Elastic knots

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Harmonic Analysis

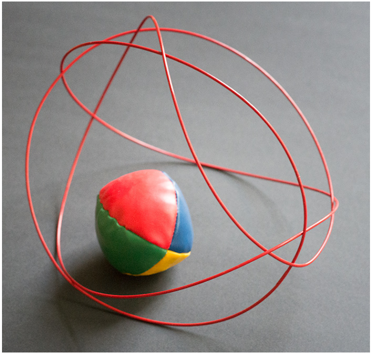
... a knotted springy wire cannot rest in stable equilibrium
without points of self-contact—an experimentally observable fact.

This fact leads to a rather curious "topologically constrained" variational problem;
what actually happens if one forms a knot in a piece of springy wire?

Experiments yield some beautiful curves with impressive symmetry ...

— J. Langer & D. A. Singer 1984

Self-obstacle problem
The solution itself
defines the obstacle



Lots of knots

Examples. Shoelace, rubber band, wires, submarine communications cables, protein molecules, solar coronal loops, ...

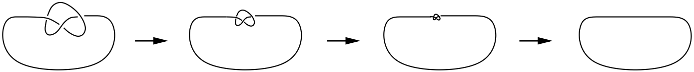
Characteristics of these objects

- centerline: embedded curve, rectifiable, ...
    - curvature ($\rightarrow$ bending energy [Bernoulli 1739])
- diameter: thickness ($\rightarrow$ reach [Federer '59])
    - impermeability
    - topology ($\rightarrow$ knot type)
- twist
- further physical properties (shear, friction, ...)

Vocabulary

Knot is an embedded closed curve $u : \mathbb{R}/\mathbb{Z} \to \mathbb{R}^3$.

Ambient isotopy deforms two curves continuously into each other, without self-intersections or pulling-tight.



Knot classes are equivalence classes w. r. t. ambient isotopy.

Unknot or **trivial knot** is any element of the knot class containing the round circle.

Knot classes are classified by the least number of crossings.

A simple model for long slender objects

Examples. Shoelace, rubber band, wires, submarine communications cables, protein molecules, solar coronal loops, ...

The centerline of these objects can be modeled by a curve $u : I \to \mathbb{R}^3$.

Bending energy [D. Bernoulli, 1739]

$$E_0(u) = \frac{1}{2} \int_I k(s)^2 \, \mathrm{d}s, \qquad u \in H^2$$

- Simplified model: ignoring twist
- Γ-limit of three-dimensional nonlinear elasticity [Mora & Müller '03]
- Applications in models for cell filaments, textile fabrication processes, computer graphics, ...
- Gradient flow [Polden ; Dziuk, Kuwert, Schätzle ; Deckelnick & Dziuk ; Barrett, Garcke, Nürnberg ; Bartels ; Dall'Acqua, Lin, Pozzi ; ...]

Minimizing the bending energy within isotopy classes

Bending energy [D. Bernoulli, 1739]

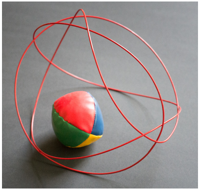
$$E_0(u) = \frac{1}{2}\int_I k(s)^2\, ds, \qquad u \in H^2$$

Aim. Find global minimizers within nontrivial knot classes.

Theorem [Langer & Singer '85]

The circle is the only (local) minimizer of the bending energy in $\mathbb{R}^3$.

Consequence. No bending energy minimizers within a nontrivial knot class. Limits of minimal sequences belong to the weak H^2-boundary.



Problem. In the case of the trefoil knot there is a one-parameter family of such limits.

Strategy. Regularization by a self-avoiding functional that separates different isotopy classes by infinite barriers.

Regularization by a self-avoiding functional

Variational problem [von der Mosel '98]

$$E_{\varrho}(u) = \frac{1}{2}\int_I k(s)^2\,\mathrm{d}s + \varrho\mathcal{R}(u) \to \min!$$

Also see [Gallotti & Pierre-Louis '07; Sossinsky '10; Gerlach et al. '17]

- $\mathcal{R}$ is a self-avoiding functional $\rightsquigarrow$ impermeability
- Limit curves as $\varrho \searrow 0$ are called elastic knots
- Existence of minimizers for any $\varrho > 0$
- Computational challenge: strong forces related to bending effects have to be compensated by repulsive forces related to $\mathcal{R}$ to avoid self-intersections
- Consider a suitable gradient descent
  - Smooth functional $\mathcal{R} = \mathrm{TP}$ [Buck & Orloff '95; Gonzalez & Maddocks '99]
  - Discrete H^2 gradient flow [Bartels & R. '18]

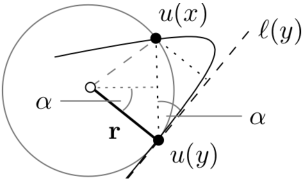
Self-avoidance

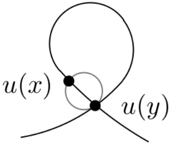
Tangent-point energies

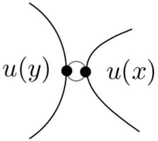
Modeling “thickness” by a smooth functional

$$\mathrm{TP}(u) = \frac{1}{2^q q} \iint_{\mathbb{R}/\mathbb{Z}\times\mathbb{R}/\mathbb{Z}} \frac{\mathrm{d}x\,\mathrm{d}y}{r_u(x,y)^q}, \qquad q > 2,$$

where $r_u(x, y)$ denotes the radius of circle tangential at $u(y)$ and intersecting in $u(x)$. [Gonzalez & Maddocks ’99]







- TP is highly non-local, $\frac{1}{r_u(x,y)} \xrightarrow{x\to y} k(y)$
- self-avoiding property [Strzelecki & von der Mosel ’10]
- characterization of energy spaces [Blatt ’13] $\rightsquigarrow W^{2-1/q,q}$
- numerical advantage: smoothness, no “intrinsic terms”, two-dimensional integration domain

Tangent-point energies

Modeling “thickness” by a smooth functional

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where $r_u(x,y)$ denotes the radius of circle tangential at $u(y)$ and intersecting in $u(x)$. [Gonzalez & Maddocks ’99]

We have

$$r_u(x,y) = \frac{|u(x)-u(y)|^2}{2\,\mathrm{dist}(u(x),\ell(y))} = \frac{|u(x)-u(y)|^2}{2\,|u'(y)\wedge(u(x)-u(y))|}$$

where $\ell(y) = u(y) + \mathbb{R}u'(y)$, so

$$\mathrm{TP}(u) = \frac{1}{q} \iint_{\mathbb{R}/\mathbb{Z}\times\mathbb{R}/\mathbb{Z}} \frac{|u'(y)\wedge(u(x)-u(y))|^q}{|u(x)-u(y)|^{2q}}\,\mathrm{d}x\,\mathrm{d}y.$$

The importance of being bi-Lipschitz

The bi-Lipschitz constant of an arclength parametrized curve $u : \mathbb{R}/\mathbb{Z} \to \mathbb{R}^3$ is defined via

$$\mathrm{biL}(u) = \sup_{x,y\in\mathbb{R}/\mathbb{Z},\, x\neq y} \frac{|x-y|}{|u(x)-u(y)|} \qquad (\geq 1)\,.$$

Lemma (Uniform bi-Lipschitz estimate) [Blatt & R. '15]

There is a uniform bound $C_{M,q} < \infty$ such that if $\mathrm{TP}(u) \leq M$ then

$$|x-y|_{\mathbb{R}/\mathbb{Z}} \leq C_{M,q}\,|u(x)-u(y)| \qquad \text{for all } x,y \in \mathbb{R}/\mathbb{Z}.$$

$\rightsquigarrow$ biL cannot be controlled merely by the Sobolev norm.

The importance of being bi-Lipschitz

Lemma
There is a uniform bound $C_{M,q} < \infty$ such that if $\mathrm{TP}(u) \leq M$ then

$$|x - y|_{\mathbb{R}/\mathbb{Z}} \leq C_{M,q} \, |u(x) - u(y)| \qquad \text{for all } x, y \in \mathbb{R}/\mathbb{Z}.$$

Corollary (Self-avoidance)

Let $(u_k)_{k \in \mathbb{N}}$ pointwise converge to a curve $u_\infty \in C^0(\mathbb{R}/\mathbb{Z}, \mathbb{R}^3)$ with a self-intersection: there are $x, y \in \mathbb{R}/\mathbb{Z}$, $x \neq y$ with $u_\infty(x) = u_\infty(y)$. Then $\mathrm{TP}(u_k) \to \infty$ as $k \to \infty$.

Proof. Assuming the contrary, we infer the existence of a constant $C < \infty$ with $0 < |x - y|_{\mathbb{R}/\mathbb{Z}} \leq C \, |u_k(x) - u_k(y)| \xrightarrow{k \to \infty} 0$. □

The first variation

Theorem [Blatt & R. '15]

TP is continuously differentiable on embedded $W^{2-1/q,q}$-curves,

$$\delta\,\mathrm{TP}(u)[w] \le C_q(\mathrm{biL}\,u)^{2q+2}\,\|u'\|_{L^\infty}^{q-1}\,\|u'\|_{W^{1-1/q,q}}\,\|w'\|_{W^{1-1/q,q}}\,.$$

If $u,\varphi \in W^{2-1/q,q}(\mathbb{R}/\mathbb{Z},\mathbb{R}^3)$, $q\in(2,\infty)$, u embedded and parametrized by arc-length with $u' \perp \varphi'$

$$\delta\,\mathrm{TP}(u)[\varphi] = \mathcal{M}_0(u;u,\varphi) + \mathcal{M}_0(u;\varphi,u) - 2\mathcal{A}_0(u;u,\varphi)$$

where

$$\mathcal{M}_0(u;v,w) = \iint_{\mathbb{R}/\mathbb{Z}\times\mathbb{R}/\mathbb{Z}} \frac{|u'(y)\wedge(u(x)-u(y))|^{q-2}}{|u(x)-u(y)|^{2q}}\times$$

$$\times\,\langle u'(y)\wedge(u(x)-u(y))\,,v'(y)\wedge(w(x)-w(y))\rangle\;\mathrm{d}x\,\mathrm{d}y,$$

$$\mathcal{A}_0(u;v,w) = \iint_{\mathbb{R}/\mathbb{Z}\times\mathbb{R}/\mathbb{Z}} \frac{|u'(y)\wedge(u(x)-u(y))|^{q}}{|u(x)-u(y)|^{2q+2}}\times$$

$$\times\,\langle v(x)-v(y), w(x)-w(y)\rangle\;\mathrm{d}x\,\mathrm{d}y.$$

Numerical scheme

Approximating elastic knots

Prescribing arclength parametrization $|u'| \equiv 1$ gives $k = |u''|$.

We perform a discretization of the H^2 gradient flow

$$(u_t, \phi)_{H^2} = -(u'', \phi'')_{L^2} - \varrho\delta\,\mathrm{TP}(u)[\phi] \qquad \text{for all } \phi \in H^2, \phi' \perp u'$$

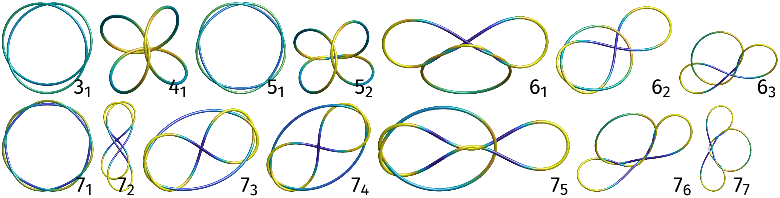
- subject to initial and boundary conditions (periodicity),
- incorporating the linearized arc-length condition $u_t' \perp u'$,
- based on piecewise cubic finite elements.

Theorem (Stability) [Bartels & R. '18]

The corresponding semi-discrete scheme produces a sequence $(u_k)_{k=0,\dots,L}$ such that

- the energy $E(u_k)$ is decreasing and
- the arclength violation error $\left\| |[u^k]'|^2 - 1 \right\|_{L^\infty}$ is unconditionally bounded by the time step size.

Approximating elastic knots



Which of these are global minimizers of E_ϱ within their knot class?

Elastic knots (i.e., limits of these minimizers as $\varrho \searrow 0$) are (likely to be)

- circular for BB knots [Gallotti & Pierre-Louis '07; Diao et al. '20]
- planar for Figure-eight [Avvakumov & Sossinsky '14; Bartels & R. '18]

Question. Are elastic knots always planar or spherical?
Possibly not [Avvakumov & Sossinsky '14]

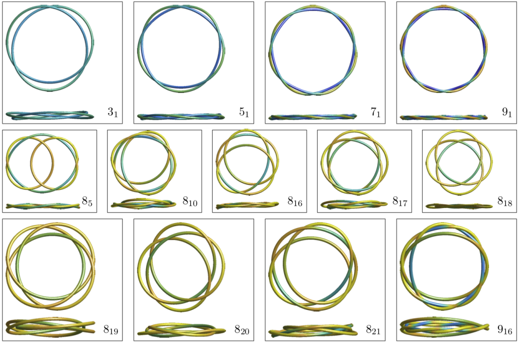
BB knots

bridge number minimal number of local minima of $\langle u, \nu \rangle$ over $\nu \in \mathbb{S}^2$

braid index minimal number of strands required in a circular representation of the knot class

A knot class is **BB** if bridge index = braid index.

- All torus knots; 8_5, 8_{10}, 8_{16}–8_{21}, 9_{16}
- 33 knots with 10 crossings, 17 with 11, 119 with 12



Theorem [Diao, Ernst, R. ’20]

The number of BB knots with a given crossing number n grows exponentially with n.

[Bartels & R. ’18]

BB knots — heuristics

Let $u : \mathbb{R}/\mathbb{Z} \to \mathbb{R}^3$ be embedded, BB, and parametrized by arclength.

$$E_\varrho(u) \geq \int_{\mathbb{R}/\mathbb{Z}} |u''(s)|^2 \, \mathrm{d}s \geq \left(\int_{\mathbb{R}/\mathbb{Z}} |u''(s)| \, \mathrm{d}s \right)^2 = (\mathrm{TC}(u))^2 \geq (2\pi \mathrm{bridge})^2$$

On the other hand, we may find an admissible comparison curve $\tilde{u}$ close to the braid-times covered circle with

$$E_\varrho(\tilde{u}) \leq \underbrace{\int_{\mathbb{R}/\mathbb{Z}} |\tilde{u}''(s)|^2 \, \mathrm{d}s}_{\leq (2\pi \mathrm{braid})^2 + \mathcal{O}(\vartheta^{2/3})} + \mathcal{O}(\vartheta^{2/3}).$$

Assuming that u is the global minimizer, we find that

$$E_\varrho(u) = (2\pi \mathrm{braid})^2 + \mathcal{O}(\vartheta^{2/3}).$$

If $\varrho \searrow 0$ we find that u has constant curvature.

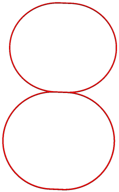
Symmetric elastic knots

Let $\mathscr{C}_{\text{symm}} = \{u \in H^2(\mathbb{R}/\mathbb{Z}, \mathbb{R}^3) \mid |u'| = 1, u \in \mathcal{K} \cap \mathcal{S}\}$ for some isotopy class $\mathcal{K}$ and a symmetry group $\mathcal{S}$.

- Proceeding as before, we consider a sequence of minimizers as $\varrho \searrow 0$.
- Due to the principle of symmetric criticality [Palais '79] these are critical points of E_ϱ for $\varrho > 0$.
- The limit curve is called a symmetric elastic knot.

Theorem [Gilsbach, R., von der Mosel '21]

The (dihedrally) symmetric elastic trefoil is the tangential pair of co-planar circles with exactly one point in common.



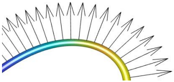
We expect an analogous result to hold for general torus knot classes.

Let’s twist!

A refined model for long slender objects

We attach a frame $F \in H^1(I, \mathrm{SO}(3))$ to the curve such that $F(s) = [t(s), b(s), d(s)]$ where

- $t = u'/|u'|$ is the unit tangent,
- b and $d = u' \times b$ are the directors that track the twisting of the frame about the centerline.



Elastic energy

$$E(u,b) = \frac{C_b}{2} \int_I |t'(s)|^2 \, ds + \frac{C_t}{2} \int_I (b'(s) \cdot d(s))^2 \, ds, \qquad u \in H^2, b \in H^1$$

Special case of a very general theory [Antman ; Maddocks et al. ; Audoly et al. ; Starostin & van der Heijden ; Neukirch et al. ; Coleman & Swigon ; Goriely et al. ; Singer et al. ; ...]

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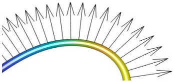


Elastic energy

$$E(u, b) = \frac{c_b}{2} \int_I |t'(s)|^2 \, ds + \frac{c_t}{2} \int_I (b'(s) \cdot d(s))^2 \, ds, \qquad u \in H^2, b \in H^1$$

Formal derivation from a general three-dimensional hyperelastic model imposes $c_b \geq 2c_t$ [Mora & Müller '03; Bartels '19].

A model for inextensible and impermeable rods

Let $u \in H^2(I, \mathbb{R}^3)$, $b \in H^1(I, \mathbb{R}^3)$.

Regularized energy

$$E_\varrho(u, b) = \frac{c_b}{2} \int_I |t'(s)|^2 \, ds + \frac{c_t}{2} \int_I (b'(s) \cdot d(s))^2 \, ds + \varrho \, \mathrm{TP}(u)$$

- Tangent-point functional TP prevents curves from leaving the isotopy class.
- Computational challenge: strong forces related to bending / twisting effects have to be compensated by tangent-point functional to avoid self-intersections
- Existence of minimizers for $c_b > 0$, $c_t \geq 0$, $\varrho \geq 0$

Gradient descent

$d_t u^k = \dfrac{u^k - u^{k-1}}{\tau}$ denotes the backward difference quotient.

$\mathcal{F}_h$ and $\mathcal{E}_h$ are tangent spaces.

1. Choose an initial pair $(u_h, b_h) \in \mathcal{A}_h$, a step size $\tau > 0$, and let $k = 1$.
2. Compute $d_t u_h^k \in \mathcal{F}_h[u_h^{k-1}]$ s.th. for all $w_h \in \mathcal{F}_h[u_h^{k-1}]$
$$(d_t u_h^k, w_h)_{H^2} + c_\mathrm{b}([u_h^k]'', w_h'') + \varepsilon^{-1}([u_h^k]' \cdot b_h^{k-1}, w_h' \cdot b_h^{k-1})_h$$
$$= c_\mathrm{t}\left([\mathbb{Q}_h b_h^{k-1}] \cdot [u_h^{k-1}]'', [\mathbb{Q}_h b_h^{k-1}] \cdot [w_h]''\right) - \varrho\delta\,\mathrm{TP}(u_h^{k-1})[w_h].$$
3. Compute $d_t b_h^k \in \mathcal{E}_h[b_h^{k-1}]$ s.th. for all $r_h \in \mathcal{F}_h[b_h^{k-1}]$.
$$(d_t b_h^k, r_h)_{H^1} + c_\mathrm{t}([b_h^k]', r_h') + \varepsilon^{-1}([u_h^k]' \cdot b_h^k, [u_h^k]' \cdot r_h)_h$$
$$= c_\mathrm{t}\left([\mathbb{Q}_h b_h^{k-1}] \cdot [u_h^k]'', [\mathbb{Q}_h r_h] \cdot [u_h^k]''\right).$$
4. Stop the iteration if the difference quotients are too small or set $k \to k+1$ otherwise.

Stability result [Bartels, R. '19]

Theorem ($\theta = 1$, $\varrho = 0$)

The algorithm is well defined and produces a sequence $(u_h^k, b_h^k)_{k=0,1,\dots}$ such that for all $L \geq 0$ we have

$$E_{\varepsilon,0}^h(u_h^L, b_h^L) + \tau \sum_{k=1}^{L} \left(\|d_t u_h^k\|_{H^2}^2 + \|d_t b_h^k\|_{H^1}^2 \right) \leq E_{\varepsilon,0}^h(u_h^0, b_h^0).$$

The iteration is energy decreasing, convergent, and the unit-length violation is controlled via

$$\max_{k=0,\dots,L} \left(\| |[u_h^k]'|^2 - 1 \|_{L^\infty} + \| |b_h^k|^2 - 1 \|_{L^\infty} \right) \leq \tau c_\star E_{\varepsilon,0}^h(u_h^0, b_h^0),$$

where $c_\star > 0$ only depends on the metrics.

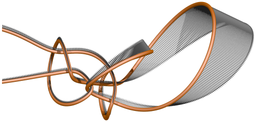
As Riemannian as you can get

How to efficiently untangle cable spaghetti?

Problem. Parameter-dependent restriction on time step size

Idea. Consider an ODE based on a metric that allows for large motions away from regions of almost self-contact.

- The space $\mathcal{C}$ of embedded curves is a Riemannian manifold [Neuberger '97; Michor & Mumford '06; Heeren et al. '14; ...]
- Definition of a metric G inspired by $\mathcal{R}$ (degenerating on non-embedded curves)
- Smooth repulsive energy $\mathcal{E}$ gives rise to a field $\mathrm{grad}_G(\mathcal{E})$.



Theorem [R. & Schumacher '20]

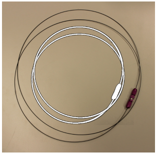
The gradient $\mathrm{grad}_G(\mathcal{E})$ is a well-defined, locally Lipschitz continuous vector field on $\mathcal{C}$. There is a unique short-time solution to the ODE

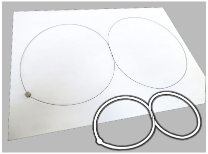
$$\partial_t u_t = -\mathrm{grad}_G(\mathcal{E})|_{u_t}.$$

Summary

- identify global minimizers of bending or elastic energy within knot classes
- rigorous results for two-bridge torus knots
- simulations based on robust numerical schemes

- future aspects
  - extend the setting to higher dimensions
  - consider the non-euclidean case (preferred curvature)
  - bifurcation analysis?
  - twisted trefoil





Thank you!

More information and Simulations at
https://www.tu-chemnitz.de/mathematik/harmonische_analysis/reiter/research/