Untangling and Tangling Elastic Knots

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France-Taiwan Joint Conference on Nonlinear PDE
CIRM, Marseille
March 27, 2008
This is a joint work with Dr. Hartmut Schwetlick, Department of Mathematical Sciences, University of Bath
Outline of Part I: Motivations

1. The Smale Conjecture on the Space of Unknotted Knots
   - The Smale Conjecture
   - Searching for a Physical Procedure in Unknotting

2. Mechanical Modelling of Biopolymers (e.g., DNA or Bacteria Fibre)
   - Supercoiling
   - Over-Damped Dynamics
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Outline of Part II: Untangling Elastic Knots

3 Variational Approaches
- The Möbius Energy
- The Bending Energy

4 Our Setting on the Gradient Flow and Main Results
- Gradient Flows of Elastic Knots
- The Existence of Solutions and Asymptotics
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Outline of Part III: Tangling Elastic Knots

5. **The Total Energy**
   - The Twisting Energy
   - The Variational Problem

6. **The Gradient Flow and Main Results**
   - The Gradient Flow
   - The Existence of Solutions and Asymptotics
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Part I

Motivations
The Smale conjecture: the space of all smooth, unknotted, simple, closed loops is homotopic equivalent to the space of round loops ($\simeq \mathbb{RP}^2$).

This conjecture was confirmed by A. Hatcher, *A proof of the Smale conjecture, Diff($S^3$) $\simeq O(4)$*, Ann. Math., 1983.
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It has been suggested in the article, Freedman, He and Wang, *M"obius energy of knots and unknots*, Ann. Math., 1994: there may exist some physical procedure that will evolve a "tangled" but unknotted simple loop through embeddings into a round circle.
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This picture comes from the article:
Pohl, DNA and differential geometry, Math. Intelligencer,
Supercoiling of a Bacterial Fiber: Bacillus subtilis

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One direction to go is static theory of the supercoiling phenomena (as obstacle problems in elasticity theory). Some progress have been made, for examples by Swigon and Coleman (bifurcation), and Maddocks and his group (global curvature), Schuricht and Von der Mosel (existence and regularity of minimizers).

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Dynamic theory taking into account supercoiling is quite challenging.
In recent years, there is a large interest in the dynamics of twisted biopolymers such as DNA, filaments of Bacillus subtilis, or folded proteins.

The dynamics of these biopolymer filaments is very important in understanding certain mechanism of their functioning.

However, it still remains very complicated. The scientific computations for these dynamics are still too slow and expensive.

An over-damped dynamics of these models provides an approach to study some details.
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Part II

Untangling Elastic Knots
3 Variational Approaches
- The Möbius Energy
- The Bending Energy

4 Our Setting on the Gradient Flow and Main Results
- Gradient Flows of Elastic Knots
- The Existence of Solutions and Asymptotics
Definition of the Möbius Energy

Let \( f : \mathbb{R}/\mathbb{Z} \to \mathbb{R}^3 \) be a \( C^2 \) smooth and closed space curve. Define the electrostatic energy functional of knots by

\[
\mathcal{E}^{(p)}[f] = \iint_{\mathbb{R}/\mathbb{Z} \times \mathbb{R}/\mathbb{Z}} \left[ \frac{1}{|f(y) - f(x)|^p} - \frac{1}{D(f(y), f(x))^p} \right] |f'(y)||f'(x)| \, dx \, dy,
\]

where \( p \geq 1 \), and the improper integral is defined by its principal value, i.e.,

\[
\iint g(x, y) \, dx \, dy = \lim_{\epsilon \to 0^+} \iint_{|x-y| \geq \epsilon} g(x, y) \, dx \, dy.
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- \( \mathcal{E}^{(p)} \) is a renormalized electrostatic energy.
- \( \mathcal{E}^{(2)} \) is the so-called Möbius energy.
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Let $f : \mathbb{R}/\mathbb{Z} \to \mathbb{R}^3$ be a $C^2$ smooth and closed space curve. Define the electrostatic energy functional of knots by

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Below we denote the Möbius Energy $\mathcal{E}^{(2)}$ by $\mathcal{E}_M$.

- The Möbius energy is $C^2$ self-repulsive, i.e., $\mathcal{E}_M[f] \to +\infty$, as $f$ is continuously deformed into an immersion (with self-intersection) in $C^2$ topology.
- The Möbius energy is conformally invariant.
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He considered the gradient flow:

$$\partial_t f = -\nabla \mathcal{E}_M[f].$$  \hspace{1cm} (1)

He showed the short time existence for smooth solutions of Eq.(1).

However, by the conformal invariant property of Möbius energy, one can construct a sequence of knots with decreasing energy which pulls tightly and eventually becomes a round circle.

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The Pull-Tight of Knots with Decreasing Möbius Energy

A Round Circle
Up to our knowledge, nobody has excluded the case of “pull-tight” in the heat flow of Möbius energy. Thus, it is suspicious to derive the long time existence for smooth solutions of the heat flow of Möbius energy.
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Elastic Knots

By adding a bending energy,

$$\mathcal{K}[f] = \frac{1}{2} \int |\kappa|^2 \, ds,$$

to a Möbius energy, we define a new energy functional of knots, i.e.,

$$\mathcal{E}[f] := \frac{1}{2} \int |\kappa|^2 \, ds + \gamma \cdot \mathcal{E}_M[f],$$

where $\kappa = \frac{d^2 f}{ds^2}$ is the curvature vector of $f$, $s$ is the arclength parameter of $f$, and $\gamma > 0$ is a constant.
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On the Gradient Flows

Now we consider the gradient flow of the elastic knot energy $\mathcal{E}_\lambda$,

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\mathcal{E}_\lambda[f] := \frac{1}{2} \int |\kappa|^2 \, ds + \lambda \cdot \int ds + \gamma \cdot \mathcal{E}_M[f],
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\partial_t f = -\nabla \mathcal{E}_\lambda[f] = -\nabla_s^2 \kappa - \frac{|\kappa|^2}{2} \kappa + \lambda \cdot \kappa - \gamma \cdot \mathcal{H}_f, \quad (2)
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where $\nabla_s g = (\partial_s g) ^\perp$, $\lambda > 0$ is a constant (or a Lagrange multiplier for preserving total length), $\mathcal{H}_f : \mathbb{R}/\mathbb{Z} \to \mathbb{R}^3$ is defined by

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\nabla_h \mathcal{E}_M[f] = \int_{\mathbb{R}/\mathbb{Z}} \langle \mathcal{H}_f(x), h(x) \rangle \cdot |f'(x)| \, dx,
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Now we consider the gradient flow of the elastic knot energy $E_{\lambda}$,

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On the Gradient Flows

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\[ \mathcal{H}_f(x) = 2 \cdot \text{(p.v.)} \int_{\mathbb{R}/\mathbb{Z}} \left[ \frac{2 \cdot P_{f'}(x)(f(y) - f(x))}{|f(y) - f(x)|^2} - \kappa(x) \right] \frac{|f'(y)|}{|f(y) - f(x)|^2} dy. \]

Here, \( P_{f'}(x) : \mathbb{R}^3 \rightarrow \mathbb{R}^3 \), defined by

\[ P_{f'}(x)(z) := z - \frac{\langle z, f'(x) \rangle f'(x)}{|f'(x)|^2}, \]

is the orthogonal projection of \( \mathbb{R}^3 \) onto the normal vector plane to \( f \) at \( f(x) \). Note that it is elementary to show

\[ f \in C^{3+k,\alpha}(\mathbb{R}/\mathbb{Z}; \mathbb{R}^3) \Rightarrow \mathcal{H}_f \in C^{k,\beta}(\mathbb{R}/\mathbb{Z}; \mathbb{R}^3), \]

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where \( 0 < \beta < \alpha \leq 1 \). Thus, \( \mathcal{H}_f \) is a closed and smooth space curve as long as \( f \) is a closed and sufficiently smooth space curve.
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Short Time Existence

- From [He,CPAM,2000], the major term in the linearized operator of $\mathcal{H}_f = \nabla \mathcal{E}_M[f]$ is a pseudo-differential operator, $\Delta^{3/2}$, whose order is less than 4, the highest order in $\partial_t f = -\nabla \mathcal{E}_\lambda[f] = -\nabla \mathcal{K}_\lambda[f] - \gamma \cdot \mathcal{H}_f$.

- Therefore, in standard linearization argument for short-time existence, $\nabla \mathcal{H}_f$ is still a compact operator between the relevant parabolic functional spaces.

- Hence, the short time existence for $C^\infty$ smooth solutions of

$$\partial_t f = -\nabla \mathcal{E}_\lambda[f] = -\nabla^2_s \kappa - \frac{|\kappa|^2}{2} \kappa + \lambda \cdot \kappa - \gamma \cdot \mathcal{H}_f,$$

Short Time Existence

- From [He, CPAM, 2000], the major term in the linearized operator of $\mathcal{H}_f = \nabla \mathcal{E}_M[f]$ is a pseudo-differential operator, $\triangle^{3/2}$, whose order is less than 4, the highest order in $\partial_t f = -\nabla \mathcal{E}_\lambda[f] = -\nabla \mathcal{K}_\lambda[f] - \gamma \cdot \mathcal{H}_f$.

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Long Time Existence

To prove long time existence of solutions, we wish to derive global bounds for the higher Sobolev norms of the curvature. Since their evolution is given by

\[ \nabla_t \nabla^m_s \kappa = -\nabla^4_s \nabla^m_s \kappa + \text{tensors of lesser order}. \]

Therefore we arrive at

\[ \frac{d}{dt} \frac{1}{2} \int |\nabla^m_s \kappa|^2 \, ds + \int |\nabla^{m+2}_s \kappa|^2 \, ds = \text{terms of less order}. \]

Now we need to estimate the “terms of less order” to have

\[ \frac{d}{dt} \frac{1}{2} \int |\nabla^m_s \kappa|^2 \, ds + \varepsilon^2 \cdot \int |\nabla^{m+2}_s \kappa|^2 \, ds \leq \text{uniformly bounded constant}. \]
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In fact, it can be written as

\[
\frac{d}{dt} \frac{1}{2} \int |\nabla^m_s \kappa|^2 \, ds + \int |\nabla^{m+2}_s \kappa|^2 \, ds
\]

\[
= \int \langle P^{m+2}_3 (\kappa) + P^m_5 (\kappa), \nabla^m_s \kappa \rangle + \lambda \cdot \langle P^{m+2}_1 (\kappa) + P^m_3 (\kappa), \nabla^m_s \kappa \rangle \, ds
\]

\[
+ \gamma \cdot \left[ \int \langle \mathcal{H}_f, (-1)^{m+2} \nabla^{2m+2}_s \kappa \rangle \, ds + \int \mathcal{H}_f * P^{2m}_3 (\kappa) \, ds \right],
\]

where the notation \( P^\mu \nu (\phi) \) is defined below. Notice, the structure of this differential equation is important in our proof. For example, as we consider \( L^p \)-norm of elastic energy (i.e., \( \| \kappa \|_{L^p} \)), our proof doesn’t work.
In fact, it can be written as

\[
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\]

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Long Time Existence

- The Notation \( P^\mu_\nu (\phi) \): 

For normal vector fields \( \phi_1, \cdots, \phi_k \) along \( f \), we denote by \( \phi_1 \ast \ast \ast \phi_k \) a term of the type

\[
\phi_1 \ast \ast \ast \phi_k = \begin{cases} 
\langle \phi_{i_1}, \phi_{i_2} \rangle \cdots \langle \phi_{i_{k-1}}, \phi_{i_k} \rangle, & \text{for } k \text{ even}, \\
\langle \phi_{i_1}, \phi_{i_2} \rangle \cdots \langle \phi_{i_{k-2}}, \phi_{i_{k-1}} \rangle \cdot \phi_{i_k}, & \text{for } k \text{ odd},
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\]

where \( i_1, \cdots, i_k \) is any permutation of \( 1, \cdots, k \). Slightly more generally, we allow some of the \( \phi_i \) to be functions, in which case the \( \ast \)-product reduces to multiplication. Thus for a normal vector field \( \phi \) along \( f \), we denote by \( P^\mu_\nu (\phi) \) any linear combination of terms of the type \( \nabla^i_{s_1} \phi \ast \cdots \ast \nabla^i_{s_\nu} \phi \) with universal constant coefficients, where \( \mu = i_1 + \cdots + i_\nu \) is the total number of derivatives.
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For normal vector fields $\phi_1, \cdots, \phi_k$ along $f$, we denote by $\phi_1 \star \cdots \star \phi_k$ a term of the type

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Long Time Existence

- We need the lemmas below to estimate the terms of less order.

**Lemma (Gagliardo-Nirenberg interpolation inequality)**

Let $\kappa : I \rightarrow \mathbb{R}^n$ be a smooth vector field. If $\mu + \frac{1}{2}\nu < 2k + 1$, then $\gamma < 2$ and we have for any $\varepsilon > 0$,

$$
\int_I |P_{\nu}^{\mu}(\kappa)| \, ds \leq \varepsilon \int_I |\nabla_s^k \kappa|^2 \, ds + c \varepsilon^{\frac{-\gamma}{2-\gamma}} \left( \int_I |\kappa|^2 \, ds \right)^{\frac{\nu-\gamma}{2-\gamma}}
$$

$$
+ c \left( \int_I |\kappa|^2 \, ds \right)^{\mu+\nu-1},
$$

where $c = c(n, k, \mu, \nu)$.
To estimate terms involving $\mathcal{H}_f$, one further needs

**Lemma (L- and Schwetlick)**

Let $f : \mathbb{R}/\mathbb{Z} \to \mathbb{R}^3$ be a $C^{3,1}$ function, $\ell^{-1} \leq \mathcal{L}[f] \leq \ell$, and $\mathcal{E}_M[f] \leq b$, for some positive constants $\ell$ and $b$. Then

\[
\left( \int_1^\infty \left| \mathcal{H}_f(s) \right|^2 \, ds \right)^{\frac{1}{2}} \leq C(\ell, b, \|\kappa\|_{L^2}) \cdot \left[ \delta^{-3} + \delta^{1/2} \cdot \left( 1 + \sum_{i=0}^{6} \|\kappa\|_{m+2,2}^{2-i/4} \right) \right],
\]

for all sufficiently small $\delta > 0$. 

Sketch of the Proof of Lemma

Recall the integral formula of $\mathcal{H}_f$

$$\mathcal{H}_f(x) = \left(\frac{2 \cdot \mathbb{P}_{f'_\perp(x)}(f(y) - f(x))}{|f(y) - f(x)|^2} - \kappa(x)\right) \frac{|f'(y)|}{|f(y) - f(x)|^2} dy,$$

and

Lemma (O’Hara, Topology, 1991)

Let $f : \mathbb{R}/\mathbb{Z} \to \mathbb{R}^3$ be a smooth knot. For any $b \in \mathbb{R}$ there is a positive constant $C = C(b)$ such that if $E_M[f] \leq b$ then $|f(s) - f(t)| \geq C \cdot d(s, t)$ for any $s, t \in S^1$, where $d(s, t)$ is the shortest arclength between $f(s)$ and $f(t)$ along the space curve $f$. 
Sketch of the Proof of Lemma

Recall the integral formula of $\mathcal{H}_f$

$$\mathcal{H}_f(x) = 2 \cdot \int_{\mathbb{R}/\mathbb{Z}} \left[ \frac{2 \cdot \mathbb{P}_{f'}(x)(f(y) - f(x))}{|f(y) - f(x)|^2} - \kappa(x) \right] \frac{|f'(y)|}{|f(y) - f(x)|^2} dy,$$

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**Lemma (O’Hara, Topology, 1991)**

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Sketch of the Proof of Lemma

- Decomposition of the Integral

For each fixed $s \in I$, we may decompose the integral formula of $\mathcal{H}_f$ as

$$\mathcal{H}_f(s) = (\mathcal{H}_f)_1(s) + (\mathcal{H}_f)_2(s),$$

where

$$(\mathcal{H}_f)_1(s) := (\text{p.v.}) 2 \cdot \int_{l_\delta} (\cdots) \, ds',$$

$$(\mathcal{H}_f)_2(s) := (\text{p.v.}) 2 \cdot \int_{l_\delta^c} (\cdots) \, ds',$$

$l_\delta = l_\delta(s) := \{ s' \in I : |s' - s| \leq \delta \}$, and $l_\delta^c = l_\delta^c(s) := I \setminus l_\delta(s)$. 
Sketch of the Proof of Lemma

- To estimate \( \left( \int_I |(\mathcal{H}_f)_1(s)|^2 \, ds \right)^{1/2} \).

We apply power series expansions, i.e., for \(|\sigma| < \delta\),

\[
f(s+\sigma) = f(s) + f'(s)\sigma + \frac{f''(s)}{2!} \sigma^2 + \frac{f^{(3)}(s)}{3!} \sigma^3 + \frac{1}{3!} \int_s^{s+\sigma} (s+\sigma-t)^3 f^{(4)}(t) \, dt
\]

- To estimate \( \left( \int_I |(\mathcal{H}_f)_2(s)|^2 \, ds \right)^{1/2} \).

We apply O’Hara’s Lemma.
Uniform bounds of the total length:

**Lemma (L- and Schwetlick)**

*If the initial curve is smooth, then the total length of $f$, $\mathcal{L}[f]$, remains uniformly bounded away from 0 and $\infty$ during the gradient flow of $\mathcal{E}_\lambda$. In fact,*

$$\frac{2\pi^2}{\mathcal{E}_\lambda[f_0]} \leq \mathcal{L}[f] \leq \frac{\mathcal{E}_\lambda[f_0]}{\lambda}.$$
Now one applies the lemmas to estimate the terms of less order.

\[ \left| \int \left< P_{3}^{m+2}(\kappa) + P_{5}^{m}(\kappa), \nabla_{s}^{m}\kappa \right> + \lambda \cdot \left< P_{1}^{m+2}(\kappa) + P_{3}^{m}(\kappa), \nabla_{s}^{m}\kappa \right> ds \right| \]

\[ \leq C \cdot \| \kappa \|_{L^{2}}^{p(m)} \cdot \left( \| \kappa \|_{m+2,2}^{2-\frac{1}{m+2}} + \| \kappa \|_{m+2,2}^{2-\frac{2}{m+2}} + \| \kappa \|_{m+2,2}^{2-\frac{3}{m+2}} \right) \]

\[ \leq C \cdot \left( \| \kappa \|_{m+2,2}^{2-\frac{1}{m+2}} + \| \kappa \|_{m+2,2}^{2-\frac{2}{m+2}} + \| \kappa \|_{m+2,2}^{2-\frac{3}{m+2}} \right), \]

where \( C = C_{m}(\lambda, \mathcal{E}[f_{0}]) \);
Long Time Existence

and,

$$\gamma \cdot \left| \int_I \langle \mathcal{H}_f, (-1)^{m+2} \nabla_s^{2m+2} \kappa \rangle \, ds + \int_I \mathcal{H}_f * P_3^{2m}(\kappa) \, ds \right|$$

$$\leq C \cdot \left[ \delta^{-3} + \delta^{1/2} \left( 1 + \sum_{i=0}^{6} \| \kappa \|_{m+2,2}^{2-i/4} \right) \right] \left[ \| \kappa \|_{m+2,2}^{2-2/m+2} + \| \kappa \|_{m+2,2}^{2-3/m+2} \right],$$

where $C = C_m(\gamma, \lambda, \mathcal{E}[f_0]).$
By combining these estimates and applying the interpolation inequality again, one has
\[
\frac{d}{dt} \frac{1}{2} \int_I |\nabla_s^m \kappa|^2 \, ds + \int_I |\nabla_s^{m+2} \kappa|^2 \, ds \\
\leq \left[ \varepsilon + \gamma \cdot \delta^{1/2} \cdot C_m(\gamma, \lambda, \mathcal{E}[f_0]) \right] \cdot \int_I |\nabla_s^{m+2} \kappa|^2 \, ds + C_m(\gamma, \lambda, \delta, \mathcal{E}[f_0]),
\]

By choosing sufficiently small $\delta$ and $\varepsilon$,
\[
\frac{d}{dt} \frac{1}{2} \int_I |\nabla_s^m \kappa|^2 \, ds + \frac{1}{2} \cdot \int_I |\nabla_s^{m+2} \kappa|^2 \, ds \leq C_m(\gamma, \lambda, \mathcal{E}[f_0]), \quad (4)
\]
Long Time Existence

- By combining these estimates and applying the interpolation inequality again, one has

\[
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\leq \left[ \varepsilon + \gamma \cdot \delta^{1/2} \cdot C_m(\gamma, \lambda, \mathcal{E}[f_0]) \right] \cdot \int_I |\nabla_s^{m+2} \kappa|^2 \, ds + C_m(\gamma, \lambda, \delta, \mathcal{E}[f_0]),
\]

- By choosing sufficiently small $\delta$ and $\varepsilon$,

\[
\frac{d}{dt} \frac{1}{2} \int_I |\nabla_s^m \kappa|^2 \, ds + \frac{1}{2} \cdot \int_I |\nabla_s^{m+2} \kappa|^2 \, ds \leq C_m(\gamma, \lambda, \mathcal{E}[f_0]), \quad (4)
\]
Notice that by the fact

$$\partial_s \varphi = \nabla_s \varphi + \langle \varphi, \kappa \rangle \, T,$$  \hspace{1cm} \text{(5)}

where $\varphi \in (T)^\perp$, by applying Poincare inequality twice on $\partial_s^{m+2} \kappa$, and by using the interpolation inequality, one derives

$$\int |\nabla_s^{m+2} \kappa|^2 \, ds \geq C(\mathcal{L}[f]) \cdot \int |\nabla_s^m \kappa|^2 \, ds - C_m(\|\kappa\|_{L^2}).$$

Thus, we have the differential inequality

$$\frac{d}{dt} \int |\nabla_s^m \kappa|^2 \, ds + c^2 \cdot \int |\nabla_s^{m+2} \kappa|^2 \, ds \leq C_m(\gamma, \lambda, \mathcal{E}[f_0]),$$

which implies

$$\|\nabla_s^m \kappa\|_{L^2} \leq C_m(\gamma, \lambda, \mathcal{E}[f_0], \|\nabla_s^m \kappa\|_{L^2}^2(0)), \forall m \in \mathbb{Z}^+.$$
Long Time Existence

- Notice that by the fact

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which implies

\[ \|\nabla_s^m \kappa\|_{L^2} \leq C_m(\gamma, \lambda, \mathcal{E}[f_0], \|\nabla_s^m \kappa\|_{L^2}(0)), \forall m \in \mathbb{Z}^+. \]
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Long Time Existence

- The uniform upper bounds of $\|\partial_s^m \kappa\|_{L^2}$ now follows from letting $\varphi = \nabla_s^{m-1} \kappa$ in Eq.(5), and an induction argument on $m$.

- Thus by Sobolev embedding Theorem and an induction on $m$,

$$\|\partial_s^m \kappa\|_{L^\infty} \leq C(\gamma, \lambda, \mathcal{E}[f_0], \Lambda_1, \cdots, \Lambda_m), \quad (6)$$

where $\Lambda_i = \|\nabla_s^i \kappa\|_{L^2}^2 (0), \forall \ i \in \mathbb{Z}^+$. 

- Furthermore, we have

$$\|\partial_s^m \mathcal{H}_f\|_{L^\infty} \leq C(\gamma, \lambda, \mathcal{E}[f_0], \Lambda_1, \cdots, \Lambda_{m+2}). \quad (7)$$

This is due to Eq.(6) and the fact in Eq.(3), i.e.,

$$f \in C^{3+k,\alpha}(\mathbb{R}/\mathbb{Z}; \mathbb{R}^3) \Rightarrow \mathcal{H}_f \in C^{k,\beta}(\mathbb{R}/\mathbb{Z}; \mathbb{R}^3)$$
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Asymptotics

We first choose a subsequence of curves \( f(t, \cdot) \), which converges smoothly to a smooth limit curve \( f_\infty \) as \( t \to \infty \) after reparametrization of arclength and translations. Then by applying Eqs.(6), (7), and the lemma below, we can derive the estimates

\[
\| \nabla_t (\nabla_s^m \kappa) \|_{L^\infty} \leq C(\gamma, \lambda, E[f_0], \Lambda_1, \cdots, \Lambda_{m+4}), \forall m \geq 0. \tag{8}
\]

**Lemma (L- and Schwetlick)**

Let \( f \) be a solution of Eq.(2). Then \( \phi_m = \nabla_s^m \kappa \), \( m \in \mathbb{Z}^+ \), satisfy

\[
\nabla_t \phi_m + \nabla_s^4 \phi_m
\]

\[
= P_3^{m+2} (\kappa) + \lambda \cdot (\nabla_s^{m+2} \kappa + P_3^m (\kappa)) + \frac{1}{2} \cdot (P_3^{m+2} (\kappa) + P_5^m (\kappa))
\]

\[
+ \gamma \cdot (\nabla_s^{m+2} \mathcal{H}_f + P_2^m (\kappa) \ast \mathcal{H}_f).
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Asymptotics

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*Let \( f \) be a solution of Eq. (2). Then \( \phi_m = \nabla_s^m \kappa, \ m \in \mathbb{Z}^+, \) satisfy*

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Asymptotics

Let

\[ u(t) := \int_I |\partial_t f|^2 \, ds. \]

Note that the first equality in the energy identity

\[ \frac{d}{dt} E_\lambda [f_t] = -\int_I |\partial_t f|^2 \, ds = -\int_I |-\nabla_s^2 \kappa - \frac{|\kappa|^2}{2} \kappa + \lambda \cdot \kappa - \gamma \cdot \mathcal{H}_f|^2 \, ds \]

implies \( u(t) \in L^1 ([0, \infty)) \). On the other hand, from using the lemma above on differentiating the energy identity, using \( L^\infty \)-estimates in Eqs. (6), (8), and using integration by parts,

\[ |u'(t)| \leq C(\gamma, \lambda, E[f_0], \Lambda_1, \cdots, \Lambda_4). \]

Thus, \( u(t) \to 0 \) as \( t \to \infty \). This implies that \( f_\infty \) is independent of \( t \). Therefore, from Eq. (2), \( f_\infty \) is an equilibrium of the energy functional \( E_\lambda \).
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Theorem (L- and Schwetlick, 2008)

For any real numbers $\lambda \in (0, \infty)$ and any smooth initial closed curve $f_0$, there exists a smooth solution to the $L^2$-gradient flow in Eq.(2). Moreover, the curves subconverge to $f_\infty$, an equilibrium of the energy functional $\mathcal{E}_\lambda$, after reparametrization by arclength and translation.

Theorem (for $\partial_t f = -\nabla \mathcal{E}$ with fixed length)

For any smooth initial closed curve $f_0$, there exists a smooth solution to the $L^2$-gradient flow in Eq.(2), which preserves total length. Moreover, the curves subconverge to $f_\infty$, an equilibrium of the energy functional $\mathcal{E}$, after reparametrization by arclength and translation.
Theorem (L- and Schwetlick, 2008)

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For any smooth initial closed curve $f_0$, there exists a smooth solution to the $L^2$-gradient flow in Eq.(2), which preserves total length. Moreover, the curves subconverge to $f_\infty$, an equilibrium of the energy functional $E$, after reparametrization by arclength and translation.
Part III

Tangling Elastic Knots
5 The Total Energy
- The Twisting Energy
- The Variational Problem

6 The Gradient Flow and Main Results
- The Gradient Flow
- The Existence of Solutions and Asymptotics
The Twisting Energy

A rod configuration $\Gamma$ is a framed curve described by
\[ \{ f(s); T(s), M_1(s), M_2(s) \}, \]
where the material frame \( \{ T, M_1, M_2 \} \) forms an orthonormal frame field along \( f \). Thus, a smooth rod configuration $\Gamma$ gives the skew-symmetric system
\[
\begin{pmatrix}
T'(s) \\
M_1'(s) \\
M_2'(s)
\end{pmatrix}
= 
\begin{pmatrix}
0 & m_1(s) & m_2(s) \\
-m_1(s) & 0 & m(s) \\
-m_2(s) & -m(s) & 0
\end{pmatrix}
\begin{pmatrix}
T(s) \\
M_1(s) \\
M_2(s)
\end{pmatrix}.
\]

The Kirchhoff elastic energy $\mathcal{E}$ of an isotropic rod $\Gamma$, is defined by
\[
\mathcal{E}[\Gamma] := \int \left[ \alpha \cdot (m_1^2 + m_2^2) + \beta \cdot m^2 \right] \, ds, \tag{9}
\]
where $\alpha > 0$ and $\beta \geq 0$ are constants. The terms involving $\alpha$ give the bending energy, while the term involving $\beta$ gives the twisting energy. It can be easily verified that $m_1^2 + m_2^2 = |\kappa|^2$ is a geometric quantity of curves.
The Twisting Energy

A rod configuration $\Gamma$ is a framed curve described by \( \{ f(s); T(s), M_1(s), M_2(s) \} \), where the material frame \( \{ T, M_1, M_2 \} \) forms an orthonormal frame field along $f$. Thus, a smooth rod configuration $\Gamma$ gives the skew-symmetric system

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\end{pmatrix}
\begin{pmatrix}
T(s) \\
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M_2(s)
\end{pmatrix}.
$$

The Kirchhoff elastic energy $E$ of an isotropic rod $\Gamma$, is defined by

$$
E[\Gamma] := \int_{\Gamma} \left[ \alpha \cdot (m_1^2 + m_2^2) + \beta \cdot m^2 \right] ds, \quad (9)
$$

where $\alpha > 0$ and $\beta \geq 0$ are constants. The terms involving $\alpha$ give the bending energy, while the term involving $\beta$ gives the twisting energy. It can be easily verified that $m_1^2 + m_2^2 = |\kappa|^2$ is a geometric quantity of curves.
The natural frames of the curve discussed by Bishop form the orthonormal frames along a given curve $f$, which can be uniquely determined by fixing it at a given point on the centerline and solving the skew-symmetric system,

$$
\begin{pmatrix}
T'(s) \\
U'(s) \\
V'(s)
\end{pmatrix} = \begin{pmatrix}
0 & * & * \\
* & 0 & 0 \\
* & 0 & 0
\end{pmatrix} \begin{pmatrix}
T(s) \\
U(s) \\
V(s)
\end{pmatrix}.
$$

As we denote by $\theta$ the angle from $U$ to $M_1$, it can be verified that $m(s) = \theta'(s)$. Since a natural frame can be thought as a frame without twisting, $m(s)$ in Eq.(9) is called **twisting rate**. Thus the elastic energy in Eq.(9) becomes

$$
\mathcal{E} [\Gamma] = \int \left[ \alpha \cdot |\kappa|^2 + \beta \cdot (\theta')^2 \right] ds.
$$

(10)
The natural frames of the curve discussed by Bishop form the orthonormal frames along a given curve $f$, which can be uniquely determined by fixing it at a given point on the centerline and solving the skew-symmetric system,

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As we denote by $\theta$ the angle from $U$ to $M_1$, it can be verified that $m(s) = \theta'(s)$. Since a natural frame can be thought as a frame without twisting, $m(s)$ in Eq.(9) is called twisting rate. Thus the elastic energy in Eq.(9) becomes

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\mathcal{E} [\Gamma] = \int_{\Gamma} [\alpha \cdot |\kappa|^2 + \beta \cdot (\theta')^2] \, ds. \tag{10}
\]
We will use the term \((f(s), \theta(s))\) to represent the rod configuration \(\Gamma\), which is the curve-angle representation.

Because of the twisting energy, we need to establish the end-point conditions (or “boundary” value conditions) which will be imposed through the Călugăreanu-White-Fuller formula

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Lk[\Gamma] = Tw[\Gamma] + Wr[f]
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(11)
The linking number, twisting number, and writhing number of $\Gamma$ are defined by

\[
Lk[\Gamma] := \frac{1}{4\pi} \int \int_{s \in I \atop \sigma \in I} \frac{\langle f(s) - g_\epsilon(\sigma), f'(s) \times g_\epsilon'(\sigma) \rangle}{|f(s) - g_\epsilon(\sigma)|^3} \, ds \wedge d\sigma, \quad (12)
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\[
Tw[\Gamma] := \frac{1}{2\pi} \int_I \langle M_1'(s), f'(s) \times M_1(s) \rangle \, ds = \frac{1}{2\pi} \int_I \theta'(s) \quad (13)
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Wr[f] := \frac{1}{4\pi} \int \int_{s \in I \atop \sigma \in I} \frac{\langle f(s) - f(\sigma), f'(s) \times f'(\sigma) \rangle}{|f(s) - f(\sigma)|^3} \, ds \wedge d\sigma. \quad (14)
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Here both $s$ and $\sigma$ represent the arclength parameterisation for $f$ and $g_\epsilon = f + \epsilon \cdot M_1$, where $\epsilon > 0$ is sufficiently small so that $f$ and $g_\epsilon$ have no intersection.
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Here both $s$ and $\sigma$ represent the arclength parameterisation for $f$ and $g_\epsilon = f + \epsilon \cdot M_1$, where $\epsilon > 0$ is sufficiently small so that $f$ and $g_\epsilon$ have no intersection.
Now we consider the total energy,

\[ \mathcal{E} [\Gamma] = \int_{\Gamma} [\alpha \cdot |\kappa|^2 + \beta \cdot (\theta')^2] \, ds + \gamma \cdot \mathcal{E}_M[f]. \] (15)

We use the topologically invariant, the linking number,

\[ \frac{\Delta \Omega}{2\pi} := Lk[\Gamma] = Tw[\Gamma] + Wr[f], \]

to set up the end-point conditions. Note that if \( f \) and \( g_\varepsilon \)
consist two closed curves the linking number is an integer-valued topological quantity, while twisting number and writhing number are only geometric quantity. The linking number continues to be an invariant under smooth perturbations of the rod configuration \( \Gamma \). In fact, one can set \( \Delta \Omega / 2\pi \) to be any real number.
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The Total Energy of Rods (framed curves)

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In order to apply our technique used before, we transform the energy of rods into that of curves. We learn from a fact that when an isotropic elastic rod attains an equilibrium state it must have a constant twisting rate.

Assuming that the twisting rate $m$ of an isotropic rod configurations $\Gamma$ is constant we can combine the definitions of elastic energy and the twisting number to deduce

$$m = \frac{2\pi}{\mathcal{L}[f]} Tw[\Gamma],$$

where $\mathcal{L}[f] = \int ds$ is the length of the centerline.
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\mathcal{F}(f) := \alpha \int_I |\kappa|^2 \, ds + \frac{\beta}{\mathcal{L}[f]} (\Delta \Omega - 2\pi \cdot Wr[f])^2 + \gamma \cdot E_M[f].
\]

As \( \beta = 0 = \gamma \), this energy functional corresponds to the Euler-Bernoulli model of elastic curves. Thus the geometric evolution considered below is also a generalization of the so-called curve-straightening flow.

We note here that in computing the writhing number, we apply Fuller’s difference of writhe formula

\[
Wr[f_1] - Wr[f_0] = \frac{1}{2\pi} \int_I \frac{\langle T_0(x) \times T_1(x), T_0'(x) + T_1'(x) \rangle}{1 + \langle T_0(x), T_1(x) \rangle} \, dx,
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This picture comes from the article: Pohl, DNA and differential geometry, Math. Intelligencer., 1980.

Chun-Chi Lin
Untangling and Tangling Elastic Knots
Now we want to tangle elastic knots by solving the variational problem stated above. We can also observe the dynamical behaviour. However, in this setting, we don’t treat the obstacle problem, which is more difficult.
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The Total Energy
- The Twisting Energy
- The Variational Problem

The Gradient Flow and Main Results
- The Gradient Flow
- The Existence of Solutions and Asymptotics
The Gradient Flow

\[ \partial_t f = 2\alpha \cdot (-\nabla^2_s \kappa - \frac{\kappa}{2}) + \lambda_2 (t) \cdot \nabla_s (T \times \kappa) + \lambda_1 \cdot \kappa - \gamma \cdot \mathcal{H}_f, \]

where

\[ \lambda_2 (t) = \frac{2\beta}{\mathcal{L}[f]} (\Delta \Omega - 2\pi \cdot \text{Wr}[f]), \]

and either \( \lambda_1 \) is a positive constant or a Lagrange multiplier for preserving total length of curves.
\[ \frac{\partial f}{\partial t} = 2\alpha \cdot ( -\nabla_s^2 \kappa - \frac{1}{2} \frac{|\kappa|^2}{\kappa} ) + \lambda_2(t) \cdot \nabla_s (T \times \kappa) + \lambda_1 \cdot \kappa - \gamma \cdot H_f, \]

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Results and A Remained Problem

- We still have the existence of smooth solutions (short time and long time) in the case of adding twisting energy. The proof parallels the one in Part II.
- Numerical implements are still in progress (it is quite demanding; one needs higher-order approximation of curves)!
- A Remained Problem: Does any one of the flows we treated here provides a physical procedure in unknotting trivial knots?
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THANK YOU FOR YOUR ATTENTION!