ORIGINAL PAPER

Evolving a Kirchhoff elastic rod without self-intersections

Chun-Chi Lin · Hartmut R. Schwetlick

Received: 24 January 2008 / Accepted: 29 February 2008 / Published online: 10 May 2008 © Springer Science+Business Media, LLC 2008

Abstract In this paper we study the problem on how to find an equilibrium state of a Kirchhoff elastic rod by evolving it in a certain way, called a geometric flow. The elastic energy of rods would decrease during the geometric flow. We show that rods remain smooth during the geometric flow as long as they stay embedded, e.g., self-penetrations do no occur. Furthermore, rods would approach an equilibrium configuration asymptotically if self-penetrations are avoided during the flow.

Keywords Geometric flows \cdot Fourth-order parabolic equations \cdot Kirchhoff elastic rods \cdot Writhe

1 Introduction

The description of the physical behavior of polymers, in particular the bending of long DNA molecules, boosted the study of elastic rod configurations. A simple mathematical model for the dynamics of polymers combines the elastic energy of the rod configuration with the assumption of over-damped dynamics, which leads to a parabolic geometric flow of Kirchhoff elastic rods. The mathematical challenge lies in the fact that the physical model imposes non-trivial boundary conditions to the centerline of the rod, which has to be considered simultaneously with the higher order parabolic flow. In [10] we derived the existence of smooth solutions up to time where inflection

C.-C. Lin (🖂)

H. R. Schwetlick

Department of Mathematics, National Taiwan Normal University, Taipei 116, Taiwan e-mail: chunlin@math.ntnu.edu.tw

Department of Mathematical Sciences, University of Bath, Bath, UK e-mail: schwetlick@maths.bath.ac.uk

points appear on the centerlines of rods. Using the Frenet frame to describe the rod configuration is very appropriate to extract the parabolic structure of the flow. However, the chosen physical boundary condition renders inflection points as singularities in the parametrization. In general inflection points will not constitute physical singularities, so that the assumption of avoiding inflection points would be too restrictive in applications. It is the main goal of this article to replace this previous restriction on inflection points by a more physical condition on the appearance of self-intersections. We resolve this issue by applying Fuller's difference of writhe formula and the so-called Călugăreanu-White-Fuller formula to set up the boundary conditions. The appearance of self-intersections is not rule out a-priorily by our flow. However, we feel that the understanding of the dynamical behavior of non-intersecting rods is a key ingredient to analyze the more realistic scenario, where self-penetrations of the rod are ruled out by an underlying dynamical model which preserves its knot type.

The analytical arguments used in this paper are extending the treatment in [10]. Since we are using Fuller's difference of writhe formula and Călugăreanu–White–Fuller formulae a number of computations get more complicated and technically different from previous approach.

Assume $f: I = \mathbb{R}/\mathbb{Z} \to \mathbb{R}^3$ is the centerline of a closed rod. Let $\gamma = |\partial_x f|$, $ds = \gamma dx$ the arclength element, and $\partial_s = \gamma^{-1}\partial_x$ the arclength differentiation. Denote by $T = \partial_s f$ the unit tangent vector, and $\kappa = \partial_s^2 f$ the curvature vector of f. 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

$$\begin{pmatrix} T'(s) \\ M'_1(s) \\ M'_2(s) \end{pmatrix} = \begin{pmatrix} 0 & m_1(s) & m_2(s) \\ -m_1(s) & 0 & m(s) \\ -m_2(s) & -m(s) & 0 \end{pmatrix} \begin{pmatrix} T(s) \\ M_1(s) \\ M_2(s) \end{pmatrix},$$

with smooth functions $m_1(s)$, $m_2(s)$, and m(s). The Kirchhoff elastic energy \mathcal{E} of an isotropic rod Γ , is defined by

$$\mathcal{E}\left[\Gamma\right] := \int_{I} \left[\alpha \cdot (m_1^2 + m_2^2) + \beta \cdot m^2\right] ds, \tag{1.1}$$

where $\alpha > 0$ and $\beta \ge 0$ 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 (e.g., see [9]). To explain the meaning of m(s), let us introduce the natural frame of the curve discussed by Bishop (see [3] or [9] p. 607 for more details). This orthonormal frame along a given curve f can be uniquely determined by fixing it 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. 1.1 is called *twisting rate*. Thus Eq. 1.1 becomes

$$\mathcal{E}\left[\Gamma\right] = \int_{I} \left[\alpha \cdot |\kappa|^2 + \beta \cdot (\theta')^2\right] ds.$$
(1.2)

Observe that, since the rod configuration Γ is entirely determined by the triple { f(s), $\theta(s)$, $M_1(0)$ }, Eq. 1.2 only depends on f and θ in { f(s), $\theta(s)$, $M_1(0)$ }. This suggests that $M_1(0)$ plays a trivial role in the analysis. Thus we will use the term $(f(s), \theta(s))$ to represent the rod configuration Γ , which is the curve-angle representation.

We define the linking number, twisting number, and writhing number of Γ by

$$Lk[\Gamma] := \frac{1}{4\pi} \int_{s \in I} \int_{\sigma \in I} \frac{\langle f(s) - g_{\epsilon}(\sigma), f'(s) \times g'_{\epsilon}(\sigma) \rangle}{|f(s) - g_{\epsilon}(\sigma)|^3} ds \wedge d\sigma,$$
(1.3)

$$Tw[\Gamma] := \frac{1}{2\pi} \int_{I} \left\langle M'_{1}(s), f'(s) \times M_{1}(s) \right\rangle \, ds = \frac{1}{2\pi} \int_{I} \theta'(s) \, ds, \qquad (1.4)$$

$$Wr[f] := \frac{1}{4\pi} \int_{s \in I} \int_{\sigma \in I} \frac{\langle f(s) - f(\sigma), f'(s) \times f'(\sigma) \rangle}{|f(s) - f(\sigma)|^3} \, ds \wedge d\sigma. \tag{1.5}$$

Here both *s* and σ represent the arclength parametrization 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.

In [10], the end point condition (or the boundary condition) was imposed through the *Călugăreanu–White–Fuller* formula

$$Lk[\Gamma] = Tw[\Gamma] + Wr[f]$$
(1.6)

using the Frenet frame along f to relate local torsion to the total twist Tw[f] of the curve. However in such a formulation, torsion is only well-defined when the curve f has no inflection points. The aim of this paper is to present an alternative approach which is capable of avoiding this restrictive assumption. The idea is to obtain the writhe of the curve by *Fuller's difference of writhe formula*

$$Wr[f_1] - Wr[f_0] = \frac{1}{2\pi} \int_{I} \frac{\langle T_0(x) \times T_1(x), T_0'(x) + T_1'(x) \rangle}{1 + \langle T_0(x), T_1(x) \rangle} \, dx, \qquad (1.7)$$

where f_0 and f_1 are two C^2 smooth curves being close in the C^1 topology (see Lemma 8).

The reader is referred to [4,6,7] and [13] for literature of the Călugăreanu–White– Fuller formula and its generalizations, and to [7] (or [1]) for literature (or rigorous proof, respectively) of Fuller's difference of writhe formulas. Fuller's difference of writhe formula is also of practical significance for the computation of the writhing number of evolving curves. If we denote by N the number of grid points chosen for the discretization the additivity induced from Eq. 1.7 implies a computational effort of order O(N) rather than $O(N^2)$.

We learn from [8] and [9] that when an isotropic elastic rod attains an equilibrium state it must have a constant twisting rate. In the following we want to show that the energy of rods with constant twisting rate can be rewritten as functional solely associated to curves.

Assuming that the twisting rate *m* of an isotropic rod configurations Γ is constant we can combine the definitions of elastic energy (1.2) and twist (1.4) to deduce

$$m = \frac{2\pi}{\mathcal{L}[f]} T w[\Gamma].$$

Here $\mathcal{L}[f] = \int_{I} ds$ is the length of the centerline. Thus, its energy can be written as

$$\mathcal{E}\left[\Gamma\right] = \alpha \int_{I} |\kappa|^2 \, ds + \frac{\beta}{\mathcal{L}[f]} \left(2\pi T w[\Gamma]\right)^2. \tag{1.8}$$

The end point condition for the rod configuration can be related to the twist $Tw[\Gamma]$ by means of topological invariants. Specifically we use the topologically invariant linking number Eq.1.6 to write

$$\frac{\Delta\Omega}{2\pi} := Lk[\Gamma] = Tw[\Gamma] + Wr[f], \qquad (1.9)$$

where we choose $\Delta\Omega$ to prescribe a value of $Lk[\Gamma]$. Note that if f and g_{ϵ} in Eq. 1.3 consist two closed curves the linking number is a (integer-valued) topological quantity, while twisting number and writhing number are not. The reader is referred to Sect. 3 of [12] for more details including the argument that the linking number continues to be an invariant under smooth perturbations of the rod configuration Γ . In fact, in such a case one can set $\frac{\Delta\Omega}{2\pi}$ to be any real number since the material frame does not necessarily have to coincide after one revolution along the curve.

Prescribing the value of the linking number we can compute the twist in the energy as

$$2\pi T w[\Gamma] = \Delta \Omega - 2\pi W r[f],$$

hence, inserting into Eq. 1.8 we obtain

$$\mathcal{E}\left[\Gamma\right] = \mathcal{F}\left[f\right],$$

where

$$\mathcal{F}[f] := \alpha \int_{I} |\kappa|^2 \, ds + \frac{\beta}{\mathcal{L}[f]} \left(\Delta \Omega - 2\pi \cdot Wr[f]\right)^2. \tag{1.10}$$

Deringer

Note that $\mathcal{F}[f]$ is solely defined by the centerline f and the choice of $\Delta\Omega$.

It is worth to mention here that as $\beta = 0$ in Eq. 1.10, this energy functional corresponds to the *Euler–Bernoulli* model of elastic rods. Thus the geometric evolution considered below is also a generalization of the so-called curve-straightening flow (for example, see [5, 11]).

We want to emphasize that the energy (1.8) is the same as the one considered by the authors in [10]. However, there the twist was related to total torsion using the self-linking number of the centerline f of the rod

$$Slk[f] = Tw[f] + Wr[f],$$

where

$$Tw[f] = \frac{1}{2\pi} \int_{I} \theta'(s) \, ds = \frac{1}{2\pi} \int_{I} \tau \, ds.$$

In the preceding approach we eliminated writhe by prescribing the difference of the two invariants, i.e.,

$$\frac{\Delta\Psi}{2\pi} := Lk[\Gamma] - Slk[f] = Tw[\Gamma] - Tw[f],$$

and hence

$$2\pi T w[\Gamma] = \Delta \Psi + 2\pi T w[f] = \Delta \Psi + \int_{I} \tau \, ds.$$

Comparing the two formulae we deduce that in order to describe the same geometric evolution of an initial curve f_0 under both flows we need to ensure that the twist of the rod configuration has to relate to the same topological invariants. This implies an identity relating the prescription values $\Delta\Omega$ and $\Delta\Psi$,

$$\Delta\Omega - \Delta\Psi = Slk[f] = Slk[f_0] = Tw[f_0] + Wr[f_0]. \tag{1.11}$$

Writing the rod energy as an energy of its centerline yields the following useful identification: Similar to the strategy in [10] one can prove that finding equilibrium rod configurations for $\mathcal{E}[\Gamma]$ is equivalent to finding equilibrium centerline curves for $\mathcal{F}[f]$. In more detail we have the equivalence

Proposition 1 Let $f : I = \mathbb{R}/\mathbb{Z} \to \mathbb{R}^3$ be the centerline of a closed rod Γ . Let $\mu > 0$ be a constant, and define

$$\mathcal{E}_{\mu} [\Gamma] := \mathcal{E} [\Gamma] + \mu \mathcal{L}[f],$$

$$\mathcal{F}_{\mu} [f] := \mathcal{F} [f] + \mu \mathcal{L}[f].$$

Then,

- (i) subject to variations of the end point condition $\Delta\Omega$ in Eq. 1.9, Γ is an equilibrium of the elastic energy \mathcal{E}_{μ} if and only if f is a critical point of the geometric functional \mathcal{F}_{μ} and the twisting rate is equal to the constant $\frac{\Delta\Omega 2\pi \cdot Wr[f]}{\mathcal{L}[f]}$ along f.
- (ii) subject to length-preserving variations of the end point condition $\Delta\Omega$ in Eq. 1.9, Γ is an equilibrium of the elastic energy \mathcal{E} if and only if f is a critical point of the geometric functional \mathcal{F} and the twisting rate is equal to the constant $\frac{\Delta\Omega - 2\pi \cdot Wr[f]}{\mathcal{L}[f]}$ along f.

Due to Proposition 1 we are able to reformulate the variational problem for equilibrium elastic rods into a variational problem for geometric curves describing their centerline.

In this article we are going to assume over-damped relaxation dynamics, that is we work on the L^2 gradient flow of \mathcal{F}_{μ} .

In Sect. 3, cf. Lemma 10, we show that this flow can be written in the form

$$\partial_t f = 2\alpha \cdot \left(-\nabla_s^2 \kappa - \frac{|\kappa|^2}{2} \kappa \right) + \lambda_2 (t) \cdot \nabla_s (T \times \kappa) + \lambda_1 \cdot \kappa.$$
 (1.12)

Here the covariant derivative $\nabla_s \eta$ denotes the normal component of $\partial_s \eta$,

$$\lambda_2(t) = \frac{2\beta}{\mathcal{L}[f]} \left(\Delta\Omega - 2\pi \cdot Wr[f]\right). \tag{1.13}$$

Furthermore, in the case of the length-preserving flow, we have

$$\lambda_{1}(t) = \frac{2\alpha \int \langle \kappa, \nabla_{s}^{2} \kappa + \frac{|\kappa|^{2}}{2} \kappa \rangle ds - \frac{2\beta}{\mathcal{L}[f]} \left(\Delta \Omega - 2\pi \cdot Wr[f]\right) \int_{I} \langle \kappa, \nabla_{s} (T \times \kappa) \rangle ds}{\int_{I} |\kappa|^{2} ds}.$$
(1.14)

If we drop the condition of length-preservation we can adopt the simpler relation $\lambda_1 = \mu$.

The main results of this article regard the long time existence of solutions of the flow with or without length-preservation.

Theorem 1 For any real numbers $\mu \in [0, \infty)$ and $\Delta\Omega$ and any smooth initial closed curve f_0 there exists a smooth solution to the L^2 -gradient flow in Eq. 1.12, until the appearance of self-intersection. If $\mu > 0$ and assuming no self-intersection during the flow, the curves subconverge to f_{∞} , an equilibrium of the energy functional \mathcal{F}_{μ} after reparametrization by arclength and translation.

Theorem 2 For any real numbers $\Delta\Omega$ and any smooth initial closed curve f_0 there exists a smooth solution to the L^2 -gradient flow in Eq. 1.12, subject to fixed length,

until the appearance of self-intersection. With the assumption of no self-intersection during the flow, the curves subconverge to f_{∞} , an equilibrium of the energy functional \mathcal{F} after reparametrization by arclength and translation.

The article is arranged as follows. To present a short and self-consistent exposition we introduce in Sect. 2 a bit of notation and collect some results from [5,10], and [1]. Section 3 contains the proofs of the main results. Finally, we present in Sect. 4 a numerical experiment to show that the new approach behaves satisfactory when points of vanishing curvature arise during the evolution of the flow.

2 Preliminaries and notations

We summarize for the reader the following identities and estimates from [5].

Lemma 1 ([5, Lemma 2.1]) Suppose ϕ is any normal field along f and $f : [0, \epsilon) \times I \to \mathbb{R}^n$ is a time dependent curve satisfying $\partial_t f = V + \varphi T$, where V is the normal velocity and $\varphi = \langle T, \partial_t f \rangle$. Then the following formulae hold.

$$\nabla_s \phi = \partial_s \phi + \langle \phi, \kappa \rangle T, \tag{2.1}$$

$$\partial_t \left(ds \right) = \left(\partial_s \varphi - \langle \kappa, V \rangle \right) ds, \tag{2.2}$$

$$\partial_t \partial_s - \partial_s \partial_t = (\langle \kappa, V \rangle - \partial_s \varphi) \,\partial_s, \tag{2.3}$$

$$\partial_t T = \nabla_s V + \varphi \cdot \kappa, \tag{2.4}$$

$$\partial_t \phi = \nabla_t \phi - \langle \nabla_s V + \varphi \kappa, \phi \rangle T, \qquad (2.5)$$

$$\nabla_t \kappa = \nabla_s^2 V + \langle \kappa, V \rangle \kappa + \varphi \cdot \nabla_s \kappa, \qquad (2.6)$$

$$(\nabla_t \nabla_s - \nabla_s \nabla_t) \phi = (\langle \kappa, V \rangle - \partial_s \varphi) \nabla_s \phi + \langle \kappa, \phi \rangle \nabla_s V - \langle \nabla_s V, \phi \rangle \cdot \kappa.$$
(2.7)

Lemma 2 ([5, Lemma 2.2]) Suppose $f : [0, t_1) \times I \to \mathbb{R}^n$ moves in a normal direction with velocity $\partial_t f = V$, ϕ is a normal vector field along f, and $\nabla_t \phi + \nabla_s^4 \phi = Y$. Then

$$\frac{d}{dt}\frac{1}{2}\int_{I}|\phi|^{2}\,ds + \int_{I}\left|\nabla_{s}^{2}\phi\right|^{2}\,ds = \int_{I}\langle Y,\phi\rangle\,ds - \frac{1}{2}\int_{I}|\phi|^{2}\,\langle\kappa,V\rangle\,ds.$$
 (2.8)

Furthermore, $\psi = \nabla_s \phi$ satisfies the equation

$$\nabla_t \psi + \nabla_s^4 \psi = \nabla_s Y + \langle \kappa, \phi \rangle \nabla_s V - \langle \nabla_s V, \phi \rangle \kappa + \langle \kappa, V \rangle \psi.$$
(2.9)

For normal vector fields ϕ_1, \ldots, ϕ_k along f, we denote by $\phi_1 * * * \phi_k$ a term of the type

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

where i_1, \ldots, i_k is any permutation of $1, \ldots, k$. Slightly more generally, we allow some of the ϕ_i to be functions, in which case the *-product reduces to multiplication.

For a normal vector field ϕ along f, we denote by $P_{\nu}^{\mu}(\phi)$ any linear combination of terms of the type $\nabla_s^{i_1}\phi * \cdots * \nabla_s^{i_\nu}\phi$ with universal constant coefficients, where $\mu = i_1 + \cdots + i_{\nu}$ is the total number of derivatives. Notice that the following formulae hold:

$$\begin{cases} \nabla_{s} \left(P_{b}^{a}(\phi) * P_{d}^{c}(\phi) \right) = \nabla_{s} P_{b}^{a}(\phi) * P_{d}^{c}(\phi) + P_{b}^{a}(\phi) * \nabla_{s} P_{d}^{c}(\phi) ,\\ P_{b}^{a}(\phi) * P_{d}^{c}(\phi) = P_{b+d}^{a+c}(\phi) , \nabla_{s} P_{d}^{c}(\phi) = P_{d}^{c+1}(\phi) . \end{cases}$$
(2.10)

Similarly, we denote by $Q_{\nu}^{\mu}(\kappa)$ the linear combination of $\partial_{s}^{i_{1}}\kappa * * * \partial_{s}^{i_{\nu}}\kappa$, where $i_{1} + \cdots + i_{\nu} = \mu$.

The following lemma states the important interpolation inequality for higher order curvature functionals.

Lemma 3 ([5, Proposition 2.5]) For any term $P_v^{\mu}(\kappa)$ with $v \ge 2$ which contains only derivatives of κ of order at most k - 1, we have

$$\int_{I} |P_{\nu}^{\mu}(\kappa)| \, ds \le c \mathcal{L}[f]^{1-\mu-\nu} \, \|\kappa\|_{2}^{\nu-\gamma} \, \|\kappa\|_{k,2}^{\gamma}, \qquad (2.11)$$

where $\gamma = \left(\mu + \frac{1}{2}\nu - 1\right)/k$, $c = c (n, k, \mu, \nu)$, and

$$\|\kappa\|_{k,p} := \sum_{i=0}^{k} \left\|\nabla_{s}^{i}\kappa\right\|_{p}, \left\|\nabla_{s}^{i}\kappa\right\|_{p} := \mathcal{L}\left[f\right]^{i+1-1/p} \left(\int_{I} \left|\nabla_{s}^{i}\kappa\right|^{p} ds\right)^{1/p}.$$

Moreover, if $\mu + \frac{1}{2}\nu < 2k + 1$ *, then* $\gamma < 2$ *and we have for any* $\varepsilon > 0$ *,*

$$\int_{I} \left| P_{\nu}^{\mu}(\kappa) \right| ds \leq \varepsilon \int_{I} |\nabla_{s}^{k} \kappa|^{2} ds + c \varepsilon^{\frac{-\gamma}{2-\gamma}} \left(\int_{I} |\kappa|^{2} ds \right)^{\frac{\nu-\gamma}{2-\gamma}} + c \left(\int_{I} |\kappa|^{2} ds \right)^{\mu+\nu-1} (2.12)$$

Lemma 4 ([5, Lemma 2.6]) We have the identities

$$\nabla_s \kappa - \partial_s \kappa = |\kappa|^2 T, \qquad (2.13)$$

$$\nabla_s^m \kappa - \partial_s^m \kappa = \sum_{i=1}^{\left[\frac{m}{2}\right]} \mathcal{Q}_{2i+1}^{m-2i}(\kappa) + \sum_{i=1}^{\left[\frac{m+1}{2}\right]} \mathcal{Q}_{2i}^{m+1-2i}(\kappa) T.$$
(2.14)

Lemma 5 ([5, Lemma 2.7]) Assume the bounds $\|\kappa\|_{L^2} \leq \Lambda_0$ and $\|\nabla_s^m \kappa\|_{L^1} \leq \Lambda_m$ for $m \geq 1$. Then for any $m \geq 1$ one has

$$\left\|\partial_{s}^{m-1}\kappa\right\|_{L^{\infty}}+\left\|\partial_{s}^{m}\kappa\right\|_{L^{1}}\leq c_{m}\left(\Lambda_{0},\ldots,\Lambda_{m}\right).$$
(2.15)

In [10] the authors proved the following extension to terms related to torsion.

Lemma 6 ([10, Lemma 3.2]) For $m \ge 2$, we have the formula,

$$\begin{split} \nabla_s^m(T\times\kappa) &= T\times\nabla_s^m\kappa + \sum_{a_1,b_1,c_1,d_1} \left[P_{b_1}^{a_1}(\kappa) \times P_{d_1}^{c_1}(\kappa) \right]^{\perp} \\ &+ \sum_{i=1,2} \sum_{a_2^{(i)},b_2^{(i)},c_2^{(i)},d_2^{(i)},e_2^{(i)},f_2^{(i)}} \left[\left(P_{b_2^i}^{a_2^i}(\kappa) \times P_{d_2^i}^{c_2^i}(\kappa) \right) * P_{f_2^i}^{e_2^i}(\kappa) \right]^{\perp} \\ &+ \sum_{i=1,2} \sum_{a_3^{(i)},b_3^{(i)},c_3^{(i)},d_3^{(i)}} \left(\left(T \times P_{b_3^{(i)}}^{a_3^{(i)}}(\kappa) \right) * P_{d_3^{(i)}}^{c_3^{(i)}}(\kappa) \right), \end{split}$$

where the sums are taken such that $(a_1 + c_1) + (b_1 + d_1)/2 = m$, $(a_2^{(i)} + c_2^{(i)} + e_2^{(i)}) + (b_2^{(i)} + d_2^{(i)} + d_2^{(i)})/2 = m - i$, and $(a_3^{(i)} + c_3^{(i)}) + (b_3^{(i)} + d_3^{(i)})/2 = m - i + 1/2$ for $i \in \{1, 2\}$.

Lemma 7 ([10, Lemma 3.3]) Let σ and $\lambda_{1,2} \in \mathbb{R}$. Suppose

$$\partial_t f = -\nabla_s^2 \kappa + \sigma |\kappa|^2 \kappa + \lambda_1 \kappa + \lambda_2 \nabla_s (T \times \kappa) \,.$$

Then the derivatives of the curvature $\phi_m = \nabla_s^m \kappa, m \ge 0$, satisfy

$$\nabla_{t}\phi_{m} + \nabla_{s}^{4}\phi_{m}$$

$$= P_{3}^{m+2}(\kappa) + \sigma \cdot \left(P_{3}^{m+2}(\kappa) + P_{5}^{m}(\kappa)\right) + \lambda_{1} \cdot \left(\nabla_{s}^{m+2}\kappa + P_{3}^{m}(\kappa)\right)$$

$$+ \lambda_{2} \cdot \left(\nabla_{s}^{m+3}(T \times \kappa) + \nabla_{s}^{m+1}(T \times \kappa) * P_{2}^{0}(\kappa) + \dots + \nabla_{s}^{1}(T \times \kappa) * P_{2}^{m}(\kappa)\right).$$
(2.16)

The statement is still true when $\lambda_i = \lambda_i$ (*t*) *depends on time.*

From [1] we collect the relevant results concerning the writhe of a curve. The first is the difference of writhe formula which implies the second result on the derivative of writhe as well.

Lemma 8 ([1, Proposition 5]) Let $\mathbb{X}_0, \mathbb{X}_1 : [0, 1] \to \mathbb{R}^3$ be two closed non selfintersecting space curves of class C^2 with regular parametrization. Let $F : [0, 1] \times$ $[0, 1] \to \mathbb{R}^3, (x, \lambda) \to \mathbb{X}_{\lambda}(x)$ be a C^0 deformation of \mathbb{X}_0 into \mathbb{X}_1 such that \mathbb{X}_{λ} are non self-intersecting space curves of class C^1 and the unit tangent $T_{\lambda}(x)$ changes continuously in λ . If $| \measuredangle (T_1(x), T_{\lambda}(x)) | < \pi$ for all $(x, \lambda) \in [0, 1] \times [0, 1]$, then

$$Wr[\mathbb{X}_{1}] - Wr[\mathbb{X}_{0}] = \frac{1}{2\pi} \int_{I} \frac{\langle T_{0}(x) \times T_{1}(x), T_{0}'(x) + T_{1}'(x) \rangle}{1 + \langle T_{0}(x), T_{1}(x) \rangle} dx.$$

🖄 Springer

Lemma 9 ([1, Corollary 8]) If $F : [0, 1] \times [0, 1] \rightarrow \mathbb{R}^3$, $(x, \lambda) \rightarrow \mathbb{X}_{\lambda}(x)$ is of class C^2 , then

$$\frac{d}{d\lambda}Wr[\mathbb{X}_{\lambda}] = -\frac{1}{2\pi} \int_{0}^{1} \left\langle \frac{\partial}{\partial\lambda}T(x,\lambda) \times T(x,\lambda), \frac{\partial}{\partial x}T(x,\lambda) \right\rangle dx, \qquad (2.17)$$

where $T(x, \lambda) = \frac{d}{dx} \mathbb{X}_{\lambda}(x) / |\frac{d}{dx} \mathbb{X}_{\lambda}(x)|$ is the unit tangent vector field along \mathbb{X}_{λ} .

3 Proof of the main results

Lemma 10 Suppose $f = f(\varepsilon, x), f: (-1, 1) \times I \to \mathbb{R}^3$, is a one-parameter smooth family of closed curves. Let

$$\mathcal{K}[f] := \frac{1}{2} \int_{I} |\kappa|^2 ds.$$

Then, one has the following deformation formulae:

$$\begin{split} & \frac{d}{d\varepsilon} \mathcal{L}[f] \lfloor_{\varepsilon=0} = -\int_{I} \langle \kappa, \partial_{\varepsilon} f \rangle \lfloor_{\varepsilon=0} ds, \\ & \frac{d}{d\varepsilon} \mathcal{K}[f] \lfloor_{\varepsilon=0} = \int_{I} \langle \nabla_{s}^{2} \kappa + \frac{|\kappa|^{2}}{2} \kappa, \partial_{\varepsilon} f \rangle \lfloor_{\varepsilon=0} ds, \\ & \frac{d}{d\varepsilon} Wr[f] = \frac{1}{2\pi} \int_{I} \langle \partial_{\varepsilon} f, \partial_{s} (T \times \kappa) \rangle ds = \frac{-1}{2\pi} \int_{I} \langle \partial_{\varepsilon} T, T \times \kappa \rangle ds. \end{split}$$

Furthermore, the Euler–Lagrange equation of \mathcal{F}_{μ} (or \mathcal{F} subject to variations of fixed length) is

$$2\alpha \cdot (-\nabla_s^2 \kappa - \frac{|\kappa|^2}{2}\kappa) + \lambda_2(t) \cdot \nabla_s(T \times \kappa) + \lambda_1 \cdot \kappa = 0, \qquad (3.1)$$

where λ_2 is defined in Eq. 1.13, and λ_1 is equal to the positive constant μ (or alternatively defined in Eq. 1.14).

Proof The first two formulae are quoted from [5] (or Lemma 3.1 of [10]).

The last one is derived from Fuller's difference of writhe formula. In other words, by Eq. 2.17,

$$\frac{d}{d\varepsilon} Wr[f_{\varepsilon}] = \frac{-1}{2\pi} \int_{I} \langle \partial_{\varepsilon} T(\varepsilon, x) \times T(\varepsilon, x), \partial_{x} T(\varepsilon, x) \rangle dx$$

$$= \frac{-1}{2\pi} \int_{I} \langle \partial_{\varepsilon} T, T \times \partial_{s} T \rangle ds = \frac{1}{2\pi} \int_{I} \langle \partial_{\varepsilon} \partial_{s} f, \kappa \times T \rangle ds$$
(by Eq. 2.3)
$$= \frac{1}{2\pi} \int_{I} \langle \kappa \times T, \partial_{s} \partial_{\varepsilon} f + \langle \kappa, \partial_{\varepsilon} f \rangle T \rangle ds$$

$$= \frac{1}{2\pi} \int_{I} \langle \kappa \times T, \partial_{s} \partial_{\varepsilon} f \rangle ds = \frac{1}{2\pi} \int_{I} \langle \partial_{s} (T \times \kappa), \partial_{\varepsilon} f \rangle ds.$$

Finally, Eq. (3.1) is a direct consequence of the deformation formulae.

Proof of Proposition 1 The proof parallels the proof of Theorem 1.1 in [10], except that the deformation formula of total torsion therein is replaced by the deformation formula of writhe in Lemma 10 above. \Box

The proofs of Theorem 1 and 2 are motivated by the arguments in [5]. The short time existence is argued the same as before (see [5] for a brief sketch or [11] for more details). We only emphasize here that the terms involving writhe (i.e., terms involving λ_1 and λ_2) in standard linearization argument for short-time existence is still a compact operator between the relevant parabolic Hölder spaces. In fact λ_1 and λ_2 in this article are the same as the λ_1 and λ_2 in [10] respectively when there is no flat point. We thus skip it here and focus on the long time existence and asymptotic behavior.

To prove global bounds we wish to estimate higher Sobolev norms of the curvature. Their evolution is given by

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

Therefore we arrive at

$$\frac{d}{dt}\frac{1}{2}\int_{I} |\nabla_{s}^{m}\kappa|^{2} ds + \int_{I} |\nabla_{s}^{m+2}\kappa|^{2} ds = \text{terms of lesser order.}$$

It will be not necessary to compute the error terms explicitly. It is sufficient to keep track of their scaling. In other words, we have to know the order of the derivatives involved.

Proof of Theorem 1 By Eqs. 2.8, 2.17, and 1.12, we have

$$\frac{d}{dt}\frac{1}{2}\int_{I}|\nabla_{s}^{m}\kappa|^{2}ds+\int_{I}|\nabla_{s}^{m+2}\kappa|^{2}ds+\lambda_{1}\int_{I}|\nabla_{s}^{m+1}\kappa|^{2}ds$$

🖄 Springer

$$= \lambda_1 \int_{I} \langle \nabla_s^m \kappa, P_3^m(\kappa) \rangle ds + \int_{I} \langle \nabla_s^m \kappa, P_3^{m+2}(\kappa) + P_5^m(\kappa) \rangle ds$$
$$+ \lambda_2(t) \int_{I} \langle \nabla_s^m \kappa, \nabla_s^{m+3}(T \times \kappa) + \nabla_s^{m+1}(T \times \kappa) * P_2^0(\kappa)$$
$$+ \dots + \nabla_s^1(T \times \kappa) * P_2^m(\kappa) \rangle ds.$$
(3.2)

From Lemma 10, one can verify

$$\frac{d}{dt}\mathcal{F}_{\mu}[f] = 2\alpha \frac{d}{dt}\mathcal{K}[f] - \frac{4\pi\beta}{\mathcal{L}[f]} (\Delta\Omega - 2\pi \cdot Wr[f]) \frac{d}{dt}Wr[f] + \lambda_{1} \cdot \frac{d}{dt}\mathcal{L}[f]$$

$$= \int_{I} \langle 2\alpha (\nabla_{s}^{2}\kappa + \frac{|\kappa|^{2}}{2}\kappa) - \lambda_{2}(t) \nabla_{s}(T \times \kappa) - \lambda_{1}\kappa, \partial_{t}f \rangle ds$$

$$= -\int_{I} |2\alpha (-\nabla_{s}^{2}\kappa - \frac{|\kappa|^{2}}{2}\kappa) + \lambda_{2}(t) \nabla_{s}(T \times \kappa) + \lambda_{1}\kappa|^{2}ds$$

$$\leq 0.$$
(3.3)

Thus, we yield that $\mathcal{F}_{\mu}[f]$ is nonincreasing as t increases. Hence

$$\frac{\beta}{\mathcal{L}[f]} \left(\Delta\Omega - 2\pi \cdot Wr[f]\right)^2 \le \mathcal{F}_{\mu}[f] \le \mathcal{F}_{\mu}[f_0]. \tag{3.4}$$

Note that by Fenchel-Fary inequality of closed space curves, we have

$$\int_{I} |\kappa| ds \ge 2\pi,\tag{3.5}$$

and then by applying Hölder's inequality, we have

$$(2\pi)^2 \le \mathcal{L}[f] \cdot \int_{I} |\kappa|^2 ds.$$
(3.6)

From Eq. 3.3 and the definition of \mathcal{F}_{μ} , we have

$$\mu \cdot \mathcal{L}[f] \le \mathcal{F}_{\mu}[f] \le \mathcal{F}_{\mu}[f_0]. \tag{3.7}$$

Now by combining Eqs. 3.6 and 3.7, we derive uniformly upper and lower bounds of length $\mathcal{L}[f]$,

$$\frac{\alpha \cdot (2\pi)^2}{\mathcal{F}_{\mu}[f_0]} \le \mathcal{L}[f] \le \frac{\mathcal{F}_{\mu}[f_0]}{\mu}.$$
(3.8)

Deringer

Note that combining Eqs. 3.6 and 3.8 also gives a uniformly positive lower bound of $\|\kappa\|_{L^2}$, i.e.,

$$\int_{I} |\kappa|^2 ds \ge \frac{\mu \cdot (2\pi)^2}{\mathcal{F}_{\mu} [f_0]}$$

By the definition of λ_2 and Eqs. 3.7, 3.8 and 3.4,

$$|\lambda_{2}(t)| \leq 2\sqrt{\frac{\beta \cdot \mathcal{F}_{\mu}[f]}{\mathcal{L}[f]}} \leq \frac{\sqrt{\beta}}{\pi \cdot \sqrt{\alpha}} \mathcal{F}_{\mu}[f_{0}] \leq C\left(\left\|\partial_{s}^{2} f_{0}\right\|_{L^{2}}, \Delta\Omega, \alpha, \beta, \mu, L_{0}\right).$$
(3.9)

Furthermore, by Eqs. 1.10 and 3.3,

$$\|\kappa\|_{L^2}^2 \le C\left(\left\|\partial_s^2 f_0\right\|_{L^2}, \Delta\Omega, \alpha, \beta, \mu, L_0\right).$$
(3.10)

Moreover, by Eq. 2.2, we have

$$\frac{d}{dt}\mathcal{L}[f] + \frac{1}{2}\int_{I} |\nabla_{s}\kappa|^{2}ds < C\left(\left\|\partial_{s}^{2}f_{0}\right\|_{L^{2}}, \Delta\Omega, \alpha, \beta, \mu, L_{0}\right).$$
(3.11)

By applying Eqs. 2.12, 3.9, 3.10, and Lemma 6, the right hand side of Eq. 3.2 satisfies the inequality,

$$R.H.S. \text{ of Eq. } 3.2 \le \varepsilon \int_{I} \left| \nabla_{s}^{m+2} \kappa \right|^{2} ds + C \left(\left\| \partial_{s}^{2} f_{0} \right\|_{L^{2}}, \Delta \Omega, \alpha, \beta, \mu, L_{0}, m, \varepsilon \right).$$

$$(3.12)$$

Since $\lambda_1 = \mu > 0$ in Eq. 3.2 and by combining with Eq. 3.12, we have

$$\frac{d}{dt} \int_{I} |\nabla_{s}^{m} \kappa|^{2} ds + \int_{I} |\nabla_{s}^{m+2} \kappa|^{2} ds \leq C \left(\left\| \partial_{s}^{2} f_{0} \right\|_{L^{2}}, \Delta \Omega, \alpha, \beta, \mu, L_{0}, m \right). (3.13)$$

Note that by Eq. 2.1,

$$\begin{aligned} |\partial_s^2 \nabla_s^m \kappa|^2 &= |\nabla_s^{m+2} \kappa|^2 + \langle \kappa, \nabla_s^m \kappa \rangle |\kappa|^2 - 2 \langle \kappa, \nabla_s^{m+2} \kappa \rangle \langle \kappa, \nabla_s^m \kappa \rangle \\ &+ 4 \langle \kappa, \nabla_s^{m+1} \kappa \rangle^2 + 4 \langle \kappa, \nabla_s^{m+1} \kappa \rangle \langle \nabla_s \kappa, \nabla_s^m \kappa \rangle + \langle \nabla_s \kappa, \nabla_s^m \kappa \rangle^2 \,, \end{aligned}$$

and

$$|\partial_s \nabla_s^m \kappa|^2 = |\nabla_s^{m+1} \kappa|^2 + \langle \kappa, \nabla_s^m \kappa \rangle^2.$$

Deringer

Then, by applying Eq. 2.12 and Poincare inequality, we have

$$\begin{split} \int_{I} |\nabla_{s}^{m+2}\kappa|^{2} ds &\geq \int_{I} |\partial_{s}^{2} \nabla_{s}^{m}\kappa|^{2} ds - \varepsilon \int_{I} |\nabla_{s}^{m+2}\kappa|^{2} ds - C\left(\varepsilon, \left\|\partial_{s}^{2} f\right\|_{L^{2}}\right) \\ &\geq 2c_{0} \int_{I} |\partial_{s} \nabla_{s}^{m}\kappa|^{2} ds - \varepsilon \int_{I} |\nabla_{s}^{m+2}\kappa|^{2} ds - C\left(\varepsilon, \left\|\partial_{s}^{2} f\right\|_{L^{2}}\right) \\ &\geq 2c_{0} \int_{I} |\nabla_{s}^{m+1}\kappa|^{2} ds - 2\varepsilon \int_{I} |\nabla_{s}^{m+2}\kappa|^{2} ds - 2C\left(\varepsilon, \left\|\partial_{s}^{2} f\right\|_{L^{2}}\right). \end{split}$$

By choosing sufficiently small $\varepsilon > 0$,

$$\int_{I} |\nabla_s^{m+2}\kappa|^2 ds \ge c_0 \int_{I} |\nabla_s^{m+1}\kappa|^2 ds - C\left(\left\|\partial_s^2 f\right\|_{L^2}\right),\tag{3.14}$$

for some $c_0 > 0$. Thus by Eqs. 3.14, 3.13 and 3.10, we have

$$\frac{d}{dt} \int_{I} |\nabla_{s}^{m} \kappa|^{2} ds + c_{0}^{2} \int_{I} |\nabla_{s}^{m} \kappa|^{2} ds \leq C \left(\left\| \partial_{s}^{2} f_{0} \right\|_{L^{2}}, \Delta \Omega, \alpha, \beta, \mu, L_{0}, m \right).$$

Therefore, this differential inequality implies

$$\left\|\nabla_{s}^{m}\kappa\right\|_{L^{2}}^{2}(t) \leq \left\|\nabla_{s}^{m}\kappa\right\|_{L^{2}}^{2}(0) + C\left(\left\|\partial_{s}^{2}f_{0}\right\|_{L^{2}}, \Delta\Omega, \alpha, \beta, \mu, L_{0}, m\right), \quad (3.15)$$

for all $m \ge 0$. Notice that one has the estimate,

$$\left\|\partial_s^{m-1}\kappa\right\|_{L^{\infty}} \le c \cdot \left\|\partial_s^m\kappa\right\|_{L^1}, \quad \forall \ m \ge 1.$$
(3.16)

Now, by an induction argument on m and using Lemma 4, 5, Eqs. 3.15, 3.16, 3.8 and Hölder's inequality, we derive the inequalities,

$$\left\|\nabla_{s}^{m}\kappa\right\|_{L^{\infty}}+\left\|\partial_{s}^{m}\kappa\right\|_{L^{\infty}}\leq C\left(\left\|\partial_{s}^{2}f_{0}\right\|_{L^{2}},\Delta\Omega,\alpha,\beta,\mu,L_{0},m\right),\quad\forall m\geq0.$$
(3.17)

This gives uniform bound for $\|\partial_s^m \kappa\|_{L^{\infty}}$ for each *m*.

On the asymptotic behavior of the flow, we choose a subsequence of curves $f(t, \cdot)$ which converges smoothly to a curve f_{∞} , after reparametrization of arclength and translations. Lemma 7 and Eq. 3.17 imply

$$\left\|\nabla_{t}\left(\nabla_{s}^{m}\kappa\right)\right\|_{L^{\infty}} \leq C\left(\left\|\partial_{s}^{2}f_{0}\right\|_{L^{2}}, \Delta\Omega, \alpha, \beta, \mu, L_{0}, m\right), \quad \forall \ m \geq 0.$$
(3.18)

From Eq. 3.17 and 3.18, one sees that for $u(t) := \int |\partial_t f|^2 ds$, the inequality

$$|u'(t)| \leq C\left(\left\|\partial_s^2 f_0\right\|_{L^2}, \Delta\Omega, \alpha, \beta, \mu, L_0\right),$$

holds. On the other hand, the energy identity, Eq. 3.23, implies $u(t) \in L^1([0, \infty))$. Therefore, $u(t) \to 0$ as $t \to \infty$. In other words, f_∞ is independent of t and thus, by Eq.1.12, is an equilibrium of \mathcal{F} . Now, by Proposition 1, the proof is finished.

Proof of Theorem 2 One again works with Eq. 3.2 to obtain integral estimates. The main difference is that $\lambda_1 = \lambda_1(t)$, given by Eq. 1.14, is time dependent and thus might not stay positive. In this situation we need to use different trick from the argument in the proof of Theorem 1 to estimate the terms involving $\lambda_1(t)$ in Eq. 3.2.

We first note that, by applying Eq. 3.5 and Hölder's inequality, we have a uniformly positive lower bound of $\|\kappa\|_{L^2}^2$, i.e.,

$$\|\kappa\|_{L^2}^2 \ge \frac{4\pi^2}{L_0} > 0. \tag{3.19}$$

Then by the definition of λ_2 and Eq. 3.4, we have

$$|\lambda_{2}(t)| \leq 2\sqrt{\frac{\beta \cdot \mathcal{F}_{\mu}[f_{0}]}{L_{0}}} \leq C\left(\left\|\partial_{s}^{2}f_{0}\right\|_{L^{2}}, \Delta\Omega, \alpha, \beta, \mu, L_{0}\right).$$
(3.20)

Thus by Eqs. 1.14, 3.19 and 2.11, we have

$$\begin{aligned} &|\lambda_{1}(t)| \\ &\leq C\left(\left\|\partial_{s}^{2}f_{0}\right\|_{L^{2}}, \Delta\Omega, \alpha, \beta, L_{0}\right) \cdot \int_{I} \left(\left|P_{2}^{2}(\kappa)\right| + \left|P_{4}^{0}(\kappa)\right| + \left|P_{2}^{1}(\kappa)\right|\right) ds \\ &\leq C \cdot \left(\left\|\kappa\right\|_{m+2,2}^{\frac{2}{m+2}} \cdot \left\|\kappa\right\|_{2}^{2-\frac{2}{m+2}} + \left\|\kappa\right\|_{m+2,2}^{\frac{1}{m+2}} \cdot \left\|\kappa\right\|_{2}^{4-\frac{2}{m+2}} + \left\|\kappa\right\|_{m+2,2}^{\frac{1}{m+2}} \cdot \left\|\kappa\right\|_{2}^{2-\frac{1}{m+2}}\right). \end{aligned}$$

On the other hand, by applying Eq. 2.11, we have

$$\left| \int_{I} \left\langle \nabla_{s}^{m} \kappa, P_{3}^{m} \left(\kappa \right) \right\rangle ds \right| \leq \int_{I} \left| P_{4}^{2m} \left(\kappa \right) \right| ds \leq c \left(m, \mathcal{L}\left[f \right] \right) \cdot \left\| \kappa \right\|_{m+2,2}^{2-\frac{3}{m+2}} \cdot \left\| \kappa \right\|_{2}^{2+\frac{3}{m+2}}$$

Therefore,

$$\begin{aligned} |\lambda_{1}(t) \int_{I} \langle \nabla_{s}^{m} \kappa, P_{3}^{m}(\kappa) \rangle ds | \\ &\leq C \left(\left\| \partial_{s}^{2} f_{0} \right\|_{L^{2}}, \Delta\Omega, \alpha, \beta, L_{0}, m \right) \cdot \left(\left\| \kappa \right\|_{m+2,2}^{2-\frac{1}{m+2}} + \left\| \kappa \right\|_{m+2,2}^{2-\frac{2}{m+2}} \right) \\ &\leq \varepsilon \int_{I} \left| \nabla_{s}^{m+2} \kappa \right|^{2} ds + C \left(\left\| \partial_{s}^{2} f_{0} \right\|_{L^{2}}, \Delta\Omega, \alpha, \beta, \mu, L_{0}, m, \varepsilon \right), \end{aligned}$$
(3.21)

🖉 Springer

where the last inequality comes form applying Young's inequality and applying

$$\|\kappa\|_{k,2}^{2} \leq c(k) \cdot \left(\left\| \nabla_{s}^{k} \kappa \right\|_{2}^{2} + \|\kappa\|_{2}^{2} \right).$$
(3.22)

Notice that Eq. 3.22 comes from a standard interpolation inequality (see [2]).

Now we only need to estimate $\lambda_1(t) \cdot \int_I |\nabla_s^{m+1}\kappa|^2 ds$, which is the borderline case as applying the interpolation argument. In fact the interpolation argument fails here. Fortunately the scaling argument, which we learn from [5], still works here. In other words, as we rescale f by $f^{(\rho)} = p + \rho (f - p)$, it is easy to very that

$$\mathcal{K}\left[f^{(\rho)}\right] = \frac{1}{\rho}\mathcal{K}\left[f\right], Wr\left[f^{(\rho)}\right] = Wr\left[f\right], \text{and}\mathcal{L}\left[f^{(\rho)}\right] = \rho\mathcal{L}\left[f\right].$$

By taking the derivative of $\mathcal{F}[f^{(\rho)}]$ at $\rho = 1$ and using Eq. 1.12, we have

$$2\alpha \mathcal{K}[f] - \lambda_1 \mathcal{L}[f] = -\frac{d}{d\rho} \mathcal{F}\left[f^{(\rho)}\right] \downarrow_{\rho=1} = \int_I \langle \partial_t f, f - p \rangle \, ds.$$

By choosing p = p(t) to be $p = L^{-1} \int_{I} f ds$, we have the inequality,

$$-\lambda_1(t) \le L^{1/2} \|\partial_t f\|_{L^2}.$$

Then the energy identity,

$$\frac{d}{dt}\mathcal{F}[f_t] = -\int_{I} |\partial_t f|^2 \, ds, \qquad (3.23)$$

implies the estimate,

$$\int_{0}^{t} \left(\lambda_{1}^{-}(\tau)\right)^{2} d\tau \leq C\left(\left\|\partial_{s}^{2} f_{0}\right\|_{L^{2}}, \Delta\Omega, \alpha, \beta, \mu, L_{0}\right),$$

where $\lambda_1^-(t) = -\min\{0, \lambda_1(t)\}\)$. Note that, by Hölder's inequality and integration by parts, we have

$$-\lambda_{1} \int_{I} \left| \nabla_{s}^{m+1} \kappa \right|^{2} ds \leq \varepsilon \cdot \int_{I} \left| \nabla_{s}^{m+2} \kappa \right|^{2} ds + c \left(\varepsilon \right) \cdot \left(\lambda_{1}^{-} \right)^{2} \cdot \int_{I} \left| \nabla_{s}^{m} \kappa \right|^{2} ds.$$

$$(3.24)$$

🖉 Springer

Below we denote by $C_i = C_i \left(\left\| \partial_s^2 f_0 \right\|_{L^2}, \Delta\Omega, \alpha, \beta, L_0, m \right) > 0, \forall i \in \mathbb{Z}$. Then by Eqs. 3.2, 3.12, 3.21, 3.24, we have

$$\frac{d}{dt} \int_{I} \left| \nabla_{s}^{m} \kappa \right|^{2} ds + C_{1} \cdot \int_{I} \left| \nabla_{s}^{m+2} \kappa \right|^{2} ds \leq C_{2} \cdot \left(1 + (\lambda_{1}^{-}(t)^{2}) \cdot \int_{I} \left| \nabla_{s}^{m} \kappa \right|^{2} ds \right),$$
(3.25)

for some sufficiently small number $\varepsilon = \varepsilon \left(\left\| \partial_s^2 f_0 \right\|_{L^2}, \Delta \Omega, \alpha, \beta, L_0, m \right) > 0$. By applying Eq. 2.1 and Poincaré inequality twice to the term $\int_{I} |\nabla_s^{m+2} \kappa|^2 ds$ in Eq. 3.25, we have

$$\frac{d}{dt} \int_{I} |\nabla_{s}^{m} \kappa|^{2} ds + C_{3} \cdot \int_{I} |\nabla_{s}^{m} \kappa|^{2} ds \leq C_{2} \cdot \left(1 + (\lambda_{1}^{-}(t)^{2}) \cdot \int_{I} |\nabla_{s}^{m} \kappa|^{2} ds\right).$$

Let

$$u_m(t) := \exp\left(C_1 \cdot t\right) \cdot \int_{I} \left|\nabla_s^m \kappa\right|^2 ds.$$

By applying Gronwall inequality to Eq. 3.25, we have

$$u_m(t) \leq e^{a(t)} \cdot \left(u_m(0) + C_4 \cdot \int_0^t e^{C_1 \cdot \tau} d\tau \right),$$

where

$$a(t) = \int_{0}^{t} C_{5} \cdot (\lambda_{1}^{-}(\tau))^{2} d\tau \leq C \left(\left\| \partial_{s}^{2} f_{0} \right\|_{L^{2}}, \Delta \Omega, \alpha, \beta, L_{0}, m \right).$$

Therefore, we obtain

$$\begin{aligned} \left\| \nabla_{s}^{m} \kappa \right\|_{L^{2}}^{2}(t) &\leq C\left(\left\| \partial_{s}^{2} f_{0} \right\|_{L^{2}}, \Delta \Omega, \alpha, \beta, L_{0}, m \right) \cdot \left(1 + e^{-C_{1} \cdot t} \cdot \left\| \nabla_{s}^{m} \kappa \right\|_{L^{2}}^{2}(0) \right) \\ &\leq C\left(\left\| \partial_{s}^{2} f_{0} \right\|_{L^{2}}, \Delta \Omega, \alpha, \beta, L_{0}, m \right), \end{aligned}$$

for all $m \ge 0$. In addition, from the definition of λ_1 in Eq. 1.14, we conclude that $|\lambda_1| \le C \left(\left\| \partial_s^2 f_0 \right\|_{L^2}, \Delta\Omega, \alpha, \beta, L_0 \right)$. The rest of proof proceeds the same as those in Theorem 1.

4 Numerical simulations

4.1 Introduction

To illustrate the results numerically we extend the algorithm in [10] to the new description. Exploiting the divergence form of the main part in the evolution equation and the partition into a 2nd order parabolic–elliptic system for the position vector f and the curvature vector κ we write

$$\partial_t f + \partial_s \left(\partial_s \kappa + \frac{3}{2} |\kappa|^2 T - \lambda_2 T \times \kappa \right) = \lambda_1 \kappa, \tag{4.1}$$

$$\partial_s^2 f = \kappa \tag{4.2}$$

and discretize the problem using an semi-implicit scheme in time and piecewise-affine finite elements for the space dependence.

Now we have to deal with the computation for the writhe Wr[f] of the curve. Using the double integral definition only for the initial curve and turning to the difference of writhe formula for subsequent time steps we can hope to keep the additional computational effort reasonable.

4.2 Computational experiments

We conclude with a numerical experiment showing the appearance of a situation where the flow considered previously in [10] almost immediately runs into an inflection point scenario whereas the new flow shows an improved behavior seemingly un-effected by the appearance of inflection points. The initial curve is chosen to be of helical shape bent into a closed curve. This means that total torsion is large initially.

Figure 1 shows the curve obtained by evolving the initial curve under the newly proposed flow Eq. 1.12 for a short time $t_1 = 0.02$. Because of the short time interval the curve plotted is nearly unchanged from the helical initial curve we started with.

On the other hand we will see in following figures that the evolution under the old flow does not produce a reliable result. Obeying the relation of the prescription values $\Delta\Omega$ and $\Delta\Psi$ in Eq. 1.11 we choose the same initial curve to be evolved by the flow in [10]. Whereas we expect the evolution to new and old flow to be the same the latter one is pushing the curve very fast into a configuration where the curvature vector almost vanishes. Since this is causing the numerical computation of the torsion to fail badly the discretized flow deviates strongly from its analytical original even before the appearance of the actual inflection point. We want to mention that this is exactly the situation we wanted to address with the newly proposed formulation.

We show the variation of the energy of the curve over time in Fig. 2. Clearly, the expectation would be that the gradient flow reduces the energy which is failing to be true for the numerical computation of the old flow. The following plots should help to explain the reason for this failure. In Fig. 3 we plot (the logarithm of) the minimal length of the curvature vector along the curve. In both cases this quantity is decreasing initially but in the old flow the computation of torsion gets increasingly inaccurate if the curvature vector is too small. We show this in Fig. 4 by plotting the evolution of



Fig. 1 The curve at t_1 , evolved under the new flow



Fig. 2 Energy $\mathcal{F}[f]$

total torsion over time. Comparing the plot with the previous Fig.3 we see that the smallness of $|\kappa|^2$ causes the numerical implementation of the old flow to overestimate the correct value of total torsion after about 180 time steps (approx. 0.01 units in real time for the time step size k = 0.001 chosen). Since computation of total torsion affects the values for the Lagrange multipliers $\lambda_{1,2}$ in the old flow, this failure will



Fig. 3 Minimum value of $\log |\kappa|^2$



Fig. 4 Total torsion

kick the curve evolution onto a very different trajectory, in particular, away from the trajectory drawn by the new flow. Note that the new flow would also fail to compute torsion reliable but the value does not enter the computation of the speed so that the evolution continues in a reasonable way.

Acknowledgements This work was partially supported by the Taiwan National Science Council Grant 95-2115-M-003-002. We also thank Prof. Tsung-Min Hwang at Department of Mathematics in National Taiwan Normal University for his help with the Matlab codes in the numerical experiment.

References

- 1. J. Aldinger, I. Klapper, M. Tabor, Formulae for the calculation and estimation of writhe. J. Knot Theory Ramifications **4**(3), 343–372 (1995)
- 2. T. Aubin, Nonlinear analysis on manifolds. Monge-Ampère equations, Grundlehren der Mathematischen Wissenschaften, 252. (Springer-Verlag, New York, 1982)
- 3. R. Bishop, There is more than one way to frame a curve. Amer. Math. Monthly 82, 118–133 (1975)
- G. Călugăreanu, Sur les classes d'isotopie des nœuds tridimensionnels et leurs invariants. Czechoslovak Math. J. 11(86), 588–625 (1961)
- 5. G. Dziuk, E. Kuwert, R. Schätzle, Evolution of elastic curves in \mathbb{R}^n , existence and computation. SIAM J. Math. Anal. **33**(5), 1228–1245 (2002)
- 6. F.B. Fuller, The writhing number of a space curve. Proc. Nat. Acad. Sci. U.S.A. 68, 815–819 (1971)
- F.B. Fuller, Decomposition of the linking number of a closed ribbon: a problem from molecular biology. Proc. Nat. Acad. Sci. U.S.A. 75(8), 3557–3561 (1978)
- T. Ivey, D. Singer, Knot types, homotopies and stability of closed elastic rods. Proc. London Math. Soc. (3) 79(2), 429–450 (1999)
- 9. J. Langer, D. Singer, Lagrangian aspects of the Kirchhoff elastic rod. SIAM Rev. 38(4), 605-618 (1996)
- C.C. Lin, H.R. Schwetlick, On the geometric flow of Kirchhoff elastic rods. SIAM J. Appl. Math. 65(2), 720–736 (2004/05)
- 11. A. Polden, *Curves and surfaces of least total curvature and fourth-order flows*, Ph.D. dissertation, Universität Tübingen, Tübingen, Germany, 1996
- F. Schuricht, H. von der Mosel, Euler-Lagrange equations for nonlinearly elastic rods with self-contact. Arch. Ration. Mech. Anal. 168(1), 35–82 (2003)
- 13. J.H. White, Self-linking and the Gauss integral in higher dimensions. Amer. J. Math. **91**, 693–728 (1969)