Untangling and Tangling Elastic Knots

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This is a joint work with Dr. Hartmut Schwetlick,
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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

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Part I

Motivations

The Smale Conjecture

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- This conjecture was confirmed by A. Hatcher, *A proof of the Smale conjecture, Diff($\mathbb{S}^3$) $\backsimeq O(4)$*, Ann. Math., 1983.

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Supercoiling of a Circular DNA

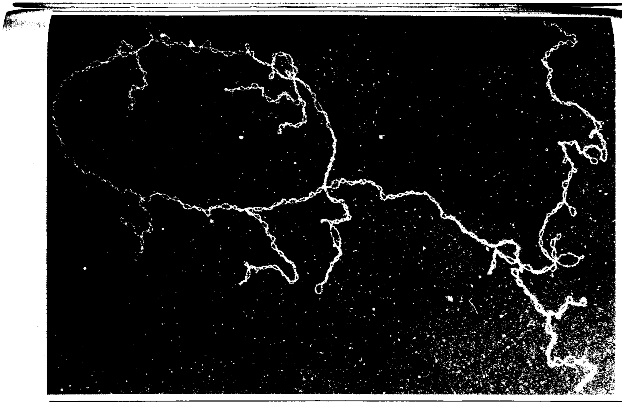
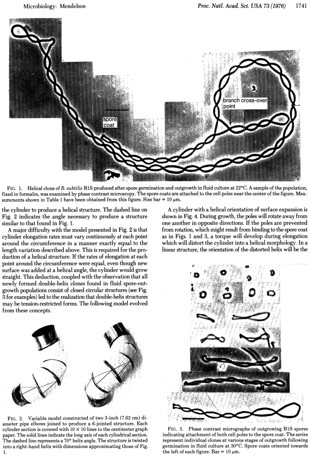


Figure 4. Electron micrograph of supercoiled circular DNA, a plasmid of *Halobacterium halobium*. Molecular weight: 10^8; 150,000 base pairs. Magnification 70000x. For details see [10]. (Courtesy of Prof. Günther Klotz).

- This picture comes from the article:
  Pohl, DNA and differential geometry, Math. Intelligencer,

Supercoiling of a Bacterial Fiber: Bacillus subtilis



Microbiology: Mendelson *Proc. Natl. Acad. Sci. USA 73 (1976)* 1741

FIG. 1. Helical clone of *B. subtilis* B1S produced after spore germination and outgrowth in fluid culture at 22°C. A sample of the population, fixed in formalin, was examined by phase contrast microscopy. The spore coats are attached to the cell poles near the center of the figure. Measurements shown in Table 1 have been obtained from this figure. Size bar = 10 μm.

the cylinder to produce a helical structure. The dashed line on Fig. 2 indicates the angle necessary to produce a structure similar to that found in Fig. 1.

A major difficulty with the model presented in Fig. 2 is that cylinder elongation rates must vary continuously at each point around the circumference in a manner exactly equal to the length variation described above. This is required for the production of a helical structure. If the rates of elongation at each point around the circumference were equal, even though new surface was added at a helical angle, the cylinder would grow straight. This deduction, coupled with the observation that all newly formed double-helix clones found in fluid spore-outgrowth populations consist of closed circular structures (see Fig. 3 for examples) led to the realization that double-helix structures may be tension-restricted forms. The following model evolved from these concepts.

FIG. 2. Variable model constructed of two 3-inch (7.62 cm) diameter pipe elbows joined to produce a 6-jointed structure. Each cylinder section is covered with 10 × 10 lines to the centimeter graph paper. The solid lines indicate the long axis of each cylindrical section. The dashed line represents a 70° helix angle. The structure is twisted into a right-hand helix with dimensions approximating those of Fig. 1.

A cylinder with a helical orientation of surface expansion is shown in Fig. 4. During growth, the poles will rotate away from one another in opposite directions. If the poles are prevented from rotation, which might result from binding to the spore coat as in Figs. 1 and 3, a torque will develop during elongation which will distort the cylinder into a helical morphology. In a linear structure, the orientation of the distorted helix will be the

FIG. 3. Phase contrast micrographs of outgrowing B1S spores indicating attachment of both cell poles to the spore coat. The series represent individual clones at various stages of outgrowth following germination in fluid culture at 30°C. Spore coats oriented towards the left of each figure. Bar = 10 μm.

- This picture comes from the article: Mendelson, PNAS, 1976.

Supercoiling

- 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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Over-Damped Dynamics

- 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

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

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

$$\iint g(x,y)\, dxdy = \lim_{\epsilon \to 0^+} \iint_{|x-y|\geq\epsilon} g(x,y)\, dxdy.$$

- $\mathcal{E}^{(p)}$ is a renormalized electrostatic energy.
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Properties of the Möbius Energy

- 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.
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Heat Flow of the Möbius Energy

- Z.X. He, *The Euler-Lagrange equation and heat flow for the Möbius energy*, Comm Pure and Applied Math., 2000.

He considered the gradient flow:

$$\partial_t f = -\nabla \mathcal{E}_M[f]. \tag{1}$$

- 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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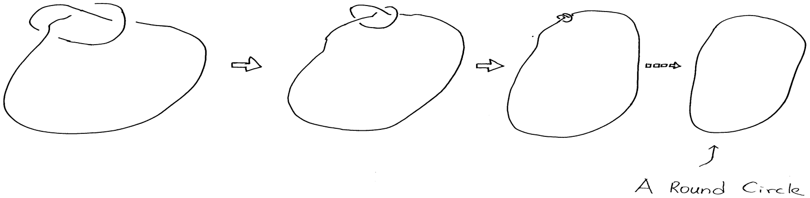
The Pull-Tight of Knots with Decreasing Möbius Energy



Long Time Existence for the Heat Flow?

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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 $\mathcal{E}_\lambda$,

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

i.e.,

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

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

$$\nabla_h \mathcal{E}_M[f] = \int_{\mathbb{R}/\mathbb{Z}} \langle \mathcal{H}_f(x), h(x) \rangle \cdot |f'(x)| \, dx,$$

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

Here, $\mathbb{P}_{f'^{\perp}(x)} : \mathbb{R}^3 \to \mathbb{R}^3$, defined by

$$\mathbb{P}_{f'^{\perp}(x)}(z) := z - \frac{\langle z, f'(x) \rangle f'(x)}{|f'(x)|^2},$$

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

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

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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Here, $\mathbb{P}_{f'^{\perp}(x)} : \mathbb{R}^3 \to \mathbb{R}^3$, defined by

$$\mathbb{P}_{f'^{\perp}(x)}(z) := z - \frac{\langle z, f'(x) \rangle f'(x)}{|f'(x)|^2},$$

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

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

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.

On the Gradient Flows

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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, $\triangle^{3/2}$, whose order is less than 4, the highest order in $\partial_t f = -\nabla \mathcal{E}_\lambda[f] = -\nabla \mathcal{K}_\lambda[f] - \gamma \cdot \mathcal{H}_f$.
- 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^∞ smooth solutions of

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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

$$\nabla_t \nabla_s^m \kappa = -\nabla_s^4 \nabla_s^m \kappa + \text{ tensors of lesser order.}$$

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$$\frac{d}{dt}\frac{1}{2}\int |\nabla_s^m \kappa|^2 \, ds + \int |\nabla_s^{m+2}\kappa|^2 \, ds = \text{ terms of less order.}$$

- Now we need to estimate the "terms of less order" to have

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- The Notation $P^{\mu}_{\nu}(\phi)$:

For normal vector fields $\phi_1, \cdots, \phi_k$ along f, we denote by $\phi_1 * * * \phi_k$ a term of the type

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

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

$$\int_I \left|P_\nu^\mu(\kappa)\right| \, ds \leq \varepsilon \int_I \left|\nabla_s^k \kappa\right|^2 ds + c\,\varepsilon^{\frac{-\gamma}{2-\gamma}} \left(\int_I |\kappa|^2 \, ds\right)^{\frac{\nu-\gamma}{2-\gamma}} + c\left(\int_I |\kappa|^2 \, ds\right)^{\mu+\nu-1},$$

where $c = c(n, k, \mu, \nu)$.

Long Time Existence

- 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, $\ell^{-1} \le \mathcal{L}[f] \le \ell$, and $\mathcal{E}_M[f] \le b$, for some positive constants ℓ and b. Then

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

for all sufficiently small $\delta > 0$.

Sketch of the Proof of Lemma

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

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

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 $\mathcal{E}_M[f]\leq b$ 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.

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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

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

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

$I_\delta = I_\delta(s) := \{s' \in I : |s' - s| \leq \delta\}$, and $I_\delta^c = I_\delta^c(s) := I \setminus I_\delta(s)$.

Sketch of the Proof of Lemma

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

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

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

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

We apply O'Hara's Lemma.

Long Time Existence

- 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 ∞ during the gradient flow of $\mathcal{E}_\lambda$. In fact,

$$\frac{2\pi^2}{\mathcal{E}_\lambda[f_0]} \leq \mathcal{L}[f] \leq \frac{\mathcal{E}_\lambda[f_0]}{\lambda}.$$

Long Time Existence

- Now one applies the lemmas to estimate the terms of less order.

$$\left|\int \langle P_3^{m+2}(\kappa) + P_5^m(\kappa), \nabla_s^m \kappa\rangle + \lambda \cdot \langle P_1^{m+2}(\kappa) + P_3^m(\kappa), \nabla_s^m \kappa\rangle \; ds\right|$$

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

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where $C = C_m(\lambda, \mathcal{E}[f_0])$;

Long Time Existence

and,

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

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

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Long Time Existence

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

$$\frac{d}{dt}\frac{1}{2}\int_I |\nabla_s^m \kappa|^2 \, ds + \int_I |\nabla_s^{m+2}\kappa|^2 \, ds$$
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- By choosing sufficiently small δ and ε,

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$$\partial_s \varphi = \nabla_s \varphi + \langle \varphi, \kappa \rangle \, T, \tag{5}$$

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

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

- Thus, we have the differential inequality

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

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- 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,

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

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

- Furthermore, we have

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

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

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Asymptotics

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

$$\|\nabla_t (\nabla_s^m \kappa)\|_{L^\infty} \le C(\gamma, \lambda, \mathcal{E}[f_0], \Lambda_1, \cdots, \Lambda_{m+4}), \ \forall\ m \ge 0. \quad (8)$$

Lemma (L- and Schwetlick)

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

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

Note that the first equality in the energy identity

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Main Results

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_∞, 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_∞, an equilibrium of the energy functional $\mathcal{E}$, after reparametrization by arclength and translation.

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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 Γ 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 Γ 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 Γ, is defined by

$$\mathcal{E}[\Gamma] := \int_I [\alpha \cdot (m_1^2 + m_2^2) + \beta \cdot m^2] \, ds, \tag{9}$$

where $\alpha > 0$ and $\beta \geq 0$ are constants. The terms involving α give the bending energy, while the term involving β gives the twisting energy. It can be easily verified that $m_1^2 + m_2^2 = |\kappa|^2$ is a geometric quantity of curves.

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$$\begin{pmatrix} T'(s) \\ M_1'(s) \\ M_2'(s) \end{pmatrix} = \begin{pmatrix} 0 & m_1(s) & m_2(s) \\ -m_1(s) & 0 & m(s) \\ -m_2(s) & -m(s) & 0 \end{pmatrix} \begin{pmatrix} T(s) \\ M_1(s) \\ M_2(s) \end{pmatrix}.$$

The Kirchhoff elastic energy $\mathcal{E}$ of an isotropic rod Γ, is defined by

$$\mathcal{E}[\Gamma] := \int_I [\alpha \cdot (m_1^2 + m_2^2) + \beta \cdot m^2] \, ds, \qquad (9)$$

where $\alpha > 0$ and $\beta \geq 0$ are constants. The terms involving α give the bending energy, while the term involving β 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

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 θ 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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The End-Point Condition

We will use the term $(f(s), \theta(s))$ to represent the rod configuration Γ, 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

$$Lk[\Gamma] = Tw[\Gamma] + Wr[f] \tag{11}$$

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The linking number, twisting number, and writhing number of Γ are defined by

$$Lk[\Gamma] := \frac{1}{4\pi}\int_{s\in I}\int_{\sigma\in I} \frac{\langle f(s)-g_\epsilon(\sigma), f'(s)\times g_\epsilon'(\sigma)\rangle}{|f(s)-g_\epsilon(\sigma)|^3}\, ds\wedge d\sigma, \quad (12)$$

$$Tw[\Gamma] := \frac{1}{2\pi}\int_I \left\langle M_1'(s), f'(s)\times M_1(s)\right\rangle\, ds = \frac{1}{2\pi}\int_I \theta'(s)\, ds, \quad (13)$$

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Here both s and σ 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_ϵ have no intersection.

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The Total Energy of Rods (framed curves)

- Now we consider the total energy,

$$\mathcal{E}\left[\Gamma\right] = \int_I \left[\alpha \cdot |\kappa|^2 + \beta \cdot (\theta')^2\right] ds + \gamma \cdot \mathcal{E}_M[f]. \qquad (15)$$

- 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_ϵ 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 Γ. In fact, one can set $\frac{\Delta\Omega}{2\pi}$ to be any real number.

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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 Γ is constant we can combine the definitions of elastic energy and the twisting number to deduce

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- 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.
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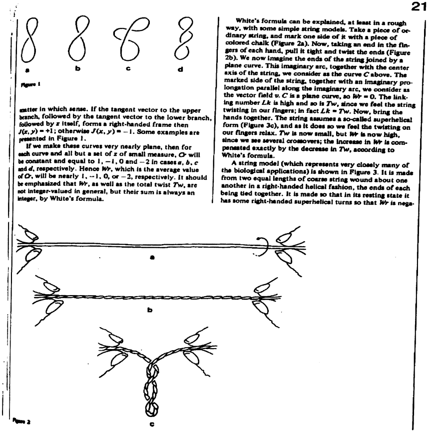
Tangling Knots by Increasing their Writhing Numbers



21

a b c d

Figure 1

matter in which sense. If the tangent vector to the upper branch, followed by the tangent vector to the lower branch, followed by x itself, forms a right-handed frame then $J(x, y) = +1$; otherwise $J(x, y) = -1$. Some examples are presented in Figure 1.

If we make these curves very nearly plane, then for each curve and all but a set of x of small measure, Cr will be constant and equal to $1, -1, 0$ and -2 in cases a, b, c and d, respectively. Hence Wr, which is the average value of Cr, will be nearly $1, -1, 0$, or -2, respectively. It should be emphasized that Wr, as well as the total twist Tw, are not integer-valued in general, but their sum is always an integer, by White's formula.

White's formula can be explained, at least in a rough way, with some simple string models. Take a piece of ordinary string, and mark one side of it with a piece of colored chalk (Figure 2a). Now, taking an end in the fingers of each hand, pull it tight and twist the ends (Figure 2b). We now imagine the ends of the string joined by a plane curve. This imaginary arc, together with the center axis of the string, we consider as the curve C above. The marked side of the string, together with an imaginary prolongation parallel along the imaginary arc, we consider as the vector field v. C is a plane curve, so $Wr = 0$. The linking number Lk is high and so is Tw, since we feel the string twisting in our fingers; in fact $Lk = Tw$. Now, bring the hands together. The string assumes a so-called superhelical form (Figure 3c), and as it does so we feel the twisting on our fingers relax. Tw is now small, but Wr is now high, since we see several crossovers; the increase in Wr is compensated exactly by the decrease in Tw, according to White's formula.

A string model (which represents very closely many of the biological applications) is shown in Figure 3. It is made from two equal lengths of coarse string wound about one another in a right-handed helical fashion, the ends of each being tied together. It is made so that in its resting state it has some right-handed superhelical turns so that Wr is nega-

a

b

c

Figure 2

- This picture comes from the article: Pohl, DNA and differential geometry, Math. Intelligencer, 1980.

Tangling Knots by Increasing their Writhing Numbers

- 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 Gradient Flow

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

where

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

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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)!
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Merci !

- THANK YOU FOR YOUR ATTENTION !