [14], but this leads to several technical difficulties which we would like to avoid here.

However, there are in fact bacteria whose genome is a single closed duplex DNA circle [28], so we are even now not too far away from "real world" problems. Of course, we are still on the level of an idealized situation that lacks a concrete biophysical model. Nevertheless, we hope for future applications of the theory presented in this survey.

Since we consider closed curves, we may extend their parametrizations to periodic functions—which is quite convenient for applying tools of harmonic analysis. Though our proofs seem to rely to a large extent on this setting, with some additional techniques a similar analysis of the energies in question should be possible for open curves.

In this text, we will provide a short outline of knot energies proposed by several authors and prove existence and regularity for a large class of knot energies. We start by giving a widely adopted definition of knot energies [24, 27].

Definition 1 (Knot functionals, knot energies and strong knot energies).
By $C^1(\mathbb{R}/\mathbb{Z},\mathbb{R}^n)$ we denote the class of all continuously differentiable functions $\mathbb{R}/\mathbb{Z}\to\mathbb{R}^n$. A *knot functional* is a mapping $C^1(\mathbb{R}/\mathbb{Z},\mathbb{R}^n)\to[0,\infty]$. A knot functional $\mathrm{KE}: C^1(\mathbb{R}/\mathbb{Z},\mathbb{R}^n)\to[0,\infty]$ is said to be a *knot energy* if it is self-repulsive, i.e., if for any sequence $(\gamma_k)_{k\in\mathbb{N}}\subset C^1$ uniform (in C^0) convergence to a non-injective curve $\gamma_\infty\in C^1$ implies

$$\mathrm{KE}(\gamma_k)\to\infty \qquad \text{as } k\to\infty. \tag{1}$$

If there are, for given $E, L>0$, only finitely many knot types having a representative with $\mathrm{KE}\le E$ and length $=L$ then KE is a *strong* knot energy.

Note that being self-repulsive is stronger than assuming that the functional is infinite on all non-injective curves.

By minimizing a knot energy one hopes to find curves having a particularly nice shape that, as indicated above, could presumably characterize a steady state in some biophysical model or help to determine the knot type.

In a broader sense, a knot energy can be seen as some sort of "measure" for the "entangledness" of a given curve. It is natural to ask to what extent a knot energy also measures smoothness and curvature.

To this end it is crucial to answer the following questions:

- Is the functional under consideration in fact a knot energy?
- Are there minimizers in every knot class?
- How smooth are those (local) minimizers?

In the next section we will present some examples of knot functional families and discuss for which parameters they are self-repulsive and non-singular. We will be able to give an affirmative answer to the first two questions raised above (Theorems 4 and 9). As to the third one, we will show that, for a certain sub-family, any stationary point is C^∞, i.e., infinitely differentiable (Theorem 10).

2. A parade of knot energies

In this section we present some families of knot functionals. Although they stem from different geometric concepts, they turn out to be quite similar from an analyst's viewpoint. This fact will become apparent in the subsequent section where we present an axiomatic form which covers all of the knot energies discussed in this section. We will use this abstract setting for simultaneously proving self-avoidance and existence of minimizers within any knot class.

Here we intend to motivate for which parameter range of the respective families we expect to find proper knot energies.

2.1. O'Hara's energies

Adapting Fukuhara's idea, O'Hara [22, 23] defined the family of knot functionals

$$\mathrm{O'H}^{(\alpha,p)}(\gamma) := \iint_{(\mathbb{R}/\mathbb{Z})^2}\left(\frac{1}{|\gamma(u)-\gamma(v)|^\alpha}-\frac{1}{D_\gamma(u,v)^\alpha}\right)^p |\gamma'(u)|\,|\gamma'(v)|\,\mathrm{d}u\,\mathrm{d}v. \tag{2}$$

Here $\alpha, p > 0$, and $\gamma \in C^{0,1}(\mathbb{R}/\mathbb{Z}, \mathbb{R}^n)$. The quantity $D_\gamma(u,v)$ measures the intrinsic distance between $\gamma(u)$ and $\gamma(v)$ on the curve γ.

As $|\gamma(u)-\gamma(v)| \le D_\gamma(u,v)$, the integrand is non-negative, so the integral takes a value in $[0,\infty]$. The first term penalizes pairs of points $(\gamma(u),\gamma(v))$ having a small Euclidean distance by taking the latter to a negative power in order to produce a singularity. As neighboring points $\gamma(u), \gamma(u+\varepsilon)$ naturally have a small Euclidean distance, we have to add some sort of regularization: substracting the intrinsic distance $D_\gamma(u,v)$ taken to the same negative power as the Euclidean distance, the singularities stemming from neighboring points are cancelled while those for distant points are essentially unaffected. Finally we average over the p-th power of this term over all pairs of points by integrating. The factors $|\gamma'(u)|\,|\gamma'(v)|$ guarantee invariance under reparametrization.

Now we have to determine the parameters $\alpha, p > 0$ for which this procedure works. We first remark $\mathrm{O'H}^{(\alpha,p)}(r\gamma) = r^{2-\alpha p}\mathrm{O'H}^{(\alpha,p)}(\gamma)$ for $r > 0$, i.e., $\mathrm{O'H}^{(\alpha,p)}$ is positively homogeneous of degree $2-\alpha p$. Therefore, in case $\alpha p > 2$ the integral blows up as the curve shrinks down.

There is an immediate heuristics why we should stick to that range. Choose a finite-energy smooth curve that contains a straight line segment. Insert a small knotted arc in that line segment producing a smooth curve. Shrinking down that knotted arc component while leaving unchanged the rest of the curve would produce a sequence of knotted arcs leaving the knot class at the limit, the so-called *pulling-tight effect*, see Figure 1. However, (1) does not apply for $\alpha p \le 2$.

Definition 2 (Preventing pulling-tight).

A knot functional is said to *prevent pulling-tight* if pulling-tight of a small knotted arc as in Figure 1 implies (1).

A formal definition is provided in O'Hara's monography [24].

From the argument sketched above we infer that a knot functional being positively homogeneous of non-negative degree it very unlikely to prevent pulling-tight.

However, self-avoidance as in the definition of knot energies does not imply the prevention of pulling-tight. A counterexample is already the first geometric knot energy $\mathrm{O'H}^{(2,1)}$ which was shown by O'Hara to be self-repulsive. But due to its invariance under the Möbius group [14] it cannot prevent a curve from being pulled tight.

In order to be self-repulsive, two perpendicular line segments must produce an energy blow-up as they approach each other. We will show that this is not the case for $\alpha p < 2$. To this end consider a curve γ_δ containing the two strands $\gamma_1(u) := (u,0,0)$ and $\gamma_2(u) = (0,u,\delta)$ for $\delta > 0$, $u \in [-1,1]$. In order to compute the respective energy values, we switch to polar coordinates, $u = r\cos\varphi$, $v = r\sin\varphi$, which gives[1]

$$\begin{aligned}
\mathrm{O'H}^{(\alpha,p)}(\gamma_\delta) &\sim \iint_{[-1,1]^2} \left(\frac{1}{|\gamma_1(u)-\gamma_2(v)|^\alpha} - \frac{1}{D(\gamma_1(u),\gamma_2(v))^\alpha} \right)^p \mathrm{d}v\,\mathrm{d}u \\
&\le \iint_{[-1,1]^2} \frac{\mathrm{d}v\,\mathrm{d}u}{(u^2+v^2+\delta^2)^{\alpha p}} \\
&\le \int_0^{\sqrt{2}} \int_0^{2\pi} \frac{r\,\mathrm{d}\varphi\,\mathrm{d}r}{(r^2+\delta^2)^{(\alpha p)/2}} \\
&\le C \int_0^{\sqrt{2}} \frac{r\,\mathrm{d}r}{(r+\delta)^{\alpha p}} \\
&\le C \int_0^{\sqrt{2}} (r+\delta)^{1-\alpha p} \\
&\overset{\alpha p<2}{\le} C \left(\left(\sqrt{2}+\delta\right)^{2-\alpha p} - \delta^{2-\alpha p} \right).
\end{aligned}$$

[1] *By writing $A \sim B$ we mean that A essentially behaves like B up to lower-order terms.*

The last term stays bounded as $\delta \searrow 0$ if $\alpha p < 2$.

On the other hand, not every functional $\mathrm{O'H}^{(\alpha,p)}$ with $\alpha p \geq 2$ leads to a suitable knot energy. In fact, for γ being parameterized by arc-length, i.e., $|\gamma'| = 1$ almost everywhere, we deduce as in [4] using $1 - \langle a, b\rangle_{\mathbb{R}^n} = \frac{1}{2}|a-b|^2$ for $a, b \in \mathbb{R}^n$, $|a| = |b| = 1$, as well as $D_\gamma(u+w,u) = |w|$

$$\begin{aligned}
\mathrm{O'H}^{(\alpha,1)}(\gamma) &= \iint_{(\mathbb{R}/\mathbb{Z})^2} \left(\frac{1}{|\gamma(u+w)-\gamma(u)|^\alpha} - \frac{1}{D_\gamma(u+w,u)^\alpha} \right) \mathrm{d}w\,\mathrm{d}u \\
&= \iint_{(\mathbb{R}/\mathbb{Z})^2} \underbrace{\left(\frac{|w|}{|\gamma(u+w)-\gamma(u)|} \right)^\alpha}_{\geq 1} \frac{1}{|w|^\alpha} \left(1 - \frac{|\gamma(u+w)-\gamma(u)|^\alpha}{|w|^\alpha} \right) \mathrm{d}w\,\mathrm{d}u \\
&\geq c \iint_{(\mathbb{R}/\mathbb{Z})^2} \frac{1}{|w|^\alpha} \left(1 - \frac{|\gamma(u+w)-\gamma(u)|^2}{|w|^2} \right) \mathrm{d}w\,\mathrm{d}u \\
&\geq c \iint_{(\mathbb{R}/\mathbb{Z})^2} \frac{1}{|w|^\alpha} \left(1 - \iint_{[0,1]^2} \langle \gamma'(u+\vartheta_1 w), \gamma'(u+\vartheta_2 w)\rangle_{\mathbb{R}^n} \,\mathrm{d}\vartheta_1\,\mathrm{d}\vartheta_2 \right) \mathrm{d}w\,\mathrm{d}u \\
&\geq \tilde{c} \iint_{(\mathbb{R}/\mathbb{Z})^2} \frac{1}{|w|^\alpha} \left(\iint_{[0,1]^2} |\gamma'(u+\vartheta_1 w) - \gamma'(u+\vartheta_2 w)|^2 \,\mathrm{d}\vartheta_1\,\mathrm{d}\vartheta_2 \right) \mathrm{d}w\,\mathrm{d}u \\
&\geq \tilde{c} \int_{\mathbb{R}/\mathbb{Z}} \int_{-1/2}^{1/2} \frac{1}{|w|^\alpha} \left(\iint_{[0,1]^2} |\gamma'(u+(\vartheta_1-\vartheta_2)w) - \gamma'(u)|^2 \,\mathrm{d}\vartheta_1\,\mathrm{d}\vartheta_2 \right) \mathrm{d}w\,\mathrm{d}u \\
&\geq \tilde{c} \iint_{[0,1]^2} \int_{\mathbb{R}/\mathbb{Z}} \int_{-1/2}^{1/2} \frac{1}{|w|^\alpha} |\gamma'(u+(\vartheta_1-\vartheta_2)w) - \gamma'(u)|^2 \,\mathrm{d}w\,\mathrm{d}u\,\mathrm{d}\vartheta_1\,\mathrm{d}\vartheta_2 \\
&\geq \tilde{c} \int_{1-\varepsilon}^{1} \int_0^\varepsilon \int_{\mathbb{R}/\mathbb{Z}} \int_{-1/2}^{1/2} \frac{1}{|w|^\alpha} |\gamma'(u+(\vartheta_1-\vartheta_2)w) - \gamma'(u)|^2 \,\mathrm{d}w\,\mathrm{d}u\,\mathrm{d}\vartheta_1\,\mathrm{d}\vartheta_2 \\
&\geq \tilde{c} \int_{1-\varepsilon}^{1} \int_0^\varepsilon \int_{\mathbb{R}/\mathbb{Z}} \int_{-(\vartheta_1-\vartheta_2)/2}^{(\vartheta_1-\vartheta_2)/2} \frac{(\vartheta_1-\vartheta_2)^{\alpha-1}}{|\tilde{w}|^\alpha} |\gamma'(u+\tilde{w}) - \gamma'(u)|^2 \,\mathrm{d}\tilde{w}\,\mathrm{d}u\,\mathrm{d}\vartheta_1\,\mathrm{d}\vartheta_2 \\
&\geq \tilde{c} \underbrace{\int_{1-\varepsilon}^{1} \int_0^\varepsilon (\vartheta_1-\vartheta_2)^{\alpha-1} \,\mathrm{d}\vartheta_1\,\mathrm{d}\vartheta_2}_{\in(0,\infty)} \int_{\mathbb{R}/\mathbb{Z}} \int_{-1/2+\varepsilon}^{1/2-\varepsilon} \frac{|\gamma'(u+\tilde{w}) - \gamma'(u)|^2}{|\tilde{w}|^\alpha} \,\mathrm{d}\tilde{w}\,\mathrm{d}u,
\end{aligned}$$

where $\varepsilon \in (0, \frac{1}{2})$. More generally, one can show

$$\mathrm{O'H}^{(\alpha,p)}(\gamma) \geq c \int_{\mathbb{R}/\mathbb{Z}} \int_{-\varepsilon}^{\varepsilon} \frac{|\gamma'(u+w) - \gamma'(u)|^{2p}}{|w|^{\alpha p}} \,\mathrm{d}w\,\mathrm{d}u \qquad \text{for } \varepsilon \ll 1,$$

see [4] for details. As for closed curves γ' cannot be constant, the right-hand side must be positive. Applying the following result which is proven in Brezis [9, Prop. 2], we then get that, in case

$$(\alpha - 2)p \geq 1, \tag{3}$$

the right hand side must be infinite for any closed curve!

Proposition 3 (Highly singular potentials).

Assume Ω is a connected open set in $\mathbb{R}^N$ and $f : \Omega \to \mathbb{R}$ is a measurable function with

$$\iint_{\Omega\times\Omega} \frac{|f(x) - f(y)|^p}{|x-y|^{N+p}} \,\mathrm{d}x\,\mathrm{d}y < \infty \qquad \textit{for some } p \in [1,\infty) \tag{4}$$

then f is constant.

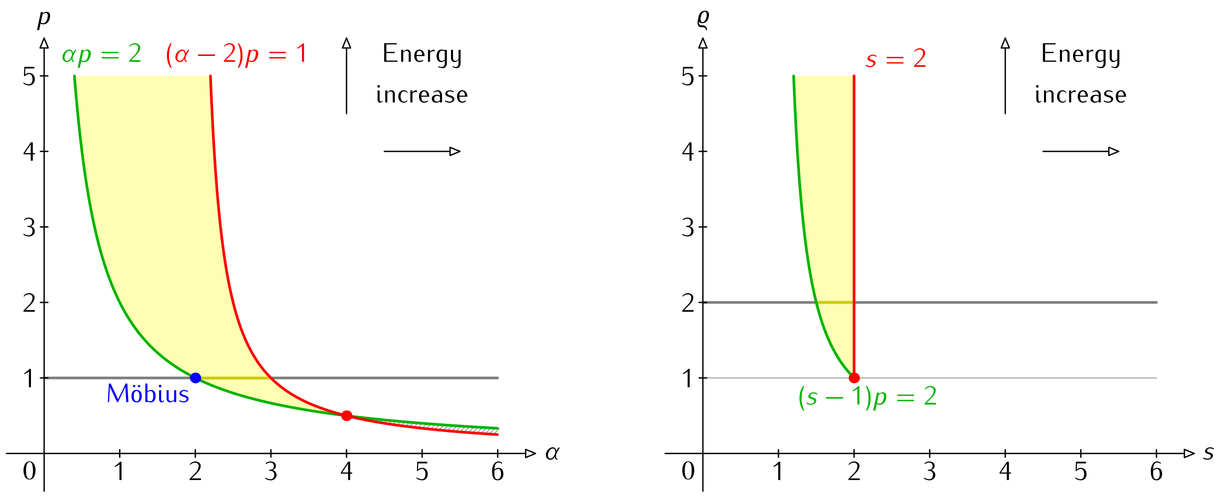

Fig 2. The range of O'Hara's energies (left); the range of abstract energies (right). On the left-hand side we depict the situation of O'Hara's energies $\mathrm{O'H}^{(\alpha,p)}$. Below the green curve, the respective functionals are not self-repulsive, thus no knot energies. On and above the red line the functionals are so singular that they only take the value infinity. The yellow area between the two curves marks the sub-critical range for which we prove self-repulsiveness and existence of minimizers in every knot class. The darker yellow line $\alpha \in (2,3)$, $p = 1$ denotes the non-degenerate sub-critical range where local minimizers are C^∞. Any functional $\mathrm{O'H}^{(\alpha,p)}$ corresponds to the abstract functional $\mathrm{KE}^{(s,\varrho)}$ where $s = \frac{\alpha}{2} - \frac{1}{2p} + 1$ and $\varrho = 2p$. The respective parameter ranges are shown on the right-hand side. The energy increase does not follow from the axioms (K_1), (K_2), (K_3), but applies for the examples discussed in this section.

An alternative way to see $\mathrm{O'H}^{(\alpha,p)} \equiv \infty$ for (3) is provided by Abrams, Cantarella et al. [1]. They prove that $\mathrm{O'H}^{(\alpha,p)}$ is (for closed curves) always globally minimized by the (round) circle. It is easy to see that it is assigned to infinite energy in case (3).

In light of these facts it is reasonable to restrict oneself to the *sub-critical range*

$$\alpha p > 2, \qquad (\alpha - 2)p < 1. \tag{5}$$

The respective parameter ranges discussed in this subsection are visualized in Figure 2 (left).

2.2. Tangent-point energies

Another important family of knot energies is the (generalized) tangent-point energy family

$$\mathrm{TP}^{(p,q)}(\gamma) = \iint_{(\mathbb{R}/\mathbb{Z})^2} \frac{\left|P^\perp_{\gamma'(u)}(\gamma(u) - \gamma(v))\right|^q}{|\gamma(u) - \gamma(v)|^p} |\gamma'(u)|\,|\gamma'(v)| \,\mathrm{d}u\,\mathrm{d}v \tag{6}$$

where $\gamma \in C^{0,1}(\mathbb{R}/\mathbb{Z}, \mathbb{R}^n)$ and

$$P_{\gamma'(u)}a := \left\langle a, \frac{\gamma'(u)}{|\gamma'(u)|} \right\rangle \frac{\gamma'(u)}{|\gamma'(u)|}, \qquad P^\perp_{\gamma'(u)}a := a - P_{\gamma'(u)}a \qquad \text{for } a \in \mathbb{R}^n \tag{7}$$

denote the projection onto the tangential and normal part along γ respectively. In case $p = 2q$ the factor $\frac{\left|P^\perp_{\gamma'(u)}(\gamma(u)-\gamma(v))\right|^q}{|\gamma(u)-\gamma(v)|^p}$ in (6) is just the q-th power of the reciprocal of the diameter of the circle being tangent to $\gamma(u)$ and passing through $\gamma(v)$.

Proceeding as for O'Hara's energies, we will show that the functionals are not self-repulsive if $p < q + 2$ while they are singular for $p \geq 2q + 1$. Therefore we will restrict our attention to the sub-critical range

$$p \in (q + 2, 2q + 1). \tag{8}$$

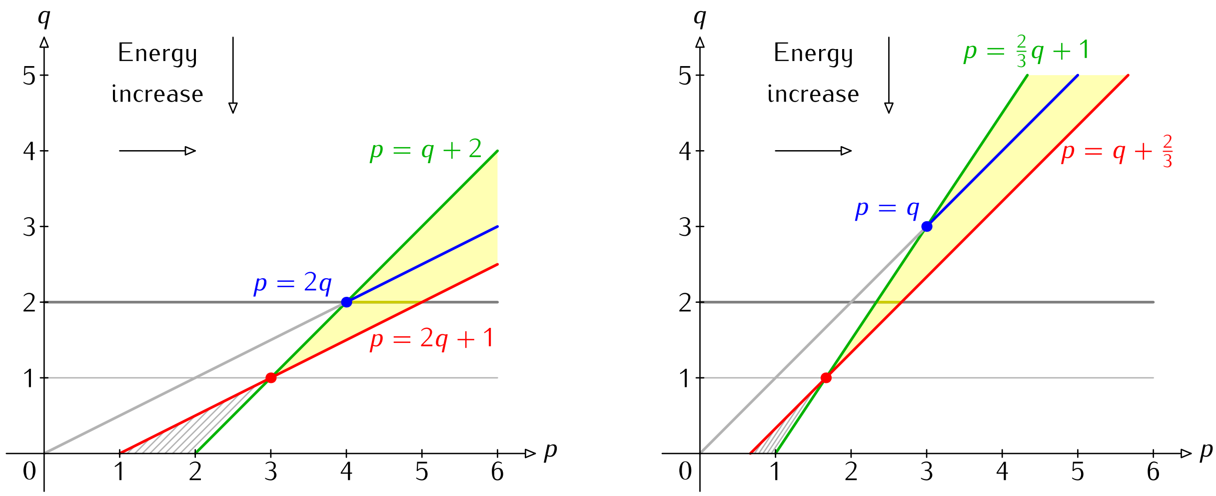

Fig 3. The ranges of the tangent-point energies (left) and the integral Menger curvature (right). Above the green line, the functionals are not self-repulsive; below the red line, they are highly singular. The yellow area marks the sub-critical range, the dark yellow line the non-degenerate sub-critical range, cf. Fig. 2. The blue line indicates the "classical" energy functionals investigated by Strzelecki et al. [26, 27]. The functionals $\mathrm{TP}^{(p,q)}$ and $\mathrm{intM}^{(p,q)}$ correspond to $\mathrm{KE}^{(s,\varrho)}$ where $s = \frac{p-1}{q}$ or $s = \frac{3p-2}{q} - 1$ respectively and $\varrho = q$, see [6, 8] for details.

This range is sketched in Figure 3. The lower bound $q+2$ is due to the fact that as before for a curve γ_δ containing the strands $\gamma_1(u) := (u,0,0)$ and $\gamma_2(u) = (0,u,\delta)$ for $\delta > 0$, $u \in [-1,1]$, one gets

$$\begin{aligned} \mathrm{TP}^{(p,q)}(\gamma_\delta) &\sim 2 \iint_{[-1,1]^2} \frac{\left(v^2+\delta^2\right)^{q/2}}{(u^2+v^2+\delta^2)^{p/2}} \,\mathrm{d}u\,\mathrm{d}v \\ &\le 2 \int_0^{\sqrt{2}} \int_0^{2\pi} \frac{\left(r^2\sin^2\varphi+\delta^2\right)^{q/2}}{(r^2+\delta^2)^{p/2}} r \,\mathrm{d}\varphi\,\mathrm{d}r \\ &\le 4\pi \int_0^{\sqrt{2}} \left(r^2+\delta^2\right)^{\frac{q-p}{2}} r \,\mathrm{d}r. \end{aligned} \tag{9}$$

The integral on the right-hand side is bounded for $\delta \searrow 0$ if $p < q+2$.

Using techniques from [3] we justify the upper bound $2q+1$ as follows. Let us again assume that γ is parametrized by arc-length. By continuity we may choose some $\delta > 0$ depending on γ such that

$$|\gamma'(u) - \gamma'(v)| \le \tfrac{1}{2}\sqrt{2} \qquad \text{for all } u \in \mathbb{R}/\mathbb{Z}, |u-v| \le \delta. \tag{10}$$

This leads to

$$\begin{aligned} &\left|P^\perp_{\gamma'(v)}(\gamma(u)-\gamma(v)) - P^\perp_{\gamma'(u)}(\gamma(u)-\gamma(v))\right|^2 \\ &= \left|\langle \gamma(u)-\gamma(v), \gamma'(v)\rangle \gamma'(v) - \langle \gamma(u)-\gamma(v), \gamma'(u)\rangle \gamma'(u)\right|^2 \\ &= \left|\langle \gamma(u)-\gamma(v), \gamma'(v)\rangle\right|^2 + \left|\langle \gamma(u)-\gamma(v), \gamma'(u)\rangle\right|^2 \\ &\quad - 2\langle \gamma(u)-\gamma(v), \gamma'(u)\rangle \langle \gamma(u)-\gamma(v), \gamma'(v)\rangle \langle \gamma'(u), \gamma'(v)\rangle \\ &= \left|\langle \gamma(u)-\gamma(v), \gamma'(v)\rangle - \langle \gamma(u)-\gamma(v), \gamma'(u)\rangle\right|^2 \\ &\quad + \langle \gamma(u)-\gamma(v), \gamma'(u)\rangle \langle \gamma(u)-\gamma(v), \gamma'(v)\rangle \left|\gamma'(u)-\gamma'(v)\right|^2 \\ &\ge \left|\gamma'(u)-\gamma'(v)\right|^2 |u-v|^2 \int_0^1 \underbrace{\langle \gamma'(u+\vartheta_1(v-u)), \gamma'(u)\rangle}_{=1-\frac{1}{2}|\gamma'(u+\vartheta_1(v-u))-\gamma'(u)|^2 \ge \frac{3}{4}} \mathrm{d}\vartheta_1 \int_0^1 \underbrace{\langle \gamma'(u+\vartheta_2(v-u)), \gamma'(v)\rangle}_{\ge \frac{3}{4}} \mathrm{d}\vartheta_2 \end{aligned}$$

$$\geq \tfrac{9}{16}\left|u-v\right|^2\left|\gamma'(u)-\gamma'(v)\right|^2$$

which in turn allows to estimate using $|\gamma(u)-\gamma(v)| \leq |u-v|$

$$\begin{aligned}
\mathrm{TP}^{(p,q)}(\gamma) &= \iint_{(\mathbb{R}/\mathbb{Z})^2} \frac{\left|P^{\perp}_{\gamma'(u)}\left(\gamma(u)-\gamma(v)\right)\right|^q}{|\gamma(u)-\gamma(v)|^p}\,\mathrm{d}u\,\mathrm{d}v \\
&= \tfrac{1}{2}\iint_{(\mathbb{R}/\mathbb{Z})^2} \frac{\left|P^{\perp}_{\gamma'(v)}\left(\gamma(u)-\gamma(v)\right)\right|^q + \left|P^{\perp}_{\gamma'(u)}\left(\gamma(u)-\gamma(v)\right)\right|^q}{|\gamma(u)-\gamma(v)|^p}\,\mathrm{d}u\,\mathrm{d}v \\
&\geq \tilde{c}_q \iint_{(\mathbb{R}/\mathbb{Z})^2} \frac{\left|P^{\perp}_{\gamma'(v)}\left(\gamma(u)-\gamma(v)\right) - P^{\perp}_{\gamma'(u)}\left(\gamma(u)-\gamma(v)\right)\right|^q}{|\gamma(u)-\gamma(v)|^p}\,\mathrm{d}u\,\mathrm{d}v \\
&\geq c_{p,q}\iint_{|u-v|\leq\delta} \frac{|u-v|^q\,|\gamma'(u)-\gamma'(v)|^q}{|\gamma(u)-\gamma(v)|^p}\,\mathrm{d}u\,\mathrm{d}v \\
&\geq c_{p,q}\iint_{|u-v|\leq\delta} \frac{|\gamma'(u)-\gamma'(v)|^q}{|u-v|^{p-q}}\,\mathrm{d}u\,\mathrm{d}v.
\end{aligned}$$

Applying Proposition 3, we again get that for $p > 2q+1$ the energy is only finite for pieces of one straight line.

2.3. Integral Menger curvature

Instead of the circle passing through one point and being tangent to another we can also consider the *circumcircle*, i.e. the circle passing through three distinct points $x, y, z \in \mathbb{R}^n$. The circumcircle radius is given by

$$R(x,y,z) := \frac{|y-z|\,|y-x|\,|z-x|}{2\,|(y-x)\wedge(z-x)|} = \frac{|y-z|}{2\sin\sphericalangle(y-x, z-x)}, \qquad x,y,z \in \mathbb{R}^n. \tag{11}$$

Decoupling powers in the nominator and denominator we arrive at

$$R^{(p,q)}(x,y,z) := \frac{(|y-z|\,|y-x|\,|z-x|)^p}{|(y-x)\wedge(z-x)|^q} = \frac{|y-z|^p\,|y-x|^{p-q}\,|z-x|^{p-q}}{\sin\sphericalangle(y-x,z-x)^q}$$

which is the integrand of the *generalized integral Menger curvature* functionals [8]

$$\mathrm{intM}^{(p,q)}(\gamma) := \iiint_{(\mathbb{R}/\mathbb{Z})^3} \frac{|\gamma'(u)|\,|\gamma'(u+v)|\,|\gamma'(u+w)|}{R^{(p,q)}(\gamma(u),\gamma(u+v),\gamma(u+w))}\,\mathrm{d}w\,\mathrm{d}v\,\mathrm{d}u, \qquad p,q>0. \tag{12}$$

Due to the three dimensional integration domain the situation is a little bit more involved. In order to exclude the case $p < \frac{2}{3}q+1$ we again look at a curve γ_δ containing the strands $\gamma_1(u) := (u,0,0)$ and $\gamma_2(u) = (0,u,\delta)$ for $\delta > 0$, $u \in [-1,1]$. Applying spherical coordinates $u = r\cos\vartheta$, $v = r\sin\vartheta\cos\varphi$, $w = r\sin\vartheta\sin\varphi$, leads us to

$$\begin{aligned}
\mathrm{intM}^{(p,q)}(\gamma_\delta) &\sim C\iiint_{[-1,1]^3} \frac{\left(\delta^2+u^2\right)^{q/2}}{|v-w|^{p-q}\,(\delta^2+u^2+v^2)^{p/2}\,(\delta^2+u^2+w^2)^{p/2}}\,\mathrm{d}w\,\mathrm{d}v\,\mathrm{d}u \\
&\leq C\iiint_{[-1,1]^3} \frac{\left(\delta^2+u^2\right)^{(q-p)/2}}{|v-w|^{p-q}\,(\delta^2+u^2+v^2+w^2)^{p/2}}\,\mathrm{d}w\,\mathrm{d}v\,\mathrm{d}u \\
&\leq C\int_0^{\sqrt{3}}\int_0^{\pi} \frac{\left(\delta^2+r^2\cos^2\vartheta\right)^{(q-p)/2} r^2\sin\vartheta}{r^{p-q}\sin^{p-q}\vartheta\,(\delta^2+r^2)^{p/2}}\,\mathrm{d}\vartheta\,\mathrm{d}r\,\underbrace{\int_0^{2\pi}\frac{\mathrm{d}\varphi}{|\cos\varphi-\sin\varphi|^{p-q}}}_{\leq C}
\end{aligned}$$

$$
\begin{aligned}
&\le C \int_0^{\sqrt{3}} \left(\int_{[0,\frac{\pi}{4}]\cup[\frac{3\pi}{4},\pi]} \frac{\left(\delta^2+r^2\right)^{(q-p)/2} \,\mathrm{d}\vartheta}{r^{p-q-2} \underbrace{\sin^{p-q-1}\vartheta}_{\ge 1} \left(\delta^2+r^2\right)^{p/2}} + \int_{\frac{\pi}{4}}^{\frac{3\pi}{4}} \frac{\left(\delta^2+r^2\cos^2\vartheta\right)^{(q-p)/2} r\sin\vartheta}{r^{p-q-1}\sin^{p-q}\vartheta \left(\delta^2+r^2\right)^{p/2}} \,\mathrm{d}\vartheta \right) \mathrm{d}r \\
&\le C \int_0^{\sqrt{3}} \left((\delta+r)^{-3p+2q+2} + r^{-p+q+1} (\delta+r)^{-p} \int_0^r \left(\delta^2+\sigma^2\right)^{(q-p)/2} \mathrm{d}\sigma \right) \mathrm{d}r \\
&\le C \left(1-\delta^{-3p+2q+3}\right).
\end{aligned}
$$

Proceeding in a similar way as for the tangent-point energies, we infer the restriction $p < q + \frac{2}{3}$ to exclude the highly singular range, see [5, 8].

2.4. Ropelength

In this subsection we briefly mention a special case which is related to the integral Menger curvature family. In fact, it corresponds to the limit case $p = q \to \infty$.

Taking the infimum of (11) over all points of the curve γ, we obtain a notion of *thickness*. This particular definition which goes back to Gonzalez and Maddocks [17] has the advantage over other definitions not to require any initial regularity of the curve.

It is elementary to see that *ropelength*, i.e. the quotient of length over thickness, is a knot energy. Ropelength minimizers are referred to as *ideal knots*. As taking infima is a non-smooth operation, one cannot proceed by the techniques presented in this text.

The existence of ideal knots has been proven in [18], [13], and [16]; they have at least a Lipschitz continuous tangent (if parametrized by arc-length). For further information we refer to [11] and references therein.

3. Existence of minimizers

In this section we discuss the existence of minimizers in any knot class. There is almost nothing known about the shape of those minimizers up to the fact that circles are unique minimizers among all closed curves for O'Hara's energies [1].

In order not to prove the existence result for minimizers of O'Hara's energies, tangent point energies and integral Menger curvature separately, we gather all the properties of these energies we need in one abstract framework:

For $k \in \mathbb{N}$, $k > 1$, we let $f^{(s,\varrho)} : C^1(\mathbb{R}/\mathbb{Z},\mathbb{R}^n) \times (\mathbb{R}/\mathbb{Z})^k \to [0,\infty]$ be a measurable non-negative function and define the energy of a curve γ by

$$
\mathrm{KE}^{(s,\varrho)}(\gamma) := \left\| f^{(s,\varrho)}(\gamma;\cdots) \right\|_{L^1((\mathbb{R}/\mathbb{Z})^k)} = \underset{(\mathbb{R}/\mathbb{Z})^k}{\int\cdots\int} f^{(s,\varrho)}(\gamma;u_1,\ldots,u_k)\,\mathrm{d}u_1\cdots\mathrm{d}u_k.
$$

We assume that $f^{(s,\varrho)}$ and $\mathrm{KE}^{(s,\varrho)}$ satisfy the following properties for arbitrary $\gamma \in C^1(\mathbb{R}/\mathbb{Z},\mathbb{R}^n)$.

- (K_1) We have $f^{(s,\varrho)}(r\gamma + x;\cdots) = r^{-(s-1-1/\varrho)} f^{(s,\varrho)}(\gamma;\cdots)$ for all $r > 0$ and $x \in \mathbb{R}^n$. Furthermore, $\mathrm{KE}^{(s,\varrho)}(\gamma)$ is invariant under reparametrization of γ.
- (K_2) If $f^{(s,\varrho)}(\gamma;\cdots)$ vanishes on $U_1 \times \cdots \times U_k$ where $U_j \subset \mathbb{R}/\mathbb{Z}$, $j = 1,\ldots,k$, then the image of γ restricted to $\bigcup_{j=1}^k U_j$ is collinear, i.e., lies on a straight line.
- (K_3) For any $C > 0$ there is some $C' = C'(C) > 0$ such that $\mathrm{KE}^{(s,\varrho)}(\gamma) \le C$ implies $\left\|\gamma'\right\|_{C^{0,s-1-1/\varrho}} \le C'$ for any arc-length parametrized curve γ.

It is not difficult to see that $\mathrm{O'H}^{(\alpha,p)}$, $\mathrm{TP}^{(p,q)}$, and $\mathrm{intM}^{(p,q)}$ satisfy (K_1) and (K_2) for appropriatly chosen s and ϱ. However, in order to prove (K_3) one can either use an approach based on fractional Sobolev spaces and Morrey's embeding theorem, see [6–8], or use a sophisticated scaling argument as shown in [21], [26], and [27].

Theorem 4 (Prototype knot energies in the sub-critical range).

Let (s, ϱ) belong to the sub-critical range, i.e.,

$$s \in (1 + \tfrac{1}{\varrho}, 2), \qquad \varrho \in (1, \infty). \tag{13}$$

The prototype functional $\mathrm{KE}^{(s,\varrho)} : C^1(\mathbb{R}/\mathbb{Z}, \mathbb{R}^n) \to [0, \infty]$ given by

$$\mathrm{KE}^{(s,\varrho)}(\gamma) := \left\| f^{(s,\varrho)}(\gamma; \cdots) \right\|_{L^1((\mathbb{R}/\mathbb{Z})^k)} = \int \cdots \int_{(\mathbb{R}/\mathbb{Z})^k} f^{(s,\varrho)}(\gamma; u_1, \ldots, u_k) \, \mathrm{d}u_1 \cdots \mathrm{d}u_k$$

is a strong knot energy that prevents pulling-tight.

Proof. Pulling-tight produces a singularity of the tangent which is excluded by (K_3). Strong self-repulsiveness is proven in Proposition 8. □

Note that $\mathrm{KE}^{(s,\varrho)}(\gamma)$ might be infinite although $\gamma \in C^{1,s-1-1/\varrho}$ is an embedded arc-length parametrized curve. However, in all the cases discussed here, the energy values are finite for sufficiently regular embedded curves, for example curves having a Lipschitz continuous tangent.

We start with a rigorous proof of bi-Lipschitz continuity providing a bi-Lipschitz constant depending only on the energy, not on the curve itself.

Proposition 5 (Uniform bi-Lipschitz estimate).

For every $M < \infty$ and (13) there is a constant $C(M) < \infty$ such that any embedded curve $\gamma \in C^1(\mathbb{R}/\mathbb{Z}, \mathbb{R}^n)$ parametrized by arc-length with

$$\mathrm{KE}^{(s,\varrho)}(\gamma) \leq M \tag{14}$$

satisfies the bi-Lipschitz estimate

$$|u - v| \leq C(M) \, |\gamma(u) - \gamma(v)| \qquad \text{for all } u, v \in \mathbb{R}/\mathbb{Z}.$$

We will give an easy proof that essentially boils down to combining the regularity from (K_3) with a scaling argument. The following lemma will be one of the essential parts in the proof. We define for two arc-length parametrized curves $\gamma_i : I_i \to \mathbb{R}$, $i = 1, 2$, I_1, I_2 open intervals,

$$\begin{aligned} \mathrm{KE}^{(s,\varrho)}(\gamma_1, \gamma_2) := &\int \cdots \int_{I_1^k} f^{(s,\varrho)}(\gamma; u_1, \ldots, u_k) \, \mathrm{d}u_1 \cdots \mathrm{d}u_k + \\ &+ \int \cdots \int_{I_2^k} f^{(s,\varrho)}(\gamma; u_1, \ldots, u_k) \, \mathrm{d}u_1 \cdots \mathrm{d}u_k + \\ &+ \int \cdots \int_{I_1 \times I_2^{k-1}} f^{(s,\varrho)}(\gamma; u_1, \ldots, u_k) \, \mathrm{d}u_1 \cdots \mathrm{d}u_k \end{aligned}$$

in order to state

Lemma 6.

Let $\alpha \in (0, 1)$. For $\mu > 0$ let M_μ denote the set of all pairs (γ_1, γ_2) of embedded arc-length parametrized curves $\gamma_i \in C^1([-\frac{1}{2}, \frac{1}{2}], \mathbb{R}^n)$ satisfying

- $|\gamma_1(0) - \gamma_2(0)| = 1$,
- $\gamma_1'(0) \perp (\gamma_1(0) - \gamma_2(0)) \perp \gamma_2'(0)$,

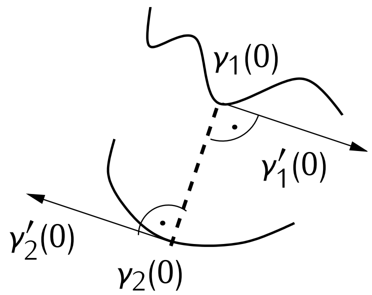

Fig 4. The situation in Lemma 6. Note that γ_1 and γ_2 are always disjoint.

- $\|\gamma_i'\|_{C^{0,\alpha}} \leq \mu, \qquad i = 1, 2.$

Then there is some $c = c(\alpha, \mu) > 0$ *with*

$$\mathrm{KE}^{(s,\varrho)}(\gamma_1, \gamma_2) \geq c \qquad \textit{for all } (\gamma_1, \gamma_2) \in M_\mu.$$

Proof. We will show that $\mathrm{KE}^{(s,\varrho)}(\cdot,\cdot)$ attains its minimum c on M_μ. From this we immediately infer $c > 0$ for, otherwise, $\mathrm{KE}^{(s,\varrho)}(\gamma_1, \gamma_2) = 0$ implies by (K_2) that both γ_1 and γ_2 are part of one single straight line. This contradicts the fact that M_μ does not contain straight lines by the first two properties.

Let $(\gamma_1^{(n)}, \gamma_2^{(n)})$ be a minimizing sequence in M_μ, i.e., we have

$$\lim_{n\to\infty} \mathrm{KE}^{(s,\varrho)}(\gamma_1^{(n)}, \gamma_2^{(n)}) = \inf_{M_\mu} \mathrm{KE}^{(s,\varrho)}(\cdot,\cdot).$$

Subtracting $\gamma_1(0)$ from *both* curves, i.e., setting

$$\tilde{\gamma}_i^{(n)}(\tau) := \gamma_i^{(n)}(\tau) - \gamma_1(0), \qquad i = 1, 2,$$

and using the Arzelà-Ascoli theorem (due to the third property), we may pass to a subsequence

$$\tilde{\gamma}_i^{(n)} \to \tilde{\gamma}_i \qquad \text{in } C^1.$$

Furthermore, $(\tilde{\gamma}_1, \tilde{\gamma}_2) \in M_\mu$ since M_μ is closed under convergence in C^1. Since, by Fatou's lemma, the functional $\mathrm{KE}^{(s,\varrho)}$ is lower semi-continuous with respect to C^1 convergence, we obtain

$$\inf_{M_\mu} \mathrm{KE}^{(s,\varrho)}(\cdot,\cdot) \leq \mathrm{KE}^{(s,\varrho)}(\tilde{\gamma}_1, \tilde{\gamma}_2) \leq \lim_{n\to\infty} \mathrm{KE}^{(s,\varrho)}(\tilde{\gamma}_1^{(n)}, \tilde{\gamma}_2^{(n)}) \overset{(K_1)}{=} \lim_{n\to\infty} \mathrm{KE}^{(s,\varrho)}(\gamma_1^{(n)}, \gamma_2^{(n)}) = \inf_{M_\mu} \mathrm{KE}^{(s,\varrho)}(\cdot,\cdot).$$

□

Let us use this lemma to give the

Proof of Propsition 5. Applying (K_3) to (14) we obtain

$$\|\gamma'\|_{C^{0,\alpha}} \leq C'(M)$$

for $\alpha = s - 1 - \frac{1}{\varrho} > 0$. As an immediate consequence there is a $\delta = \delta(\alpha, C') > 0$ such that

$$|u - v| \leq 2|\gamma(u) - \gamma(v)|$$

for all $u, v \in \mathbb{R}/\mathbb{Z}$ with $|u - v| \leq \delta$. Let now

$$S := \inf \left\{ |\gamma(u) - \gamma(v)| \,\middle|\, u, v \in \mathbb{R}/\mathbb{Z}, |u - v| \geq \delta \right\} \leq \tfrac{1}{2}.$$

We will complete the proof by estimating S from below. Using the compactness of $\{u, v \in \mathbb{R}/\mathbb{Z}, |u - v| \geq \delta\}$, there are $s, t \in \mathbb{R}/\mathbb{Z}$ with $|s - t| \geq \delta$ and

$$|\gamma(s) - \gamma(t)| = S.$$

In case $|s - t| = \delta$ we infer

$$2S = 2|\gamma(s) - \gamma(t)| \geq \delta$$

and hence

$$|u - v| \leq \tfrac{1}{2} \leq \frac{S}{\delta} \leq \frac{|\gamma(u) - \gamma(v)|}{\delta(\alpha, C')}$$

for all $u, v \in \mathbb{R}/\mathbb{Z}$ with $|u - v| \geq \delta$. This proves the proposition in this case. If, on the other hand, $|s - t| > \delta$ then the minimality of $|\gamma(s) - \gamma(t)|$ implies

$$\gamma'(s) \perp (\gamma(s) - \gamma(t)) \perp \gamma'(t).$$

We let for $\tau \in [-\frac{1}{2}, \frac{1}{2}]$

$$\gamma_1(\tau) := \tfrac{1}{S}\gamma(s + S\tau) \qquad \text{and} \qquad \gamma_2(\tau) := \tfrac{1}{S}\gamma(t + S\tau).$$

Since

$$\left\|\gamma_i'\right\|_{C^{0,\alpha}} \leq \left\|\gamma'\right\|_{C^{0,\alpha}} \qquad (\leq C'(M))$$

we may apply Lemma 6 which gives

$$\mathrm{KE}^{(s,\varrho)}(\gamma_1, \gamma_2) \geq c(\alpha, C') > 0.$$

Together with

$$\mathrm{KE}^{(s,\varrho)}(\gamma_1, \gamma_2) = S^{s-1-1/\varrho}\mathrm{KE}^{(s,\varrho)}(S\gamma_1, S\gamma_2) \leq S^{s-1-1/\varrho}\mathrm{KE}^{(s,\varrho)}(\gamma),$$

where we used (K_1) twice, this leads to

$$S \geq \left(\frac{c(\alpha, C')}{\mathrm{KE}^{(s,\varrho)}(\gamma)}\right)^{\frac{1}{s-1-1/\varrho}} \geq \left(\frac{c(\alpha, C')}{M}\right)^{\frac{1}{s-1-1/\varrho}}.$$

Hence,

$$|u - v| \leq \tfrac{1}{2} \leq \frac{|\gamma(u) - \gamma(v)|}{2S} \leq C(M)\,|\gamma(u) - \gamma(v)|$$

for all $u, v \in \mathbb{R}/\mathbb{Z}$ with $|u - v| \geq \delta$. □

We are now in the position to prove the following mighty

Theorem 7 (Compactness).

For each $M < \infty$ and (13) the set

$$A_M := \left\{ \gamma \in C^1(\mathbb{R}/\mathbb{Z}, \mathbb{R}^n) \,\middle|\, \gamma \text{ embedded}, |\gamma'| \equiv 1, \mathrm{KE}^{(s,\varrho)}(\gamma) \leq M \right\}$$

is sequentially compact in C^1 up to translations.

Proof. By (K_3) there are $C' = C'(M) < \infty$ and $\alpha > 0$ such that

$$\left\|\gamma'\right\|_{C^{0,\alpha}} \leq C'$$

for all $\gamma \in A_M$ and hence

$$\left\|\tilde{\gamma}\right\|_{C^{1,\alpha}} \leq C' + 1$$

where $\tilde{\gamma}(u) := \gamma(u) - \gamma(0)$. Furthermore, from Proposition 5 we infer the bi-Lipschitz estimate

$$|u - v| \leq C(M)|\gamma(u) - \gamma(v)|$$

for all $\gamma \in A_M$, $u, v \in \mathbb{R}/\mathbb{Z}$. Considering a sequence $(\gamma_n)_{n\in\mathbb{N}} \subset A_M$ we obtain

$$\left\|\tilde{\gamma}_n\right\|_{C^{1,\alpha}} \leq C' + 1 \qquad \text{for any } n \in \mathbb{N}$$

and hence, after passing to suitable subsequence,

$$\tilde{\gamma}_n \to \gamma_0 \qquad \text{in } C^1.$$

Since γ_n was parametrized by arc-length, γ_0 is still parametrized by arc-length and still

$$|u - v| \leq C(M)|\gamma_0(u) - \gamma_0(v)|$$

for all $u, v \in \mathbb{R}/\mathbb{Z}$. So, especially, γ_0 is embedded. From lower semi-continuity with respect to C^1 convergence we infer

$$\mathrm{KE}^{(s,\varrho)}(\gamma_0) \leq \liminf_{n\to\infty} \mathrm{KE}^{(s,\varrho)}(\gamma_n) \leq M.$$

So $\gamma_0 \in A_M$. □

Let us conclude this section by deriving two simple corollaries of this sequential compactness and the lower semi-continuity of the energies with respect to C^1-convergence.

The first one states that, on the sub-critical range (13), the prototype energies $\mathrm{KE}^{(s,\varrho)}$ are in fact knot energies as defined in the introduction. The second one, already announced in the introduction, ensures that there exist minimizers of the energies within every knot class—which are then smooth by Theorem 10.

Proposition 8 ($\mathrm{KE}^{(s,\varrho)}$ is a strong knot energy).

Let (13) hold.

- *If $(\gamma_k)_{k\in\mathbb{N}} \subset C^1$ is a sequence uniformly converging (in C^0) to a non-injective curve $\gamma_\infty \in C^1$ then $\mathrm{KE}^{(s,\varrho)}(\gamma_k) \to \infty$.*
- *For given $E, L > 0$ there are only finitely many knot types having a representative with $\mathrm{KE}^{(s,\varrho)} \leq E$ and length $= L$.*

Proof. The first statement immediately follows from the bi-Lipschitz estimate in Proposition 5.

To show the second statement, let us assume that it was wrong, i.e., that there are curves $(\gamma_k)_{k\in\mathbb{N}}$ of length L, all belonging to different knot classes, with energy less than E. Of course we can assume $L = 1$. By Theorem 7, after suitable translations and passing to a subsequence, there is some $\gamma_0 \in A_M$ with $\gamma_n \to \gamma_0$ in C^1. As the intersection of every knot class with C^1 is an open set in C^1 [2, Cor. 1.5] (see [25] for an explicit construction), this implies that almost all γ_k belong to the same knot class as γ_0, which is a contradiction. □

Theorem 9 (Existence of minimizers in knot classes).
In the sub-critical case (13) there is a minimizer of $\mathrm{KE}^{(s,\varrho)}$ *in any knot class* $\mathfrak{K}$.

Proof. Let $(\gamma_k)_{k\in\mathbb{N}} \in C^1$, $|\gamma_k'| \equiv 1$, be a minimal sequence of embedded curves for $\mathrm{KE}^{(s,\varrho)}$ in a given knot class $\mathfrak{K}$, i.e., let

$$\lim_{k\to\infty} \mathrm{KE}^{(s,\varrho)}(\gamma_k) = \inf_{C^1\cap\mathfrak{K}} \mathrm{KE}^{(s,\varrho)}.$$

After passing to a subsequence and suitable translations, we hence obtain by Theorem 7 an embedded arc-length parametrized $\gamma_0 \in C^1$ with $\gamma_k \to \gamma_0$ in C^1. Again by [2, 25] the curve γ_0 belongs to the same knot class as the elements of the minimal sequence $(\gamma_k)_{k\in\mathbb{N}}$. The lower semi-continuity of $\mathrm{KE}^{(s,\varrho)}$ furthermore implies that

$$\inf_{C^1\cap\mathfrak{K}} \mathrm{KE}^{(s,\varrho)} \le \mathrm{KE}^{(s,\varrho)}(\gamma_0) \le \lim_{n\to\infty} \mathrm{KE}^{(s,\varrho)}(\gamma_n) = \inf_{C^1\cap\mathfrak{K}} \mathrm{KE}^{(s,\varrho)}.$$

Hence, γ_0 is the minimizer we have been searching for. □

By the same reasoning one derives the existence of a global minimizer of $\mathrm{KE}^{(s,\varrho)}$.

4. Regularity of stationary points

The aim of this section is to outline the proof of

Theorem 10 (Regularity of local minimizers).
Any local minimizer of $\mathrm{O'H}^{(\alpha,1)}$, $\alpha \in (2,3)$, $\mathrm{TP}^{(p,2)}$, $p \in (4,5)$, *and* $\mathrm{intM}^{(p,2)}$, $p \in (\frac{7}{3}, \frac{8}{3})$, *is* C^∞*-smooth.*

The parameter ranges in the above statement are referred to as the *non-degenerate sub-critical case* which is depicted as yellow line in Figures 2 and 3. For the abstract energies $\mathrm{KE}^{(\cdot,\cdot)}$ this is equivalent to

$$s \in (\tfrac{3}{2}, 2), \qquad \varrho = 2. \tag{15}$$

In contrast to the previous section, we do not provide an axiomatic approach as this would demand quite a lot of additional requirements. Therefore, mainly due to convenience, our analysis presented below reflects the case where $\mathrm{KE}^{(\cdot,\cdot)}$ stands for either $\mathrm{O'H}^{(\cdot,\cdot)}$, $\mathrm{TP}^{(\cdot,\cdot)}$, or $\mathrm{intM}^{(\cdot,\cdot)}$. However, our argument can be adopted for similar problems.

Recall that $\mathrm{O'H}^{(\alpha,p)}$ corresponds to $\mathrm{KE}^{\left(\frac{\alpha}{2}-\frac{1}{2p}+1,2p\right)}$, $\mathrm{TP}^{(p,q)}$ to $\mathrm{KE}^{\left(\frac{p-1}{q},q\right)}$, $\mathrm{intM}^{(p,q)}$ to $\mathrm{KE}^{\left(\frac{3p-2}{q}-1,q\right)}$.

We now sketch the strategy of proof for C^∞-smoothness of local $\mathrm{KE}^{(s,2)}$-minimizers in the non-degenerate sub-critical case (15). All details are to be found in [6–8].

The first task is to compute the first variation

$$\delta\mathrm{KE}^{(s,2)}(\gamma; h) := \lim_{\tau\to 0} \frac{\mathrm{KE}^{(s,2)}(\gamma+\tau h) - \mathrm{KE}^{(s,2)}(\gamma)}{\tau}. \tag{16}$$

Any local minimizer γ of $\mathrm{KE}^{(s,2)}$ is a *stationary point*, i.e., it satisfies the *Euler-Lagrange equation*

$$\delta\mathrm{KE}^{(s,2)}(\gamma; h) + \lambda \langle \gamma', h' \rangle_{L^2} = 0 \qquad \text{for all } h \in C^\infty(\mathbb{R}/\mathbb{Z}, \mathbb{R}^n) \tag{17}$$

where $\lambda \in \mathbb{R}$ is a Lagrange parameter stemming from the side condition (fixed length) and the L^2-scalar product is defined in (20) below. We will prove Theorem 10 by exploiting this identity in the following way: a suitable decomposition allows to concentrate the highest-order term on the left-hand side of the equation while the right-hand side turns out to be a lower-order term. By a so-called *bootstrapping* argument we inductively deduce that the curve γ is more and more regular. Consequently, the statement in Theorem 10 holds even for stationary points. In the sequel we sketch the main steps being prerequired for its proof.

Computing the first variation demands a quite subtle argument for O'Hara's energies $\mathrm{O'H}^{(\alpha,p)}$ while it is rather straightforward for $\mathrm{TP}^{(p,q)}$ and $\mathrm{intM}^{(p,q)}$.

In order to start a bootstrapping process, we decompose $\delta\mathrm{KE}^{(s,2)}$ into the sum of a bilinear elliptic term $Q^{(s)}$ and a remainder term $R^{(s)}$ of lower order, i.e.,

$$\delta\mathrm{KE}^{(s,2)}(\gamma; h) = Q^{(s)}(\gamma; h) + R^{(s)}(\gamma; h). \tag{18}$$

The general idea how to construct $Q^{(s)}$ is just to "linearize" the integrand of $\delta\mathrm{KE}^{(s,2)}$, e.g. by replacing negative powers of $|\gamma(u) - \gamma(v)|$ by the corresponding ones of $|u - v|$.

We will briefly illustrate this idea by exemplifying it for $\mathrm{O'H}^{(2,\alpha)}$, $\alpha \in (2, 3)$. The first variation at an arc-length parametrized (sufficiently smooth) embedded curve is given by

$$\delta\mathrm{O'H}^{(2,\alpha)}(\gamma; h) = \lim_{\varepsilon \searrow 0} \iint_{\substack{u,v\in\mathbb{R}/\mathbb{Z} \\ |u-v|\geq\varepsilon}} \left((\alpha - 2)\frac{\langle \gamma'(u), h'(u)\rangle}{|u - v|^{\alpha}} + 2\frac{\langle \gamma'(u), h'(u)\rangle}{|\gamma(u) - \gamma(v)|^{\alpha}} - \alpha\frac{\langle \gamma(u) - \gamma(v), h(u) - h(v)\rangle}{|\gamma(u) - \gamma(v)|^{\alpha+2}} \right) \mathrm{d}u\,\mathrm{d}v.$$

Linearizing as indicated above leads to

$$Q^{(\frac{\alpha+1}{2})}(\gamma; h) = \alpha \lim_{\varepsilon \searrow 0} \iint_{\substack{u,v\in\mathbb{R}/\mathbb{Z} \\ |u-v|\geq\varepsilon}} \left(\frac{\langle \gamma'(u), h'(u)\rangle}{|u - v|^{\alpha}} - \frac{\langle \gamma(u) - \gamma(v), h(u) - h(v)\rangle}{|u - v|^{\alpha+2}} \right) \mathrm{d}u\,\mathrm{d}v. \tag{19}$$

The remainder is then obtained by computing the difference according to (18)

$$\begin{aligned} R^{\left(\frac{\alpha+1}{2}\right)}(\gamma; h) = 2 &\iint_{u,v\in\mathbb{R}/\mathbb{Z}} \langle \gamma'(u), h'(u)\rangle \left(\frac{1}{|\gamma(u) - \gamma(v)|^{\alpha}} - \frac{1}{|w|^{\alpha}} \right) \mathrm{d}u\,\mathrm{d}v \\ &- \alpha \iint_{u,v\in\mathbb{R}/\mathbb{Z}} \langle \gamma(u) - \gamma(v), h(u) - h(v)\rangle \left(\frac{1}{|\gamma(u) - \gamma(v)|^{\alpha+2}} - \frac{1}{|w|^{\alpha+2}} \right) \mathrm{d}u\,\mathrm{d}v, \end{aligned}$$

where the limits $\varepsilon \searrow 0$ may be omitted, see [7] for details.

Here it becomes apparent that the setting $\varrho = 2$ corresponds to the Hilbert case which is characterized by the existence of a scalar product

$$\langle f, g\rangle_{L^2} := \int_0^1 \langle f(u), g(u)\rangle_{\mathbb{C}^n}\,\mathrm{d}u \qquad \text{for } f, g \in L^2(\mathbb{R}/\mathbb{Z}, \mathbb{C}^n). \tag{20}$$

This enables us to apply the theory of Fourier series. Recall that we may express a function f by its Fourier series

$$\sum_{k\in\mathbb{Z}} \hat{f} e^{2\pi i k x}$$

where $\hat{f}_k := \int_0^1 f(x)e^{-2\pi i k x}\,\mathrm{d}x$ is the k-th Fourier coefficient. A function f belongs to $L^2(\mathbb{R}/\mathbb{Z}, \mathbb{R}^n)$ if and only if the sequence of its Fourier coefficients belongs to ℓ^2, i.e., they are square summable,

$$\sum_{k\in\mathbb{Z}} \left|\hat{f}_k\right|^2 < \infty.$$

In this case $f(x) = \sum_{k\in\mathbb{Z}} \hat{f} e^{2\pi ikx}$ for almost every $x \in \mathbb{R}/\mathbb{Z}$. On the level of Fourier coefficients regularity is expressed by multiplication of powers of k, more precisely, $\widehat{f'} = 2\pi ik\hat{f}$ and $\widehat{f''} = -4\pi^2k^2\hat{f}$. Therefore, in order to prove $f \in C^\infty$, we have to show

$$\left(|k|^\sigma \hat{f}_k\right)_{k\in\mathbb{N}} \in \ell^2 \qquad \text{for arbitrarily large } \sigma > 0.$$

To this end we need an initial amount of regularity, namely

$$\left(|k|^s \hat{\gamma}_k\right)_{k\in\mathbb{N}} \in \ell^2. \tag{21}$$

In fact, this is not an additional requirement as, for the energy families presented in this text, any finite-energy curve in arc-length parametrization satisfies the latter claim already. This can be seen by the computations used to exclude the highly singular range and the fact that (21) is equivalent to $\iint_{(\mathbb{R}/\mathbb{Z})^2} \frac{|\gamma(u)-\gamma(v)|^2}{|u-v|^{1+2s}}\,\mathrm{d}u\,\mathrm{d}v < \infty$.

Now we have to investigate the regularity properties of both $Q^{(s)}$ and $R^{(s)}$. Using Parseval's theorem we obtain

$$Q^{(s)}(f;g) = \sum_{k\in\mathbb{Z}} \varrho_k \left\langle \hat{f}_k, \hat{g}_k \right\rangle_{\mathbb{C}^d} \qquad \text{where } \varrho_k = c\,|k|^{2s} + o\left(|k|^{2s}\right) \text{ as } |k| \nearrow \infty \tag{22}$$

and $c > 0$. Here $o\left(|k|^{2s}\right)$ denotes a quantity with $\frac{o\left(|k|^{2s}\right)}{|k|^{2s}} \to 0$ as $|k| \nearrow \infty$.

To see this for the example $\mathrm{O'H}^{(\alpha,2)}$, just insert the basis functions $\phi_k(t) := e^{2\pi ikt}$, $k \in \mathbb{Z}$, into (19) which gives, for basis vectors $\mathbf{e}_\ell \in \mathbb{R}^n$, $\ell = 1,\ldots,n$,

$$Q^{\left(\frac{\alpha+1}{2}\right)}(\phi_k \mathbf{e}_\ell; \phi_{k'}\mathbf{e}_{\ell'}) = \delta_{k,k'}\delta_{\ell,\ell'}c_\alpha\,|k|^{\alpha+1} + \mathcal{O}(k)$$

where $\delta_{\cdot,\cdot}$ denotes the Kronecker symbol, c_α is a positive constant, and $\frac{\mathcal{O}(k)}{|k|} \le C$ as $|k| \nearrow \infty$.

The next crucial step is to show that all terms belonging to $R^{(s)}$ have the same structure, so one can treat them simultaneously. Since the exact form of a multilinear mapping $(\mathbb{R}^n)^N \to \mathbb{R}$ will not matter in our analysis, let us introduce the "$\circledast$ notation" which represents any sort of these operators, e. g., $\langle (a \otimes b)\,c, d\rangle = a \circledast b \circledast c \circledast d$ for $a, b, c, d \in \mathbb{R}^n$. Now the term $R^{(s)}(\gamma, h)$ is a (finite) sum of expressions of type

$$\int_{\mathbb{R}/\mathbb{Z}} \int_{-1/2}^{1/2} \int \cdots \int_{[0,1]^K} g^{(s)}(u,w) \circledast h'(u + \sigma_K w)\,\mathrm{d}\theta_1 \cdots \mathrm{d}\theta_K\,\mathrm{d}w\,\mathrm{d}u$$

where

$$g^{(s)}(u,w) := \mathcal{G}^{(s)}\left(\left|\frac{\triangle\gamma}{w}\right|\right) \frac{|\gamma'(u+\sigma_1 w) - \gamma'(u+\sigma_2 w)|^2}{|w|^{2s-1}} \left(\mathop{\circledast}_{i=3}^{K-1} \gamma'(u+\sigma_i w)\right),$$

$\mathcal{G}^{(s)}$ is some analytic function defined on $[c,\infty)$, and $\sigma_i \in \{0, \theta_i\}$ for all $i = 1,\ldots,K$.

From this we can state the regularity of the remainder term as follows: if

$$\left(|k|^{s+\sigma} \hat{\gamma}_k\right)_{k\in\mathbb{N}} \in \ell^2 \qquad \text{for some } \sigma \ge 0 \tag{23}$$

then for any $\varepsilon > 0$ there is some $g = g_\varepsilon : \mathbb{R}/\mathbb{Z} \to \mathbb{R}^n$ with

$$R^{(s)}(\gamma;h) = \sum_{k\in\mathbb{Z}} \left\langle \hat{g}_k, \hat{h}_k \right\rangle_{\mathbb{C}^n} \qquad \text{and} \qquad \left(|k|^{\sigma-\varepsilon-3/2}\,\hat{g}_k\right)_{k\in\mathbb{N}} \in \ell^2. \tag{24}$$

By (22) and (24) we are able to proceed to the

Proof of Theorem 10. Rewriting (17) using (18), we arrive at

$$Q^{(s)}(\gamma; h) + \lambda \langle \gamma', h' \rangle_{L^2} + R^{(s)}(\gamma; h) = 0 \tag{25}$$

for any $h \in C^\infty(\mathbb{R}/\mathbb{Z})$. Since first variation of the length functional satisfies

$$\langle \gamma', h' \rangle_{L^2} = \sum_{k\in\mathbb{Z}} |2\pi k|^2 \left\langle \hat{\gamma}_k, \hat{h}_k \right\rangle_{\mathbb{C}^d},$$

we deduce using (22) that there is a $c > 0$ with

$$Q^{(s)}(\gamma, h) + \lambda \langle \gamma', h' \rangle_{L^2} = \sum_{k\in\mathbb{Z}} \tilde{\varrho}_k \left\langle \hat{\gamma}_k, \hat{h}_k \right\rangle_{\mathbb{C}^d} \qquad \text{where} \qquad \tilde{\varrho}_k = c\,|k|^{2s} + o\left(|k|^{2s}\right) \qquad \text{as } |k| \nearrow \infty. \tag{26}$$

Assuming (23) we infer

$$Q^{(s)}(\gamma; h) + \lambda \langle \gamma', h' \rangle_{L^2} + \sum_{k\in\mathbb{Z}} \left\langle \hat{g}_k, \hat{h}_k \right\rangle_{\mathbb{C}^n} = 0 \tag{27}$$

from applying (24) to (25). Equation (26) implies

$$\sum_{k\in\mathbb{Z}} \left\langle \tilde{\varrho}_k \hat{\gamma}_k + \hat{g}_k, \hat{h}_k \right\rangle_{\mathbb{C}^n} = 0.$$

Testing this identity with the basis functions $\hat{h}_j = \delta_{j,k}$ we obtain $\tilde{\varrho}_k \hat{\gamma}_k + \hat{g}_k = 0$ for all $k \in \mathbb{Z}$. Applying (24) yields

$$\left(\tilde{\varrho}_k\, |k|^{\sigma-\varepsilon-3/2}\, \hat{\gamma}_k\right)_{k\in\mathbb{Z}} \in \ell^2.$$

Recalling that $\tilde{\varrho}_k\, |k|^{-2s}$ converges to a positive constant as $|k| \nearrow \infty$, we are led to

$$\left(|k|^{2s+\sigma-\varepsilon-3/2}\, \hat{\gamma}_k\right)_{k\in\mathbb{Z}} \in \ell^2.$$

Choosing $\varepsilon := \frac{s}{2} - \frac{3}{4} > 0$, this reads

$$\left(|k|^{s+\sigma+\varepsilon}\, \hat{\gamma}_k\right)_{k\in\mathbb{Z}} \in \ell^2. \tag{28}$$

Consequently, compared to the initial assumption (23), we gain a positive regularity amount ε that does not depend on σ. So, starting with (21), we arrive at $\gamma \in C^\infty$ by iterating (23)–(28). □

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