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Nonlocal orientation-dependent dynamics of charged strands and ribbons

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Abstract

Time-dependent Hamiltonian dynamics is derived for a strand of charged units in $\mathbb{R}^3$ held together by both nonlocal (for example, electrostatic) and elastic interactions. The dynamical equations in the symmetry-reduced variables are written on the dual of the semidirect-product Lie algebra $so(3)\circledS(\mathbb{R}^3\oplus\mathbb{R}^3\oplus\mathbb{R}^3\oplus\mathbb{R}^3)$ with three 2-cocycles. We also demonstrate that the nonlocal interaction produces an interesting new term deriving from the coadjoint action of the Lie group $SO(3)$ on its Lie algebra $so(3)$. The new strand equations are written in conservative form by using the corresponding coadjoint actions. ***To cite this article: D.D. Holm, V. Putkaradze, C. R. Acad. Sci. Paris, Ser. I 347 (2009).***

Résumé

Dynamique non-locale des filaments électisés. Nous établir les équations de la dynamique hamiltonienne d'une courbe (chaine moléculaire) dans l'espace physique $\mathbb{R}^3$ sujette á des interactions élastiques ainsi que non-locales (électrostatiques par exemple). Les équations dynamiques des variables réduites par symétrie sont écrites sur l'espace dual de l'algèbre de Lie $so(3)\circledS(\mathbb{R}^3\oplus\mathbb{R}^3\oplus\mathbb{R}^3\oplus\mathbb{R}^3)$ (produit semidirect) avec trois 2-cocycles. Nous démontrons aussi que l'interaction non-locale produit un nouvel terme intéressant, qui dérive de l'action coadjointe du group de Lie $SO(3)$ sur son algébre $so(3)$. Les nouvelles équations du filament sont écrites sous une forme conservative grâce aux actions coadjointes correspondantes. ***Pour citer cet article : D.D. Holm, V. Putkaradze, C. R. Acad. Sci. Paris, Ser. I 347 (2009).***

Version française abrégée

Cette Note dépasse le cadre des approches à la Kirchhoff pour établir les équations de la dynamique hamiltonienne d'une courbe (chaine moléculaire) dans l'espace physique $\mathbb{R}^3$, lorsqu'elle est sujette à des interactions élastiques ainsi que non-locales (électrostatiques par exemple). Cette Note s'inspire d'une extension de la théorie des *barres géométriques parfaites* [16], qui présente l'interaction élastique dans un contexte géométrique par l'usage des *coordonnées*

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matérielles. Cette théorie a déjà été utilisée pour la description de quelques aspects de la dynamique des protéines [3]. Toutefois la généralisation des ces théories aux interactions *non-locales* (qui dépendent du temps) exige l'application de méthodes géométriques pour dériver le principe d'action (12), qui vont au-delà de l'approche à la Kirchhoff. Les équations dynamiques des variables réduites par symétrie (13), (14) sont écrites dans l'espace dual de l'algèbre de Lie $so(3) \circledS (\mathbb{R}^3 \oplus \mathbb{R}^3 \oplus \mathbb{R}^3 \oplus \mathbb{R}^3)$ (produit semidirect) avec trois 2-cocycles. De plus, les nouvelles équations du filament sont écrites sous une forme conservative (22) en utilisant les actions coadjointes correspondantes. Notre approche rend possible l'inclusion cohérente des effets électrostatiques et inertiels dans les études théoriques et numériques de la dynamique des chaines biologiques. Cela garantit aussi la conservation de l'énergie et étend les traitements Hamiltoniens à la Lie Poisson [16,8,13] afin d'englober la dépendance non-locale des variables.

1. Introduction

Consideration of biological strands as a continuum curve has a long and rich history with some notable successes [11,1,10,12]. Most studies in this approach – both for stationary and time dependent models – used the framework of the Kirchhoff model of elastic rods. That framework, however, has been so far not been able to overcome the mathematical difficulties of incorporating electrostatic (nonlocal) effects into the dynamics, by a straight-forward extension of Kirchhoff theory. Some recent progress has been made on the *stationary* solutions in the continuum framework [6]. However, no time-dependent theory considering nonlocal effects yet exists to our knowledge, as Kirchhoff's theory is formulated in the *intrinsic* frame connected with the deformed rod. Hence, the computation of distances in Euclidean space becomes non-trivial, especially in the case when distances depend on orientation, see Fig. 1 below.

This Note overcomes the problems confronted in standard Kirchhoff-based approaches by using an extension of the theory of *exact geometric rods* [16], which puts elastic interactions into a geometric framework using the *material frame* viewpoint. This theory has already been used to describe some aspects of protein dynamics [3]. However, the generalization of these theories for *time-dependent* nonlocal interactions requires geometric methods. This theory is applicable to the fast folding motion of molecular strands, or similar motion of oriented charged strands in vacuum. More accurate dynamics of stands including friction can then be considered by adding appropriate terms to the inviscid motion. However, the introduction of dissipation into the motion of biological strands is a complicated issue [11,10] that will be deferred to future work.

2. Motion of exact self-interacting geometric rods

We consider rigid conformations of charges mounted along a flexible filament at $\boldsymbol{r}(s,t)$ at distances $\boldsymbol{\eta}_k(s,t)$ and allow these charges to interact with each other via a potential (for proteins, the screened electrostatic potential). For simplicity, each charge 'bouquet' is assumed to rotate as a rigid body with respect to its origin, so $\boldsymbol{\eta}_k(s,t) := \boldsymbol{\eta}_k(s)$ and the charges are assumed mass less so the center of mass for each bouquet has its center of mass at its base. Our methods allow consideration of charges with mass, but the resulting expressions become too complicated to be presented here, without any valuable insight into mathematical structure. The parameter s is a parametrization along the filament; it can be chosen to be the arclength for inextensible filaments. For our purposes, we assume that $s \in I$ and all boundary conditions at the end of the interval I are appropriate so no boundary terms appear. Thus, the map $s \to \boldsymbol{r}(s,t)$ does not need to be an isometry. This rigid conformational rotation is illustrated in Fig. 1. Thus, the configuration of the filament is described by the two maps $s \to \boldsymbol{r}(s,t)$ with the values in $\mathbb{R}^3$ and $s \to \Lambda(s,t)$ with the values in $SO(3)$.

Suppose each rigid conformation of charges is identical and the k-th electrical charge is positioned near a given point $\boldsymbol{r}(s,t)$ of the curve at the reference state $\boldsymbol{r} + \boldsymbol{\eta}_k(s)$. Here, $\boldsymbol{\eta}_k(s)$ is a vector of constant length that determines the position of the k-th electrical charge relative to the point $\boldsymbol{r}(s,t)$ along the curve in its reference configuration. If the curve position $\boldsymbol{r}$ remains fixed, rotation is allowed only in a plane so $\Lambda \in SO(2)$ and there is only one charge $k = 1$, our model reduces to that considered in [15]. In general, the position $\mathbf{c}_k$ of the k-th charge in the rigid conformation anchored at position $\boldsymbol{r}(s,t)$ rotates to a new position with $\Lambda(s,t) \in SO(3)$ as $\mathbf{c}_k(s,t) = \boldsymbol{r}(s,t) + \Lambda(s,t)\boldsymbol{\eta}_k(s)$, where $\Lambda(s,0) = \mathrm{Id}$.

Some discussion is warranted here on the connection to previous studies. In [7], the nonlocal (for example, electrostatic) interaction force was considered for charges that were distributed along the string itself (Eq. (2.3.7)), corresponding to i.e. all $\boldsymbol{\eta}_i = 0$ of our case. This formula involved explicitly the Euclidean distance between two points on the rod, $\boldsymbol{r}(s) - \boldsymbol{r}(s')$, and a *mollifier* $M(s,s')$ making the total energy finite, necessary for electrostatic

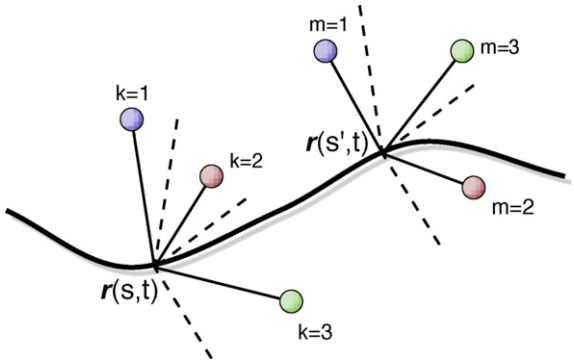

Fig. 1. Rigid conformations of charges are distributed along a curve. Dashed lines – original state, solid lines – final state.

interactions. In [1] electrostatic interactions between sufficiently nearby points on the rod were removed. The torque on the rod due to nonlocal forces was assumed to be zero. This technique has been successful in computing *stationary* rod configurations, see [6,2]. Unfortunately, in Kirchoff's approach, Euclidean distances and orientations can only be computed after the configuration of the rod is known, so the use of this technique for time-dependent simulations is difficult. In contrast, the present work derives explicit formulas for *dynamical* rod evolution for the non-trivial forces and torques, when the charges are offset from the rod's centerline.

We consider the Lagrangian L consisting of two additive parts: (i) the localized part l, including all the elastic interactions and the kinetic energy; and (ii) the nonlocal part l_{np} that describes nonlocal interactions. The localized part l of the Lagrangian depends on Λ, $\dot{\Lambda}$, Λ', $\boldsymbol{r}(s)$, $\dot{\boldsymbol{r}}$, $\boldsymbol{r}'$, where the dot denotes the time derivative and prime is the derivative with respect to parameter s. If it is left-invariant under the action of $SO(3)$, this Lagrangian may be reduced to a function of left-invariant quantities: $\Omega = \Lambda^{-1}\Lambda'$, $\omega = \Lambda^{-1}\dot{\Lambda}$, $\boldsymbol{\Gamma} = \Lambda^{-1}\boldsymbol{r}'$, $\boldsymbol{\gamma} = \Lambda^{-1}\dot{\boldsymbol{r}}$ and $\boldsymbol{\rho} = \Lambda^{-1}\boldsymbol{r}$. These quantities are maps from (s,t) with values in $so(3)$ (Ω and ω) and $\mathbb{R}^3$ ($\boldsymbol{\Gamma}$, $\boldsymbol{\gamma}$ and $\boldsymbol{\rho}$). Capital Greek letters denote derivatives in s, while lower-case Greek letters (except for $\boldsymbol{\rho}$) denote derivatives in time. Bold letters such as $\boldsymbol{\omega}$ denote vectors in $\mathbb{R}^3$ while Ω is a skew 3×3 matrix in the Lie algebra $so(3)$ whose entries correspond to vector components via the isomorphism between $so(3)$ and $\mathbb{R}^3$. For example, for any vector $\boldsymbol{v}\in\mathbb{R}^3$ one has $\Omega\boldsymbol{v} = \boldsymbol{\Omega}\times\boldsymbol{v}$; in components, this is the map $\Omega_{jk} = -\epsilon_{jkl}\Omega_l$.

The nonlocal part of the potential energy l_{np} of interaction between rigid conformations of charges at spatial coordinates s and s' along the filament depends only on the distance $d_{k,m}(s,s')$ between the k-th and m-th charges in the two conformations,

$$l_{np} = \sum_{k,m}\frac{1}{2}\int U\big(d_{k,m}(s,s')\big)\big|\boldsymbol{\Gamma}(s)\big|\big|\boldsymbol{\Gamma}(s')\big|\,\mathrm{d}s\,\mathrm{d}s', \quad d_{k,m}(s,s') = \big|\mathbf{c}_k(s) - \mathbf{c}_m(s')\big|. \tag{1}$$

Here, the terms $|\boldsymbol{\Gamma}(s)| = |\Lambda^{-1}\,\mathrm{d}\mathbf{r}/\mathrm{d}s| = |\mathrm{d}\mathbf{r}/\mathrm{d}s|$ appear because the mapping $s\to\boldsymbol{r}(s,t)$ is not isometric. Here, $U(d)$ is the potential energy between two charges, modified as necessary for $d\to 0$ so that all the integral terms written below converge. The scalar distance $d_{k,m}$ may also be expressed in terms of vectors seen from the frame of orientation of the rigid body at a point $\mathbf{x}$ along the filament, as

$$d_{k,m}(s,s') = \big|\mathbf{c}_k(s) - \mathbf{c}_m(s')\big| = \big|\boldsymbol{\kappa}(s,s') + \boldsymbol{\eta}_k(s) - \xi(s,s')\boldsymbol{\eta}_m(s')\big|, \quad \text{where} \tag{2}$$

$$\xi(s,s') = \Lambda^{-1}(s)\Lambda(s') \quad \text{and} \quad \boldsymbol{\kappa}(s,s') = \Lambda^{-1}(s)\big(\boldsymbol{r}(s) - \boldsymbol{r}(s')\big) = \boldsymbol{\rho}(s) - \xi(s,s')\boldsymbol{\rho}(s') \tag{3}$$

(suppressing the t index) are functions with the values in $\mathbb{R}^3$ and $SO(3)$, respectively. The first of these quantities is the spatial vector $\boldsymbol{r}(s) - \boldsymbol{r}(s')$ between two points on the filament, as seen from the orientation $\Lambda(s)$ of the rigid body (charge conformation) at s on the filament. The second is the *relative* orientation of the rigid bodies (charge conformations) at s and s'. A transposition identity, $\xi(s,s')^T = \xi(s',s) = \xi(s,s')^{-1}$, follows from the definition of $\xi(s,s')$ in (3). Note that both the vector $\boldsymbol{\kappa}(s,s')$ and the relative orientation $\xi(s,s')$ defined in (3) are invariant under changes of the orientation of the spatial coordinate system obtained by the left action $\boldsymbol{r}(s) - \boldsymbol{r}(s')\to O(\boldsymbol{r}(s) - \boldsymbol{r}(s'))$ and $\Lambda\to O\Lambda$ of any element O in the rotation group $SO(3)$.

In terms of these quantities, we assume the symmetry-reduced Lagrangian L may be written as the sum of a local part l and a nonlocal part l_{np}, according to

$$L(\boldsymbol{\rho},\boldsymbol{\gamma},\boldsymbol{\Gamma},\boldsymbol{\omega},\boldsymbol{\Omega},\xi)=l(\boldsymbol{\rho},\boldsymbol{\gamma},\boldsymbol{\Gamma},\boldsymbol{\omega},\boldsymbol{\Omega})+\int U\big(\boldsymbol{\kappa}(s,s'),\xi(s,s')\big)\big|\boldsymbol{\Gamma}(s)\big|\big|\boldsymbol{\Gamma}(s')\big|\,\mathrm{d}s\,\mathrm{d}s':=l+l_{np}. \tag{4}$$

3. Kinematics

Let us compute the space and time derivatives of $\boldsymbol{\rho}=\Lambda^{-1}\boldsymbol{r}\in\mathbb{R}^3$. The space ($s$) derivative of $\boldsymbol{\rho}$ (denoted by a prime) and time (t) derivative (denoted by a dot) are given by

$$\boldsymbol{\rho}'=-\Omega\boldsymbol{\rho}+\boldsymbol{\Gamma}=-\boldsymbol{\Omega}\times\boldsymbol{\rho}+\boldsymbol{\Gamma}\quad\text{and}\quad\dot{\boldsymbol{\rho}}=-\omega\boldsymbol{\rho}+\boldsymbol{\gamma}=-\boldsymbol{\omega}\times\boldsymbol{\rho}+\boldsymbol{\gamma}. \tag{5}$$

Compatibility of these formulas arises from equality of the cross-derivatives of $\boldsymbol{r}$ and Λ. Namely,

$$\dot{\boldsymbol{\Gamma}}+\boldsymbol{\omega}\times\boldsymbol{\Gamma}=\boldsymbol{\gamma}'+\boldsymbol{\Omega}\times\boldsymbol{\gamma}\quad\text{and}\quad\dot{\boldsymbol{\Omega}}=\boldsymbol{\Omega}\times\boldsymbol{\omega}+\boldsymbol{\omega}'. \tag{6}$$

4. Variations

The variations of $\boldsymbol{\rho}$, $\boldsymbol{\omega}$, $\boldsymbol{\gamma}$, $\boldsymbol{\Omega}$ and $\boldsymbol{\Gamma}$ are computed by the following steps:

$$\delta\boldsymbol{\rho}=-\Lambda^{-1}\delta\Lambda\Lambda^{-1}\boldsymbol{r}+\Lambda^{-1}\delta\boldsymbol{r}=-\Sigma\boldsymbol{\rho}+\boldsymbol{\Psi}=-\boldsymbol{\Sigma}\times\boldsymbol{\rho}+\boldsymbol{\Psi}=\boldsymbol{\rho}\times\boldsymbol{\Sigma}+\boldsymbol{\Psi}, \tag{7}$$

where one defines the left-invariant variations $\Sigma=\Lambda^{-1}\delta\Lambda\in so(3)$ and $\boldsymbol{\Psi}=\Lambda^{-1}\delta\boldsymbol{r}\in\mathbb{R}^3$. The variations $\delta\boldsymbol{\gamma}$, $\delta\boldsymbol{\Gamma}$, $\delta\boldsymbol{\omega}$ and $\delta\boldsymbol{\Omega}$ are given in terms of the left-invariant quantities Σ and $\boldsymbol{\Psi}$ by

$$\delta\boldsymbol{\gamma}=-\boldsymbol{\Sigma}\times\boldsymbol{\gamma}+\boldsymbol{\omega}\times\boldsymbol{\Psi}+\frac{\partial\boldsymbol{\Psi}}{\partial t},\quad\delta\boldsymbol{\Gamma}=-\boldsymbol{\Sigma}\times\boldsymbol{\Gamma}+\boldsymbol{\Omega}\times\boldsymbol{\Psi}+\frac{\partial\boldsymbol{\Psi}}{\partial s}, \tag{8}$$

$$\delta\boldsymbol{\omega}=\boldsymbol{\omega}\times\boldsymbol{\Sigma}+\frac{\partial\boldsymbol{\Sigma}}{\partial t}\quad\text{and}\quad\delta\boldsymbol{\Omega}=\boldsymbol{\Omega}\times\boldsymbol{\Sigma}+\frac{\partial\boldsymbol{\Sigma}}{\partial s}. \tag{9}$$

The key to understanding the nonlocal variations lies in the matrix formula

$$\xi^{-1}\delta\xi(s,s')=-\operatorname{Ad}_{\xi^{-1}(s,s')}\Sigma(s)+\Sigma(s'),\quad\text{where}\quad\operatorname{Ad}_{\xi^{-1}}\Sigma:=\xi^{-1}\Sigma\xi, \tag{10}$$

obtained from the definition of $\xi(s,s')$ in Eq. (3). The variation of $\boldsymbol{\kappa}$ in (3) is then given by

$$\delta\boldsymbol{\kappa}(s,s')=-\boldsymbol{\Sigma}(s)\times\boldsymbol{\kappa}(s,s')+\boldsymbol{\Psi}(s)-\xi(s,s')\boldsymbol{\Psi}(s'). \tag{11}$$

5. Calculation of energy variations

The equations of motion are computed from the stationary action principle $\delta S=0$, with $S=\int L\,\mathrm{d}t$ and $L=l+l_{np}$ in Eq. (4), for which

$$\begin{aligned}\delta S=\int\Big\langle\frac{\delta l}{\delta\boldsymbol{\rho}},\delta\boldsymbol{\rho}\Big\rangle+\Big\langle\frac{\delta l}{\delta\boldsymbol{\gamma}},\delta\boldsymbol{\gamma}\Big\rangle+\Big\langle\frac{\delta(l+l_{np})}{\delta\boldsymbol{\Gamma}},\delta\boldsymbol{\Gamma}\Big\rangle+\Big\langle\frac{\delta l}{\delta\omega},\delta\omega\Big\rangle\\+\Big\langle\frac{\delta l}{\delta\Omega},\delta\Omega\Big\rangle+\Big\langle\frac{\delta l_{np}}{\delta\boldsymbol{\kappa}},\delta\boldsymbol{\kappa}\Big\rangle+\Big\langle\xi^{-1}\frac{\delta l_{np}}{\delta\xi},\xi^{-1}\delta\xi\Big\rangle\mathrm{d}t=0.\end{aligned} \tag{12}$$

The terms proportional to $\boldsymbol{\Sigma}$ and $\boldsymbol{\Psi}$ give, respectively,

$$\begin{aligned}\Big(\frac{\partial}{\partial t}\frac{\delta l}{\delta\boldsymbol{\omega}}+\boldsymbol{\omega}\times\frac{\delta l}{\delta\boldsymbol{\omega}}\Big)+\Big(\frac{\partial}{\partial s}\frac{\delta l}{\delta\boldsymbol{\Omega}}\Big)+\boldsymbol{\Omega}\times\frac{\delta l}{\delta\boldsymbol{\Omega}}=\frac{\delta l}{\delta\boldsymbol{\gamma}}\times\boldsymbol{\gamma}+\frac{\delta(l+l_{np})}{\delta\boldsymbol{\Gamma}}\times\boldsymbol{\Gamma}+\frac{\delta l}{\delta\boldsymbol{\rho}}\times\boldsymbol{\rho}\\+\int\Big(\frac{\partial U}{\partial\boldsymbol{\kappa}}(s,s')\times\boldsymbol{\kappa}(s,s')+\mathbf{Z}(s,s')\Big)\big|\boldsymbol{\Gamma}(s)\big|\big|\boldsymbol{\Gamma}(s')\big|\,\mathrm{d}s',\end{aligned} \tag{13}$$

$$\begin{aligned}&\Big(\frac{\partial}{\partial t}\frac{\delta l}{\delta\boldsymbol{\gamma}}+\boldsymbol{\omega}\times\frac{\delta l}{\delta\boldsymbol{\gamma}}\Big)+\Big(\frac{\partial}{\partial s}\frac{\delta(l+l_{np})}{\delta\boldsymbol{\Gamma}}+\boldsymbol{\Omega}\times\frac{\delta l}{\delta\boldsymbol{\Gamma}}\Big)\\&\quad=\frac{\delta l}{\delta\boldsymbol{\rho}}+\int\Big(\frac{\partial U}{\partial\boldsymbol{\kappa}}(s,s')-\xi(s,s')\frac{\partial U}{\partial\boldsymbol{\kappa}}(s',s)\Big)\big|\boldsymbol{\Gamma}(s)\big|\big|\boldsymbol{\Gamma}(s')\big|\,\mathrm{d}s',\end{aligned} \tag{14}$$

$$\text{where } Z(s,s') := \mathbf{Z}(s,s')\times = \xi(s,s')\left(\frac{\partial U}{\partial \xi}(s,s')\right)^T - \frac{\partial U}{\partial \xi}(s,s')\xi^T(s,s'). \tag{15}$$

The term $Z(s,s')$ is the torque contribution from the nonlocal part of the Lagrangian we have sought. A direct calculation shows that $Z^T = -Z$, so $Z \in so(3)$. This expression appears naturally in geometric mechanics of interacting oriented bodies such as asteroids [4]. The more general theory of *reduction by stages* [5] illuminates the geometric nature of such interactions.

6. Spatial conservation laws

The physical meaning of Eqs. (13), (14) is revealed by writing them as conservation laws. For this, we invoke the following identities for the Ad- and Ad*-actions of any element $g(t) \in G$ in the Lie group on $\eta \in \mathfrak{g}$ in the Lie algebra and $\mu \in \mathfrak{g}^*$ in its dual with pairing $\langle\cdot,\cdot\rangle : \mathfrak{g}^* \times \mathfrak{g} \to \mathbb{R}$

$$\left\langle \mu, \operatorname{Ad}_{g^{-1}(t)} \frac{\partial}{\partial t} \operatorname{Ad}_{g(t)} \eta \right\rangle = \langle \mu, \operatorname{ad}_\sigma \eta \rangle \quad \text{and} \quad \left\langle \operatorname{Ad}^*_{g(t)} \frac{\partial}{\partial t} \operatorname{Ad}^*_{g^{-1}(t)} \mu, \eta \right\rangle = \langle -\operatorname{ad}^*_\sigma \mu, \eta \rangle, \tag{16}$$

where $\operatorname{Ad}^* : G \times \mathfrak{g}^* \to \mathfrak{g}^*$ is defined by $\langle \operatorname{Ad}^*_{g(t)} \mu, \eta\rangle := \langle \mu, \operatorname{Ad}_{g(t)} \eta\rangle$ and $\sigma = g^{-1}g'(t) \in \mathfrak{g}$ belongs to the Lie algebra $\mathfrak{g}$. Eqs. (13), (14) are formulated on the *dual* of the Lie algebra, so by second equation of (16),

$$\left\langle \operatorname{Ad}^*_{g(t)} \frac{\partial}{\partial t}\left(\operatorname{Ad}^*_{g^{-1}(t)} \mu(t)\right), \eta \right\rangle = \langle \dot\mu - \operatorname{ad}^*_\sigma \mu, \eta \rangle. \tag{17}$$

To derive the conservation form of Eqs. (13), (14), we consider the group $G = SE(3)$ with the group element $g = (\Lambda(s,t), \boldsymbol{r}(s,t))$, whose left-invariant time-derivative is $\sigma = (\Lambda^{-1}\dot\Lambda, \Lambda^{-1}\dot{\boldsymbol{r}}) = (\boldsymbol{\omega}, \boldsymbol{\gamma})$ and s-derivative is $(\Lambda^{-1}\Lambda', \Lambda^{-1}\boldsymbol{r}') = (\boldsymbol{\Omega}, \boldsymbol{\Gamma})$. Using the definition of ad* for the $se(3)$ Lie algebra yields, respectively:

$$\operatorname{Ad}^*_{g(t)} \frac{\partial}{\partial t}\left[\operatorname{Ad}^*_{g^{-1}(t)}\left(\frac{\delta L}{\delta \boldsymbol{\omega}}, \frac{\delta L}{\delta \boldsymbol{\gamma}}\right)\right] = \frac{\partial}{\partial t}\left(\frac{\delta L}{\delta \boldsymbol{\omega}}, \frac{\delta L}{\delta \boldsymbol{\gamma}}\right) + \left(\boldsymbol{\omega} \times \frac{\delta L}{\delta \boldsymbol{\omega}} + \boldsymbol{\gamma} \times \frac{\delta L}{\delta \boldsymbol{\gamma}}, -\boldsymbol{\omega} \times \frac{\delta L}{\delta \boldsymbol{\gamma}}\right), \tag{18}$$

$$\operatorname{Ad}^*_{g(s)} \frac{\partial}{\partial s}\left[\operatorname{Ad}^*_{g^{-1}(s)}\left(\frac{\delta L}{\delta \boldsymbol{\Omega}}, \frac{\delta L}{\delta \boldsymbol{\Gamma}}\right)\right] = \frac{\partial}{\partial s}\left(\frac{\delta L}{\delta \boldsymbol{\Omega}}, \frac{\delta L}{\delta \boldsymbol{\Gamma}}\right) + \left(\boldsymbol{\Omega} \times \frac{\delta L}{\delta \boldsymbol{\Omega}} + \boldsymbol{\Gamma} \times \frac{\delta L}{\delta \boldsymbol{\Gamma}}, -\boldsymbol{\Omega} \times \frac{\delta L}{\delta \boldsymbol{\Gamma}}\right). \tag{19}$$

Note that the nonlocal term (15) arises as the derivative of the nonlocal part of the potential with respect to Lie algebra elements $\boldsymbol{\Omega}$ and $\boldsymbol{\Gamma}$, as follows. Upon identifying coefficients of the free variations $\boldsymbol{\Sigma}\times = \Lambda^{-1}\delta\Lambda$ and $\boldsymbol{\Psi} = \Lambda^{-1}\delta\boldsymbol{r}$, we write the following identity relating different derivatives of the nonlocal potential l_{np}:

$$\delta l_{np} = \left\langle \xi^{-1}\frac{\delta l_{np}}{\delta \xi}, \xi^{-1}\delta\xi \right\rangle + \left\langle \frac{\delta l_{np}}{\delta \boldsymbol{\kappa}}, \delta\boldsymbol{\kappa} \right\rangle + \left\langle \frac{\delta l_{np}}{\delta \boldsymbol{\Gamma}}, \delta\boldsymbol{\Gamma} \right\rangle = \left\langle \frac{\delta l_{np}}{\delta \boldsymbol{\Gamma}}\bigg|_{Tot}, \delta\boldsymbol{\Gamma} \right\rangle + \left\langle \frac{\delta l_{np}}{\delta \boldsymbol{\Omega}}, \delta\boldsymbol{\Omega} \right\rangle.$$

Here, $\cdot|_{Tot}$ denotes the *total* of the derivative with respect to $\boldsymbol{\Gamma}$. Using expressions (10) for $\xi^{-1}\delta\xi$, (11) for $\delta\boldsymbol{\kappa}$, (9) for $\delta\boldsymbol{\Omega}$ and (8) for $\delta\boldsymbol{\Gamma}$, then collecting terms proportional to the free variation $\boldsymbol{\Sigma}$ yields the following identity, which implicitly defines $\delta l_{np}/\delta\boldsymbol{\Omega}$ in terms of known quantities,

$$-\frac{\partial}{\partial s}\frac{\delta l_{np}}{\delta \boldsymbol{\Omega}} + \boldsymbol{\Omega} \times \frac{\delta l_{np}}{\delta \boldsymbol{\Omega}} = \int \frac{\partial U}{\partial \boldsymbol{\kappa}}(s,s') \times \boldsymbol{\kappa}(s,s')\,\mathrm{d}s' + \int \mathbf{Z}(s,s')\,\mathrm{d}s', \tag{20}$$

where we have defined $\mathbf{Z}(s,s')$ according to (15). Likewise, identifying terms multiplying $\boldsymbol{\Psi}$ gives

$$-\frac{\partial}{\partial s}\frac{\delta l_{np}}{\delta \boldsymbol{\Gamma}}\bigg|_{Tot} + \boldsymbol{\Omega} \times \frac{\delta l_{np}}{\delta \boldsymbol{\Gamma}}\bigg|_{Tot} = \int \frac{\partial U}{\partial \boldsymbol{\kappa}}(s,s') - \xi(s,s')\frac{\partial U}{\partial \boldsymbol{\kappa}}(s',s)\,\mathrm{d}s'. \tag{21}$$

Therefore, we conclude that Eqs. (13), (14) are equivalent to the following pair of equations expressed in conservative form using variations of the total Lagrangian, $L := l + l_{np}$:

$$\frac{\partial}{\partial t}\left[\operatorname{Ad}^*_{g^{-1}(t)}\left(\frac{\delta L}{\delta \boldsymbol{\omega}}, \frac{\delta L}{\delta \boldsymbol{\gamma}}\right)\right] + \frac{\partial}{\partial s}\left[\operatorname{Ad}^*_{g^{-1}(t)}\left(\frac{\delta L}{\delta \boldsymbol{\Omega}}, \frac{\delta L}{\delta \boldsymbol{\Gamma}}\bigg|_{Tot}\right)\right] = \operatorname{Ad}^*_{g^{-1}(t)}\left(\frac{\delta L}{\delta \boldsymbol{\rho}} \times \boldsymbol{\rho}, \frac{\delta L}{\delta \boldsymbol{\rho}}\right). \tag{22}$$

The quantities $\operatorname{Ad}^*_{g^{-1}(t)}(\delta L/\delta\boldsymbol{\omega}, \delta L/\delta\boldsymbol{\gamma})$ represent, respectively, the spatial angular momentum density and the spatial linear momentum density of the strand, whose center of mass lies along its centerline. The terms $\operatorname{Ad}^*_{g^{-1}(t)}(\delta L/\delta\boldsymbol{\rho} \times$

$\boldsymbol{\rho}, \delta L/\delta \boldsymbol{\rho})$ are spatial external torques and forces, respectively, which are not expressible in conservation form. (This is similar to the situation for the heavy top.)

Note that these equations strengthen the results of [6] stating that a uniform charge along the string can be absorbed into an effective spring constant for helical shapes. Eq. (22) states that result of all nonlocal interactions can be written in conservative form as if appearing from purely elastic forces. In proving this result, the nonlocal interactions are treated using the implicit variational derivatives in Eqs. (20), (21).

7. Hamiltonian approach

On Legendre transforming the Lagrangian L to the Hamiltonian, $H(\boldsymbol{\mu}, \boldsymbol{\beta}; \boldsymbol{\Omega}, \boldsymbol{\Gamma}, \boldsymbol{\rho}) = \int (\boldsymbol{\mu} \cdot \boldsymbol{\omega} + \boldsymbol{\beta} \cdot \boldsymbol{\gamma})\, \mathrm{d}s - L(\boldsymbol{\omega}, \boldsymbol{\gamma}; \boldsymbol{\Omega}, \boldsymbol{\Gamma}, \boldsymbol{\rho})$, Eqs. (5), (6), (13) and (14) may be expressed as

$$\frac{\partial}{\partial t}\begin{bmatrix} \boldsymbol{\mu} \\ \boldsymbol{\rho} \\ \boldsymbol{\Omega} \\ \boldsymbol{\Gamma} \\ \boldsymbol{\beta} \end{bmatrix} = \begin{bmatrix} \boldsymbol{\mu}\times & \boldsymbol{\rho}\times & (\partial_s + \boldsymbol{\Omega}\times) & \boldsymbol{\Gamma}\times & \boldsymbol{\beta}\times \\ \boldsymbol{\rho}\times & 0 & 0 & 0 & Id \\ (\partial_s + \boldsymbol{\Omega}\times) & 0 & 0 & 0 & 0 \\ \boldsymbol{\Gamma}\times & 0 & 0 & 0 & (\partial_s + \boldsymbol{\Omega}\times) \\ \boldsymbol{\beta}\times & -Id & 0 & (\partial_s + \boldsymbol{\Omega}\times) & 0 \end{bmatrix} \begin{bmatrix} \delta H/\delta \boldsymbol{\mu} = \boldsymbol{\omega} \\ \delta H/\delta \boldsymbol{\rho} \\ \delta H/\delta \boldsymbol{\Omega} \\ \delta H/\delta \boldsymbol{\Gamma} \\ \delta H/\delta \boldsymbol{\beta} = \boldsymbol{\gamma} \end{bmatrix}. \tag{23}$$

This Lie–Poisson Hamiltonian matrix is dual to the semidirect-product Lie algebra $so(3) \circledS (\mathbb{R}^3 \oplus \mathbb{R}^3 \oplus \mathbb{R}^3 \oplus \mathbb{R}^3)$ with three different types of 2-cocycles defined on its normal $\mathbb{R}^3$ subalgebras. The symplectic 2-cocycle in $\{\boldsymbol{\rho}, \boldsymbol{\beta}\}$ induces the generalized 2-cocycle in $\{\boldsymbol{\Gamma}, \boldsymbol{\beta}\}$, for which $\boldsymbol{\Omega}$ is a Casimir; so $\boldsymbol{\Omega}\times$ is a constant in this 2-cocycle. In contrast, the quantity $\boldsymbol{\Omega}\times$ in the generalized 2-cocycle for $\{\boldsymbol{\mu}, \boldsymbol{\Omega}\}$ is a connection form. The latter 2-cocycle also appears in the theory of complex fluids [16,8,13]. Because of its mathematical generality, the Hamiltonian formulation derived in the Euler–Poincaré framework here appeared before in several other applications with quite different physics: (i) the $SO(3)$ version of the Yang–Mills gauge theory of classical chromohydrodynamics [9]; (ii) the theory of spin-glass dynamics [14]; (iii) the geometrically exact rod theory presented in [16]; and (iv) the complex fluids theory of [13]. In addition, the effects of nonlocal interactions are now incorporated here by computing the derivatives implicitly in Eqs. (20), (21).

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References

[1] A. Balaeff, L. Mahadevan, K. Schulten, Elastic rod model of a DNA loop in the lac operon, Phys. Rev. Lett. 83 (1999) 4900–4903.
[2] J.R. Banavar, T.X. Hoang, J.H. Maddocks, A. Maritan, C. Poletto, A. Stasiak, A. Trovato, Structural motifs of macromolecules, Proc. Natl. Acad. Sci. 104 (2007) 17283–17286.
[3] T.C. Bishop, R. Cortez, O.O. Zhmudsky, Investigation of bend and shear waves in a geometrically exact elastic rod model, J. Comp. Phys. 193 (2004) 642–665.
[4] H. Cendra, J.E. Marsden, Geometric mechanics and the dynamics of asteroid pairs, Dynamical Systems 20 (2005) 3–21.
[5] H. Cendra, J.E. Marsden, T.S. Ratiu, Lagrangian Reduction by Stages, Memoirs American Mathematical Society, vol. 152, 2001.
[6] N. Chouaieb, A. Goriely, J.H. Maddocks, Helices, Proc. Natl. Acad. Sci. 103 (2006) 9398–9403.
[7] D. Dichmann, Y. Li, J.H. Maddocks, Hamiltonian formulations and symmetries in rod mechanics, in: Mathematical Approaches to Biomolecular Structure and Dynamics, Minneapolis, MN, 1994, in: IMA Vol. Math. Appl., vol. 82, Springer, New York, 1996, pp. 71–113.
[8] F. Gay-Balmaz, T.S. Ratiu, The geometric structure of complex fluids, Adv. Appl. Math. 42 (2) (2009) 176–275.
[9] J. Gibbons, D.D. Holm, B.A. Kupershmidt, Gauge-invariant Poisson brackets for chromohydrodynamics, Phys. Lett. A 90 (1982) 281–283.
[10] R. Goldstein, A. Goriely, G. Huber, C. Wolgemuth, Bistable helixes, Phys. Rev. Lett. 84 (2000) 1631–1634.
[11] R. Goldstein, T.R. Powers, C.H. Wiggins, Viscous nonlinear dynamics of twist and writhe, Phys. Rev. Lett. 80 (1998) 5232–5235.
[12] A. Hausrath, A. Goriely, Repeat protein architectures predicted by a continuum representation of fold space, Protein Sci. 15 (2006) 1–8.
[13] D.D. Holm, Euler–Poincaré dynamics of perfect complex fluids, Geometry, Mechanics and Dynamics, Special Volume in Honor of J.E. Marsden (2001) 113–167.
[14] D.D. Holm, B.A. Kupershmidt, The analogy between spin glasses and Yang–Mills fluids, J. Math. Phys. 29 (1988) 21–30.
[15] I. Mezic, On the dynamics of molecular conformation, Proc. Natl. Acad. Sci. 103 (2006) 7542–7547.
[16] J.C. Simó, J.E. Marsden, P.S. Krishnaprasad, The Hamiltonian structure of nonlinear elasticity: The material and convective representations of solids, rods, and plates, Arch. Rational Mech. Anal. 104 (1988) 125–183.