THE DYNAMICS OF CONSERVATIVE CHARGED MOLECULAR STRANDS

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PLAN OF THE PRESENTATION

- **Dynamics of charged molecular strands**
- **Affine variational principles**
- **Dynamics of multibouquets**

DYNAMICS OF CHARGED MOLECULAR STRANDS

- Long molecules may be understood as strands of charged units.
- Dynamics depends both on the local elastic deformations of the strand and the nonlocal (screened electrostatic) interactions of charged units across the folds in the molecule.
- Electrostatic interactions depend on spatial distances and relative orientations between individual charged units in different locations.
- Full dynamical simulation: complicated, gives little insight for analytical understanding of the dynamics.
- Continuum approaches to the dynamics of molecular strands offer an alternative theoretical understanding; attractive because of the insight in finding analytical solutions. Starts with Kirchhoff [1859].
- Generalization of Kirchhoff theory to account for the torque caused by the long-range electrostatic interaction of molecules in different spatial locations along a flexible strand has not been achieved because the classical Kirchhoff theory is formulated in a frame moving with the strand, but it deals with a mixture of variables, some measured in the fixed spatial frame and some in the body frame.

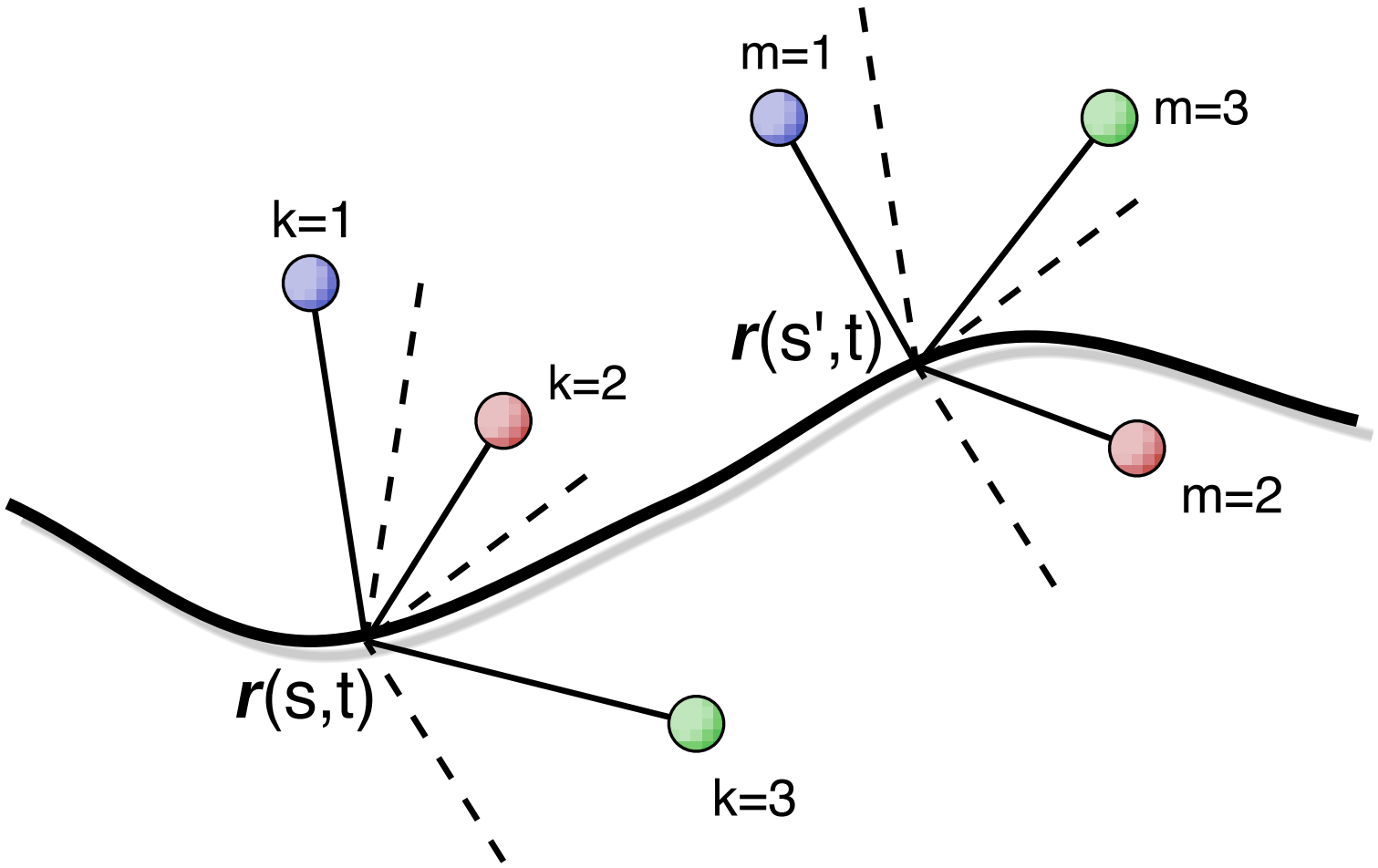
• The torque due to long-range interactions presents a particular difficulty for the mixed representations in the Kirchhoff theory, because it is applied at base points of a curve that is moving in space. That is, the spatial Euclidean distances and relative orientations of the molecules must be reconstructed at each time step during the sinuous motion and twisting of the strand before any self-consistent computation can be made of the forces and torques due to long-range electrostatic interactions.

• Even when electrostatic forces are not involved, the motion of realistic curves in space is inherently nonlocal, because of the requirement that the curve not cross itself during the dynamics. In the purely elastic Kirchhoff approach, such nonlocal considerations are neglected. Physically, however, self-intersections are prevented by the existence of a short-range potential (e.g., Lennard-Jones potential) that produces highly repulsive forces when two points along the curve approach each other. Thus, forces between segments of the strand that could be quite distant along its arc length are essential for the physical description of its dynamics.

• We solve some of these problems: we allow the treatment of both torques and forces from electrostatic interactions.

• We cast the problem of strand dynamics for an arbitrary intermolecular potential into the **convective representation**. Its methods are also applicable to the consideration of Lennard-Jones potentials and the constrained motion of non-self-interacting curves.

• This constrained motion can be generalized to allow flexible motion of the strand (time-dependent bend, twist and writhe) while also including the degrees of freedom of molecular orientation excited during the process of, say, DNA folding. According to this class of models, a DNA molecule is represented as a flexible filament or strand, along which are attached various different types of rigid conformations of sub-molecules that may *swivel* relative to each other in three dimensions under their mutual interactions. The flexibility of the filament arises physically because the electrostatic interaction between any pair of these rigid conformations either along the filament or across from one loop to another of its folds is much weaker than the internal interactions that maintain the shape of an individual charged conformation.



• We consider rigid charge conformations (RCCs) mounted along a flexible filament. We use **geometrically exact rod theory** which is expressed in the **convective representation** of continuum mechanics.

• These rigid conformations of multiple charges are allowed to interact via an effective many-body potential representing their screened electrostatic interactions. The nonlocal interactions among these RCCs depend on their spatial separations and relative orientations, which are both allowed to evolve dynamically. Thus, the inertial motion of a pair of RCCs mounted at any two spatial points $\boldsymbol{r}(s,t)$ and $\boldsymbol{r}(s',t)$ along the filament is governed by an effective potential interaction energy that depends on their separation and relative orientation.

• Filament is one-dimensional, the orientations of the rigid charged conformations mounted along it are three-dimensional.

• Example: Vinylidene fluoride (VDF) oligomer; it is approximated by a strand carrying a dipole moment whose orientation is perpendicular to the axis of the strand. The VDF oligomer strand is straight for small lengths, but it forms complex shapes due to electrostatic interactions for longer lengths.

• The theory presented here generalizes directly to the case when the dimension of the underlying manifold (filament) is greater than one: motion of charged sheets, or charged elastically deformable media.

Lagrangian representation variables: $\Lambda(s,t) \in SO(3)$, $\boldsymbol{r}(s,t) \in \mathbb{R}^3$. The vector $\boldsymbol{r}(s,t)$ is the *spatial position of the filament* and the variable $\Lambda(s,t)$ denotes the *rotation of the RCC at the point s along the filament at time t*. By taking the time and space derivatives, we find the *material velocity* $(\dot{\Lambda}(s,t), \dot{\boldsymbol{r}}(s,t))$ and the *angular and linear deformation gradients* $(\Lambda'(s,t), \boldsymbol{r}'(s,t))$, respectively. Given Λ and $\boldsymbol{r}$, we introduce notation for the following *reduced variables*

$$
\begin{aligned}
\widehat{\Omega} = \Omega &= \Lambda^{-1}\Lambda' &&\in \mathfrak{so}(3)\,,\\
\widehat{\boldsymbol{\omega}} = \omega &= \Lambda^{-1}\dot{\Lambda} &&\in \mathfrak{so}(3)\,,\\
\boldsymbol{\Gamma} &= \Lambda^{-1}\boldsymbol{r}' &&\in \mathbb{R}^3\,,\\
\boldsymbol{\gamma} &= \Lambda^{-1}\dot{\boldsymbol{r}} &&\in \mathbb{R}^3\,,\\
\boldsymbol{\rho} &= \Lambda^{-1}\boldsymbol{r} &&\in \mathbb{R}^3\,.
\end{aligned}
$$

Physical interpretation of the variables: $\boldsymbol{\rho}(s,t)$ represents the *position of the filament in space as viewed by an observer* who moves with the RCC at (s,t). The variables $\big(\boldsymbol{\Omega}(s,t), \boldsymbol{\Gamma}(s,t)\big)$ describe the *deformation gradients as viewed by an observer* who moves with the RCC. The variables $\big(\boldsymbol{\omega}(s,t), \boldsymbol{\gamma}(s,t)\big)$ describe the *body angular velocity* and the *linear velocity as viewed by an observer* who moves with the RCC.

Here $\Lambda, \boldsymbol{r}, \Omega, \omega, \boldsymbol{\Gamma}, \boldsymbol{\gamma}, \boldsymbol{\rho}$ are functions of (s,t). It is important to see these variables as time-dependent curves with values in function spaces. For example, we can interpret $\Lambda(s,t)$ as a function of space and time

$$(s,t) \in [0,L] \times \mathbb{R} \mapsto \Lambda(s,t) \in SO(3),$$

or we can see Λ as a curve in an infinite dimensional Lie group

$$t \in \mathbb{R} \mapsto \Lambda(\cdot,t) \in \mathcal{F}([0,L], SO(3)),$$

where $\mathcal{F}([0,L], SO(3))$ denotes the group of smooth functions defined on $[0,L]$ with values in $SO(3)$.

This observation is fundamental and leads to two different geometric approaches of the same equations: the **affine Euler-Poincaré** and the **covariant Lagrange-Poincaré** approaches.

Second approach is not discussed in this talk.

Energy

Curve $\boldsymbol{r}(s)$, $s \in [0, L]$ (extensible filament).

The spatial reference (undisturbed) state for the k^{th} charge:

$$\boldsymbol{r}(s) + \boldsymbol{\eta}_k(s),$$

$\boldsymbol{\eta}_k(s)$ is a vector of constant length that determines the position of the k^{th} electrical charge relative to the point $\boldsymbol{r}(s)$ along the curve in its reference configuration. The $\boldsymbol{\eta}_k(s)$ specify the shape of the rigid conformation of charges. At time t the position $\mathbf{c}_k$ of the k^{th} charge in the rigid conformation anchored at spatial position $\boldsymbol{r}(s,t)$ along the curve parametrized by s may rotate to a new position corresponding to the orientation $\Lambda(s,t)$:

$$\mathbf{c}_k(s,t) = \boldsymbol{r}(s,t) + \Lambda(s,t)\boldsymbol{\eta}_k(s)\,, \quad \text{where} \quad \Lambda(s,0) = \mathrm{Id}.$$

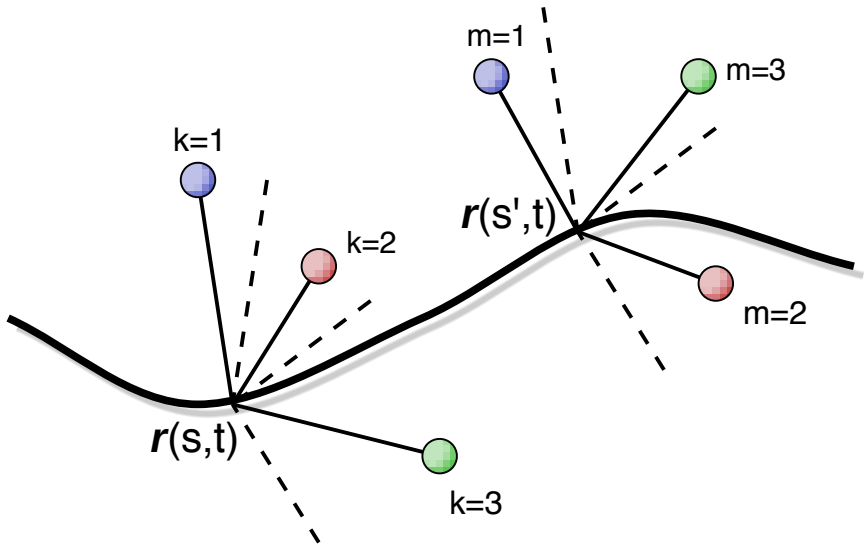
Mezić [2006], PNAS: $\Lambda \in SO(2)$, $k = 1$.

Vector of charge k at spatial position $\mathbf{c}_k(s)$, vector of charge m at spatial position $\mathbf{c}_m(s')$.

One part of the potential energy depends only on the distance

$$\begin{aligned} d_{k,m}(s,s') :&= \left|\mathbf{c}_m(s') - \mathbf{c}_k(s)\right| = \left|\Lambda^{-1}(s)\left(\mathbf{c}_m(s') - \mathbf{c}_k(s)\right)\right| \\ &= \left|\Lambda^{-1}(s)\left(\boldsymbol{r}(s') - \boldsymbol{r}(s)\right) + \Lambda^{-1}(s)\Lambda(s')\boldsymbol{\eta}_m(s') - \boldsymbol{\eta}_k(s)\right| \\ &= \left|\boldsymbol{\kappa}(s,s') + \xi(s,s')\boldsymbol{\eta}_m(s') - \boldsymbol{\eta}_k(s)\right|, \end{aligned}$$

where $\boldsymbol{\kappa}(s,s') := \Lambda^{-1}(s)\left(\boldsymbol{r}(s') - \boldsymbol{r}(s)\right) \in \mathbb{R}^3$ is the spatial vector from $\boldsymbol{r}(s)$ to $\boldsymbol{r}(s')$, as seen from the orientation $\Lambda(s)$ of the rigid charge conformation located at coordinate label s along the filament and $\xi(s,s') := \Lambda^{-1}(s)\Lambda(s') \in SO(3)$ is the relative orientation of the rigid charge conformations located at coordinate labels s and s'.



$(\xi(s,s'),\boldsymbol{\kappa}(s,s')) = (\Lambda,\boldsymbol{r})^{-1}(s)(\Lambda,\boldsymbol{r})(s')$ is left $SE(3)$-invariant.

• $E_{loc}(\boldsymbol{\Omega},\boldsymbol{\Gamma},\boldsymbol{\rho})$ local part of potential energy, represents the purely elastic part; often quadratic in $(\boldsymbol{\Omega},\boldsymbol{\Gamma})$.

• E_{np} is the nonlocal part of the potential energy determined by an interaction potential $U(d_{k,m})$:

$$-\sum_{k,m}\frac{1}{2}\int_0^L\int_0^L U\left(d_{k,m}(s,s')\right)\left|\frac{d\boldsymbol{r}}{ds}(s)\right|\left|\frac{d\boldsymbol{r}}{ds}(s')\right|\mathrm{d}s\mathrm{d}s'$$

$$=-\sum_{k,m}\frac{1}{2}\int_0^L\int_0^L U\left(d_{k,m}(s,s')\right)\left|\boldsymbol{\Gamma}(s)\right|\left|\boldsymbol{\Gamma}(s')\right|\mathrm{d}s\mathrm{d}s'$$

• Lagrangian $l = l_{loc}(\boldsymbol{\omega},\boldsymbol{\gamma},\boldsymbol{\Omega},\boldsymbol{\Gamma},\boldsymbol{\rho}) + l_{np}$, where $l_{np} = -E_{np}$, $l_{loc} = K(\boldsymbol{\omega},\boldsymbol{\gamma}) - E_{loc}(\boldsymbol{\Omega},\boldsymbol{\Gamma},\boldsymbol{\rho})$, $K(\boldsymbol{\omega},\boldsymbol{\gamma})$ kinetic energy. Assume, more generally, that $l_{np} = l_{np}(\xi,\boldsymbol{\kappa},\boldsymbol{\Gamma})$, e.g. (we shall assume this form now),

$$l_{np}(\xi,\boldsymbol{\kappa},\boldsymbol{\Gamma}) = \int_0^L\int_0^L U\Big(\xi(s,s'),\boldsymbol{\kappa}(s,s'),\boldsymbol{\Gamma}(s),\boldsymbol{\Gamma}(s')\Big)\mathrm{d}s\mathrm{d}s'$$

Filament dynamics

Idea: Get quickly equations using the Pontryagin principle; introduce Lagrange multipliers for the holonomic constraints that impose the defining relations for the five reduced variables $(\omega, \gamma, \mathbf{\Omega}, \mathbf{\Gamma}, \rho)$.

A.) **Local terms**: *The equations arise from* $\delta S = 0$, *where*

$$S = \int l(\boldsymbol{\omega}, \gamma, \mathbf{\Omega}, \mathbf{\Gamma}, \boldsymbol{\rho})\, dt + \iint \Big(\boldsymbol{\pi} \cdot \big(\Lambda^{-1} \dot{\Lambda} - \omega \big) + \mathbf{\Pi} \cdot \big(\Lambda^{-1} \Lambda' - \Omega \big) + \mathbf{R} \cdot \big(\Lambda^{-1} \boldsymbol{r} - \boldsymbol{\rho} \big) + \boldsymbol{\mu} \cdot \big(\Lambda^{-1} \dot{\boldsymbol{r}} - \boldsymbol{\gamma} \big) + \mathbf{M} \cdot \big(\Lambda^{-1} \boldsymbol{r}' - \mathbf{\Gamma} \big) \Big) ds\, dt.$$

These equations are

$$\frac{\delta l}{\delta \boldsymbol{\rho}} = \mathbf{R}, \quad \frac{\delta l}{\delta \boldsymbol{\omega}} = \boldsymbol{\pi}, \quad \frac{\delta l}{\delta \mathbf{\Omega}} = \mathbf{\Pi}, \quad \frac{\delta l}{\delta \boldsymbol{\gamma}} = \boldsymbol{\mu}, \quad \frac{\delta l}{\delta \mathbf{\Gamma}} = \mathbf{M},$$

$$\dot{\boldsymbol{\pi}} + \boldsymbol{\omega} \times \boldsymbol{\pi} + \mathbf{\Pi}' + \mathbf{\Omega} \times \mathbf{\Pi} + \boldsymbol{\gamma} \times \boldsymbol{\mu} + \mathbf{\Gamma} \times \mathbf{M} + \boldsymbol{\rho} \times \mathbf{R} = 0\,,$$

$$\dot{\boldsymbol{\mu}} + \boldsymbol{\omega} \times \boldsymbol{\mu} + \mathbf{M}' + \mathbf{\Omega} \times \mathbf{M} - \mathbf{R} = 0\,,$$

together with the constraints,

$$\Lambda^{-1} \dot{\Lambda} = \omega\,, \quad \Lambda^{-1} \Lambda' = \Omega\,, \quad \Lambda^{-1} \boldsymbol{r} = \boldsymbol{\rho}\,, \quad \Lambda^{-1} \dot{\boldsymbol{r}} = \boldsymbol{\gamma}\,, \quad \Lambda^{-1} \boldsymbol{r}' = \mathbf{\Gamma}.$$

B.) **Nonlocal terms, also via Pontryagin principle:**

Equations from the variational principle with the nonlocal action

$$S_{np} = \iiint U(\xi, \boldsymbol{\kappa}, \boldsymbol{\Gamma}) ds ds' dt + \iint \boldsymbol{m} \cdot \left(\Lambda^{-1}(s) \boldsymbol{r}'(s) - \boldsymbol{\Gamma} \right) ds dt$$

$$+ \iiint \left(X \cdot \left(\Lambda^{-1}(s) \Lambda(s') - \xi \right) + \boldsymbol{K} \cdot \left(\Lambda^{-1}(s) \left(\boldsymbol{r}(s') - \boldsymbol{r}(s) \right) - \boldsymbol{\kappa} \right) \right) ds ds' dt$$

are given by:

$$X = \frac{\partial U}{\partial \xi}, \qquad \boldsymbol{K} = \frac{\partial U}{\partial \boldsymbol{\kappa}}, \qquad \boldsymbol{m} = \frac{\partial U}{\partial \boldsymbol{\Gamma}},$$

$$\boldsymbol{\Gamma} \times \boldsymbol{m} = \int \left(\xi(s,s') X(s',s) - X(s,s') \xi^{-1}(s,s') + \boldsymbol{K}(s,s') \times \boldsymbol{\kappa}(s,s') \right) ds',$$

$$\boldsymbol{m}' + \boldsymbol{\Omega} \times \boldsymbol{m} = \int \left(\xi(s,s') \boldsymbol{K}(s',s) - \boldsymbol{K}(s,s') \right) ds',$$

together with the constraints,

$$\xi = \Lambda^{-1}(s) \Lambda(s'), \quad \boldsymbol{\kappa} = \Lambda^{-1}(s) \left(\boldsymbol{r}(s') - \boldsymbol{r}(s) \right), \quad \boldsymbol{\Gamma} = \Lambda^{-1}(s) \boldsymbol{r}'(s).$$

C.) Equations of motion

$$\widehat{Z}(s,s') := \xi(s,s')\left(\frac{\partial U}{\partial \xi}(s,s')\right)^{\mathsf{T}} - \frac{\partial U}{\partial \xi}(s,s')\xi^{\mathsf{T}}(s,s')$$

is the contribution from the nonlocal part of the Lagrangian.

$$(\partial_t + \boldsymbol{\omega}\times)\frac{\delta l_{loc}}{\delta \boldsymbol{\omega}} + (\partial_s + \boldsymbol{\Omega}\times)\frac{\delta l_{loc}}{\delta \boldsymbol{\Omega}} = \frac{\delta l_{loc}}{\delta \boldsymbol{\gamma}} \times \boldsymbol{\gamma} + \frac{\delta\left(l_{loc} + l_{np}\right)}{\delta \boldsymbol{\Gamma}} \times \boldsymbol{\Gamma}$$
$$+ \frac{\delta l_{loc}}{\delta \boldsymbol{\rho}} \times \boldsymbol{\rho} + \int \left(\frac{\partial U}{\partial \boldsymbol{\kappa}}(s,s') \times \boldsymbol{\kappa}(s,s') + \boldsymbol{Z}(s,s')\right) ds' \,,$$

$$(\partial_t + \boldsymbol{\omega}\times)\frac{\delta l_{loc}}{\delta \boldsymbol{\gamma}} + (\partial_s + \boldsymbol{\Omega}\times)\frac{\delta\left(l_{loc} + l_{np}\right)}{\delta \boldsymbol{\Gamma}}$$
$$= \frac{\delta l_{loc}}{\delta \boldsymbol{\rho}} + \int \left(\xi(s,s')\frac{\partial U}{\partial \boldsymbol{\kappa}}(s',s) - \frac{\partial U}{\partial \boldsymbol{\kappa}}(s,s')\right) ds'.$$

plus the "advection equations" (derivatives of defining relations)

$$\partial_t \boldsymbol{\rho} = -\boldsymbol{\omega} \times \boldsymbol{\rho} + \boldsymbol{\gamma}, \quad \partial_t \boldsymbol{\Gamma} + \boldsymbol{\omega} \times \boldsymbol{\Gamma} = \boldsymbol{\gamma}' + \boldsymbol{\Omega} \times \boldsymbol{\gamma}, \quad \partial_t \boldsymbol{\Omega} = \boldsymbol{\omega}' + \boldsymbol{\omega} \times \boldsymbol{\Omega}$$

- Kirchhoff filament: $\boldsymbol{\rho}$ and ξ absent.
- Pontryagin principle allows the addition of nonholonomic constraints

D.) Constrained variational principle

Variations are constrained because the variables $\boldsymbol{\rho}, \boldsymbol{\gamma}, \boldsymbol{\omega}, \boldsymbol{\Gamma}, \boldsymbol{\Omega}, \boldsymbol{\kappa}, \xi$ are defined in a very specific way; $\widehat{\boldsymbol{\Sigma}} = \boldsymbol{\Sigma} := \Lambda^{-1}\delta\Lambda$, $\boldsymbol{\Psi} = \Lambda^{-1}\delta\boldsymbol{r}$

$$\delta\boldsymbol{\rho} = \boldsymbol{\rho}\times\boldsymbol{\Sigma} + \boldsymbol{\Psi}, \qquad \delta\boldsymbol{\gamma} = \boldsymbol{\gamma}\times\boldsymbol{\Sigma} + \boldsymbol{\omega}\times\boldsymbol{\Psi} + \frac{\partial\boldsymbol{\Psi}}{\partial t}$$

$$\delta\boldsymbol{\omega} = \boldsymbol{\omega}\times\boldsymbol{\Psi} + \frac{\partial\boldsymbol{\Sigma}}{\partial t}, \qquad \delta\boldsymbol{\Gamma} = \boldsymbol{\Gamma}\times\boldsymbol{\Sigma} + \boldsymbol{\Omega}\times\boldsymbol{\Psi} + \frac{\partial\boldsymbol{\Psi}}{\partial s}$$

$$\delta\boldsymbol{\Omega} = \boldsymbol{\Omega}\times\boldsymbol{\Sigma} + \frac{\partial\boldsymbol{\Sigma}}{\partial s}, \qquad \xi^{-1}\delta\xi(s,s') = -\mathrm{Ad}_{\xi^{-1}(s,s')}\boldsymbol{\Sigma}(s) + \boldsymbol{\Sigma}(s')$$

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

$$l(\boldsymbol{\omega},\boldsymbol{\gamma},\boldsymbol{\Omega},\boldsymbol{\Gamma},\boldsymbol{\rho},\xi,\boldsymbol{\kappa}) := l_{loc} + l_{np}$$
$$= l_{loc}(\boldsymbol{\omega},\boldsymbol{\gamma},\boldsymbol{\Omega},\boldsymbol{\Gamma},\boldsymbol{\rho}) + \iint U\left(\boldsymbol{\kappa}(s,s'),\xi(s,s'),\boldsymbol{\Gamma}(s),\boldsymbol{\Gamma}(s')\right)\mathrm{d}s\mathrm{d}s'$$

The variational principle $\delta\int l\mathrm{d}t = 0$ for the constrained variations above yields the same equations of motion to which one has to add the "advection equations" to close the system.

QUESTION: What is the geometric formulation of this procedure?

AFFINE VARIATIONAL PRINCIPLES

A.) One-cocycles

Left representation of G on the vector space V^*. We can form an *affine left* representation $\theta_g(a) := ga + c(g)$, where $c \in C^\infty(G, V^*)$ is a **left group one-cocycle**, that is, it verifies the property

$$c(gh) = c(g) + gc(h), \qquad g, h \in G.$$

$$\left.\frac{d}{dt}\right|_{t=0} \theta_{\exp(t\xi)}(a) = \xi a + \mathbf{d}c(\xi), \quad \langle \xi a, v\rangle_V := -\langle a, \xi v\rangle_V$$

and

$$\langle \xi a + \mathbf{d}c(\xi), v\rangle_V = \langle \mathbf{d}c^\mathsf{T}(v) - v \diamond a,\, \xi\rangle_\mathfrak{g}\,,$$

where $\mathbf{d}c : \mathfrak{g} \to V^*$ is defined by $\mathbf{d}c(\xi) := T_e c(\xi)$, and $\mathbf{d}c^\mathsf{T} : V \to \mathfrak{g}^*$ by

$$\langle \mathbf{d}c^\mathsf{T}(v), \xi\rangle_\mathfrak{g} := \langle \mathbf{d}c(\xi), v\rangle_V, \quad \text{and} \quad \langle v \diamond a, \xi\rangle_\mathfrak{g} := \langle a, \xi v\rangle_V = -\langle \xi a, v\rangle_V$$

B.) Affine variational principle

• $L : TG \times V^* \to \mathbb{R}$ *left* invariant under affine G-action

$$g \cdot (v_h, a) := (gv_h, \theta_g(a)) = (gv_h, ga + c(g)).$$

• For $a_{ref} \in V^*$, the Lagrangian $L_{a_{ref}} : TG \to \mathbb{R}$, $L_{a_{ref}}(v_g) := L(v_g, a_{ref})$ is left $G^c_{a_{ref}}$-invariant, where $G^c_{a_{ref}}$ is the isotropy group of a_{ref} with respect to the affine action θ.

• Define $l : \mathfrak{g} \times V^* \to \mathbb{R}$ by $l := L|_{\mathfrak{g} \times V^*}$. Left G-invariance of L yields

$$l(g^{-1}v_g, \theta_{g^{-1}}(a)) = L(v_g, a)$$

for all $g \in G$, $v_g \in T_gG$, $a \in V^*$.

• Given $g(t) \in G$, let $\xi(t) := g(t)^{-1}\dot{g}(t) \in \mathfrak{g}$ and define $a(t)$ as the unique solution of the affine ODE with time dependent coefficients

$$\dot{a} = -\xi a - \mathbf{d}c(\xi),$$

with initial condition $a(0) = g(0)^{-1}a_{ref} + c\left(g(0)^{-1}\right)$. The solution is: $a(t) = \theta_{g(t)^{-1}}(a_{ref}) = g(t)^{-1}a_{ref} + c\left(g(t)^{-1}\right)$.

(i) *With a_{ref} held fixed, Hamilton's variational principle*

$$\delta \int_{t_0}^{t_1} L_{a_{ref}}(g, \dot{g}) dt = 0$$

holds, for variations $\delta g(t)$ of $g(t)$ vanishing at the endpoints.

(ii) *$g(t)$ satisfies the Euler-Lagrange equations for $L_{a_{ref}}$ on G.*

(iii) *The* **constrained affine variational principle**

$$\delta \int_{t_1}^{t_2} l(\xi(t), a(t)) dt = 0$$

holds on $\mathfrak{g} \times V^*$, using variations of the form

$$\delta\xi = \dot{\eta} + [\xi, \eta], \qquad \delta a = -\eta a - \mathbf{d}c(\eta),$$

where $\eta(t) \in \mathfrak{g}$ is any curve vanishing at the endpoints.

(iv) *The* **affine semidirect product Euler-Poincaré equations**

$$\frac{d}{dt}\frac{\delta l}{\delta \xi} = \mathrm{ad}^*_\xi \frac{\delta l}{\delta \xi} + \frac{\delta l}{\delta a} \diamond a - \mathbf{d}c^\mathsf{T}\left(\frac{\delta l}{\delta a}\right)$$

hold on $\mathfrak{g} \times V^*$.

$\diamond : V \times V^* \to \mathfrak{g}^*$ defined by $\langle v \diamond a, \xi \rangle_\mathfrak{g} := -\langle \xi a, v \rangle_V$; momentum map

C.) Affine Hamiltonian formulation

- $H : T^*G \times V^* \to \mathbb{R}$ *left* invariant under the affine G-action

$$g \cdot (\alpha_h, a) := (g\alpha_h, \theta_g(a)) = (g\alpha_h, ga + c(g)).$$

- For $a_{ref} \in V^*$, the Hamiltonian $H_{a_{ref}} : T^*G \to \mathbb{R}$, $H_{a_{ref}}(\alpha_g) := H(\alpha_g, a_{ref})$ is left $G^c_{a_{ref}}$-invariant; recall $G^c_{a_{ref}}$ is the isotropy group of a_{ref} with respect to the affine action θ.

- Let $h : \mathfrak{g}^* \times V^* \to \mathbb{R}$ by $h := H|_{\mathfrak{g}^* \times V^*}$. Left G-invariance of H yields

$$h(g^{-1}\alpha_g, \theta_{g^{-1}}(a)) = H(\alpha_g, a).$$

for all $g \in G$, $\alpha_g \in T^*_g G$, $a \in V^*$.

G-action on $T^*G \times V^*$ induced by S-action on $T^*S = T^*G \times (V \times V^*)$

$$\Psi_{(g,v)}(\alpha_h, (u, a)) := (g\alpha_h, v + gu, ga + c(g)) ;$$

cotangent lift of left translation on S plus an affine cocycle term. So think of $H : T^*G \times V^* \to \mathbb{R}$ as the Poisson reduction of a S-invariant Hamiltonian $\overline{H} : T^*S \to \mathbb{R}$ by the normal subgroup $\{e\} \times V$ since $(T^*S)/(\{e\} \times V) \cong T^*G \times V^*$.

Let $\alpha(t) \in T^*_{g(t)}G$ be a solution of $X_{H_{a_{ref}}}$ with $\alpha(0) = \mu_0 \in T^*_eG$. Then $(\mu(t), a(t)) := (g(t)^{-1}\alpha(t), \theta_{g(t)^{-1}}(a_{ref})) \in \mathfrak{g}^* \times V^*$ solution of

$$\frac{\partial}{\partial t}(\mu, a) = \left(\mathrm{ad}^*_{\frac{\delta h}{\delta \mu}} \mu - \frac{\delta h}{\delta a} \diamond a + \mathbf{d}c^{\mathsf{T}} \left(\frac{\delta h}{\delta a} \right), -\frac{\delta h}{\delta \mu} a - \mathbf{d}c \left(\frac{\delta h}{\delta \mu} \right) \right)$$

with $(\mu(0), a(0)) = (\mu_0, a_{ref})$. Affine Lie-Poisson bracket on $\mathfrak{s}^*$:

$$\{f, g\}(\mu, a) = -\left\langle \mu, \left[\frac{\delta f}{\delta \mu}, \frac{\delta g}{\delta \mu} \right] \right\rangle - \left\langle a, \frac{\delta f}{\delta \mu} \frac{\delta g}{\delta a} - \frac{\delta g}{\delta \mu} \frac{\delta f}{\delta a} \right\rangle + \left\langle \mathbf{d}c \left(\frac{\delta f}{\delta \mu} \right), \frac{\delta g}{\delta a} \right\rangle - \left\langle \mathbf{d}c \left(\frac{\delta g}{\delta \mu} \right), \frac{\delta f}{\delta a} \right\rangle.$$

Conversely, given $\alpha(0) = \mu_0 \in T^*_eG$, solution $\alpha(t)$ of $X_{H_{a_{ref}}}$ is reconstructed from the solution $(\mu(t), a(t))$ with initial conditions $(\mu(0), a(0)) = (\mu_0, a_{ref})$ by setting $\alpha(t) = g(t)\mu(t)$, where $g(t)$ is solution of $\dot{g}(t) = g(t)\frac{\delta h}{\delta \mu(t)}$ with initial condition $g(0) = e$.

Conserved quantity $\mathbf{J} : T^*S \to \mathfrak{s}^*$ associated to the action Ψ:

$$\mathbf{J}(\alpha_g, (u, b)) = (\alpha_g g^{-1} + u \diamond b - \mathbf{d}c^{\mathsf{T}}(u), b), \quad g \in G,\ \alpha_g \in T^*G,\ u \in V,\ b \in V^*.$$

Conservation of $\mathbf{J} \Rightarrow$ motion takes place on affine coadjoint orbits.

D.) Affine reduction at fixed parameter

Big problem!

Affine semidirect product reduction does not apply to the molecular strand because L is only given for $a_{ref} = 0$ and we do not know $L_{a_{ref}}$ if $a_{ref} \neq 0$ is an arbitrary element of V^*.

Extending $L_{a_{ref}}$ by G-invariance only yields a Lagrangian on $TG \times \mathcal{O}_0^c$, where $\mathcal{O}_0^c \subset V^*$ is the orbit of the affine G-action on V^*.

Fortunately, the Lagrangian $L_{a_{ref}}$ for the molecular strand is invariant under the isotropy group $G_0^c = \{g \in G \mid c(g) = 0\}$. We will see that this is enough for the extension of the affine semidirect product reduction theorem.

Hypotheses

Fix $a_{ref} \in V^*$ and assume that $L_{a_{ref}} : TG \to \mathbb{R}$ is $G^c_{a_{ref}}$-invariant.

But do not assume that $L_{a_{ref}}$ comes from a G-invariant function $L : TG \times V^* \to \mathbb{R}$. In particular, we do not have an expression of L_a when $a \neq a_{ref}$ is an arbitrary element of V^*.

To $L_{a_{ref}}$ we associate the reduced Lagrangian l on the submanifold

$$\mathfrak{g} \times \mathcal{O}^c_{a_{ref}} \subset \mathfrak{g} \times V^*, \quad \mathcal{O}^c_{a_{ref}} := \{\theta_g(a_{ref}) \mid g \in G\}$$

given by $l(\xi, \theta_g(a_{ref})) = L_{a_{ref}}(g^{-1}\xi)$.

The tangent space at a to $\mathcal{O}^c_{a_{ref}}$ is given by

$$T_a\mathcal{O}^c_{a_{ref}} = \{\mathbf{d}c(\eta) + \eta a \mid \eta \in \mathfrak{g}\}.$$

Extend the affine semidirect product reduction theorem: *$a_{ref} \in V^*$ fixed, $g(t) \in G$, $g(0) = e$. Define $\xi(t) = g(t)^{-1}\dot{g}(t) \in \mathfrak{g}$ and $a(t) := \theta_{g(t)^{-1}} a_{ref} \in V^*$. The following are equivalent*:

(i) *With a_{ref} held fixed, Hamilton's variational principle*

$$\delta \int_{t_0}^{t_1} L_{a_{ref}}(g, \dot{g}) dt = 0$$

holds for variations $\delta g(t)$ of $g(t)$ vanishing at the endpoints.
(ii) *$g(t)$ satisfies the Euler-Lagrange equations for $L_{a_{ref}}$ on G.*
(iii) *The constrained variational principle*

$$\delta \int_{t_0}^{t_1} l(\xi, a) dt = 0$$

holds on $\mathfrak{g} \times \mathcal{O}^c_{a_{ref}} \subset \mathfrak{g} \times V^*$, using variations of the form

$$\delta\xi = \frac{\partial \eta}{\partial t} + [\xi, \eta], \quad \delta a = -\eta a - \mathbf{d}c(\eta),$$

where $\eta(t) \in \mathfrak{g}$ vanishes at the endpoints.
(iv) *Extending l arbitrarily to $\mathfrak{g} \times V^*$, the affine Euler-Poincaré equations hold on the submanifold $\mathfrak{g} \times \mathcal{O}^c_{a_{ref}} \subset \mathfrak{g} \times V^*$:*

$$\frac{\partial}{\partial t}\frac{\delta l}{\delta \xi} = \mathrm{ad}^*_\xi \frac{\delta l}{\delta \xi} + \frac{\delta l}{\delta a} \diamond a - \mathbf{d}c^\mathsf{T}\left(\frac{\delta l}{\delta a}\right).$$

E.) The case $a_{ref} = 0$ and the charged strand

Charged molecular strand: $a_{ref} = 0$, so $G_0^c = \{g \in G \mid c(g) = 0\}$. Given a G_0^c-invariant Lagrangian $L_0 : TG \to \mathbb{R}$, the reduced Lagrangian l is defined on $\mathfrak{g} \times \mathcal{O}_0^c$ by

$$l(\xi, c(g^{-1})) = L_0(g\xi).$$

Work with classical Lagrangians $L_0(v_g) := K(v_g) - P(g)$, where K is the kinetic energy of a G_0^c-invariant Riemannian metric on G and the potential energy P is G_0^c-invariant. So, reduced Lagrangian is

$$l(\xi, c(g^{-1})) = K(g\xi) - P(g).$$

Note that RHS is well defined on $\mathfrak{g} \times \mathcal{O}_0^c$, i.e., it depends on g only through $c(g^{-1})$: $c(g^{-1}) = c(h^{-1}) \iff \theta_{g^{-1}}(0) = \theta_{h^{-1}}(0) \iff hg^{-1} \in G_0^c$. So $P(h) = P((hg^{-1})g) = P(g)$ by left G_0^c-invariance. Similarly for K. So $P(g) = E(c(g^{-1}))$ for a unique $E : V^* \to \mathbb{R}$ and hence

$$l(\xi, c(g^{-1})) = K(g\xi) - E(c(g^{-1})).$$

Charged strand: $P = E_{loc} + E_{np}$, E_{loc} explicitly depends only on $c(g^{-1})$, E_{np} does not have a concrete expression only in terms of $c(g^{-1})$ but it is G_0^c-invariant. K is not just G_0^c-invariant but G-invariant, so it is a function of $\xi \in \mathfrak{g}$ alone. So

$$\begin{aligned} l(\xi, c(g^{-1})) &= \underbrace{K(\xi) - E_{loc}(c(g^{-1}))}_{=l_{loc}} - E_{np}(\zeta(g), c(g^{-1})) \\ &= l_{loc}(\xi, c(g^{-1})) + l_{np}(\zeta(g), c(g^{-1})), \end{aligned}$$

where $\zeta : G \to \mathbb{R}$ is G_0^c-invariant. In terms of $(\xi, a) \in \mathfrak{g} \times \mathcal{O}_0^c$:

$$l(\xi, a) = K(\xi) - E_{loc}(a) - E_{np}(\zeta(g_a), a) = l_{loc}(\xi, a) + l_{np}(\zeta(g_a), a),$$

where $g_a \in G$ is such that $c(g_a^{-1}) = a$, determined only up to left multiplication by G_0^c. Since E_{np} is G_0^c-invariant, the function $a \mapsto E_{np}(\zeta(g_a), a)$ is well-defined – more later.

Concretely, for the charged strand we have:

$$
\begin{aligned}
G &= C^\infty([0,L], SE(3)),\\
\mathfrak{g} &= C^\infty([0,L], \mathfrak{se}(3)),\\
V^* &= \Omega^1([0,L], \mathfrak{se}(3)) \oplus C^\infty([0,L], \mathbb{R}^3),\\
V &= \mathfrak{X}([0,L], \mathbb{R}^3) \oplus C^\infty([0,L], \mathbb{R}^3)\\
c((\Lambda, \boldsymbol{r})^{-1}) &= \Big((\Lambda, \boldsymbol{r})^{-1}(\Lambda, \boldsymbol{r})', \Lambda^{-1}\boldsymbol{r}\Big) = (\Lambda^{-1}\Lambda', \Lambda^{-1}\boldsymbol{r}', \Lambda^{-1}\boldsymbol{r})\\
&= (\boldsymbol{\Omega}, \boldsymbol{\Gamma}, \boldsymbol{\rho}) \in V^*, \quad \text{one-cocycle}\\
\zeta(s, s') &= \Big(\xi(s, s'), \boldsymbol{\kappa}(s, s')\Big) = (\Lambda, \boldsymbol{r})^{-1}(s)(\Lambda, \boldsymbol{r})(s') \in SE(3)\\
&\text{so} \quad \zeta(s, \_) \in G; \quad \text{variables are}
\end{aligned}
$$

and the variables are

$$
\begin{aligned}
&(\Lambda, \boldsymbol{r}) \in G, \quad \Lambda \in C^\infty([0,L], SO(3)), \quad \boldsymbol{r} \in C^\infty([0,L], \mathbb{R}^3)\\
&(\boldsymbol{\omega}, \boldsymbol{\gamma}) \in \mathfrak{g}, \quad \boldsymbol{\omega}, \boldsymbol{\gamma} \in C^\infty([0,L], \mathbb{R}^3)\\
&(\boldsymbol{\Omega}, \boldsymbol{\Gamma}, \boldsymbol{\rho}) \in V^*, \quad \boldsymbol{\Omega} \in \Omega^1([0,L], \mathbb{R}^3), \quad \boldsymbol{\Gamma} \in \Omega^1([0,L], \mathbb{R}^3),\\
&\qquad\qquad \boldsymbol{\rho} \in C^\infty([0,L], \mathbb{R}^3)
\end{aligned}
$$

Remark: Since $a \mapsto l_{np}(\zeta(g_a), a)$ is a well-defined function of $a \in \mathcal{O}_0^c$, why write $l_{np} = l_{np}(\zeta(g_a), a)$ instead of simply $l_{np} = l_{np}(a)$? Reason: for the charged strand there is no explicit expression for $l_{np} : \mathcal{O}_0^c \to \mathbb{R}$ but it is exactly of the form $l_{np} = l_{np}(\zeta(g_a), a)$.

QUESTION: How does the variational principle for $l : \mathfrak{g} \times \mathcal{O}_0^c \to \mathbb{R}$, $l(\xi, a) = l_{loc}(\xi, a) + l_{np}(\zeta(g_a), a)$ give affine Euler-Poincaré equations

$$\frac{\partial}{\partial t}\frac{\delta l}{\delta \xi} = \mathrm{ad}^*_\xi \frac{\delta l}{\delta \xi} + \frac{\delta l}{\delta a} \diamond a - \mathbf{d}c^{\mathsf{T}}\left(\frac{\delta l}{\delta a}\right) ?$$

A term seems to be missing!

Indeed, $\delta \int L(\xi(t), c(g(t)^{-1}))\mathrm{d}t = 0$ implies

$$\frac{\partial}{\partial t}\frac{\delta l_{loc}}{\delta \xi} = \mathrm{ad}^*_\xi \frac{\delta l_{loc}}{\delta \xi} + \frac{\delta(l_{loc} + l_{np})}{\delta a} \diamond a - \mathbf{d}c^{\mathsf{T}}\left(\frac{\delta(l_{loc} + l_{np})}{\delta a}\right) + g^{-1}\frac{\delta l_{np}}{\delta \zeta} T_g \zeta.$$

Clearly, $\frac{\delta l_{loc}}{\delta \xi} = \frac{\delta l}{\delta \xi}$, so first two terms match those in the Euler-Poincaré equation. What about the other ones?

l_{np} depends *only* on $a \in \mathcal{O}_0^c$, even though we do not have an explicit formula for it! l_{np} appears as a function of $(\zeta(g), c(g^{-1}))$. Let

$$\left.\frac{\delta l_{np}}{\delta a}\right|_{Tot}$$

be the functional derivative of l_{np} viewed as a function of $a \in \mathcal{O}_0^c$.

Every curve in $\mathcal{O}_0^c$ through $a = c(g^{-1}) \in \mathcal{O}_0^c$ is $c(g_\varepsilon^{-1})$, where $g_0 = g$, we compute in two ways $\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} l_{np}(\zeta(g_\varepsilon), c(g_\varepsilon^{-1}))$ and get the identity

$$\left.\frac{\delta l_{np}}{\delta a}\right|_{Tot} \diamond a - \mathbf{d}c^{\mathsf{T}}\left(\left.\frac{\delta l_{np}}{\delta a}\right|_{Tot}\right) = \frac{\delta l_{np}}{\delta a} \diamond a - \mathbf{d}c^{\mathsf{T}}\left(\frac{\delta l_{np}}{\delta a}\right) + g^{-1}\frac{\delta l_{np}}{\delta \zeta} T_g\zeta,$$

where $a = c(g^{-1})$. Plug this and

$$\frac{\delta l}{\delta a} = \left.\frac{\delta l_{np}}{\delta a}\right|_{Tot} + \frac{\delta l_{loc}}{\delta a}.$$

in the expression above and get the affine Euler-Poincaré equations.

Remarks: All of this has

- A formulation as a conservation law.
- Circulation theorems.
- A generalization that replaces $[0, L]$ by a Riemannian manifold $\mathcal{D}$, $SO(3)$ by a Lie group $\mathcal{O}$ (order parameters), and $\mathbb{R}^3$ by a general $\mathcal{O}$-representation space E.
- A covariant (field theoretical) formulation but only for local potentials.
- A formulation in terms of quaternions.

F.) Hamiltonian formulation

Fix $a_{ref} \in V^*$, $H_{a_{ref}} : T^*G \to \mathbb{R}$ is $G^c_{a_{ref}}$-invariant defined only for this fixed value $a_{ref} \in V^*$. Expression of H_a for $a \neq a_{ref}$ does not exist. The reduced Hamiltonian is only defined on the submanifold

$$\mathfrak{g}^* \times \mathcal{O}^c_{a_{ref}} \subset \mathfrak{s}^*$$

and so the standard theorem cannot be applied.

Introduce the affine coadjoint orbit $\mathcal{O}^{\sigma}_{(\mu,a)} \subset \mathfrak{s}^*$. The left V^*-valued group one-cocycle $c : G \to V^*$ induces a left group one-cocycle $\sigma : S \to (\mathfrak{g} \circledS V)^*$ by

$$\sigma(g,u) = (u \diamond c(g) - \mathbf{d}c^{\mathsf{T}}(u), c(g)).$$

The affine coadjoint action of S on $\mathfrak{s}^*$ is hence given by

$$(g,u)(\mu,a) := \mathsf{Ad}^*_{(g,u)^{-1}}(\mu,a) + \sigma((g,u)^{-1}),$$

where $g \in G$, $u \in V$, $\mu \in \mathfrak{g}^*$, and $a \in V^*$. The connected components of the affine coadjoint orbits $\left(\mathcal{O}^{\sigma}_{(\mu,a_{ref})}, \omega^-\right)$ are the symplectic leaves of $\mathfrak{s}^*$ endowed with the affine Lie-Poisson bracket. Denote by $S^{\sigma}_{(\mu,a)}$ the isotropy group of the affine coadjoint action.

Let $H_{a_{ref}} : T^*G \to \mathbb{R}$ be $G^c_{a_{ref}}$-invariant, where $a_{ref} \in V^*$ is fixed. By $G^c_{a_{ref}}$-invariance, we obtain the reduced Hamiltonian $h : \mathfrak{g}^* \times \mathcal{O}^c_{a_{ref}} \subset \mathfrak{s}^* \to \mathbb{R}$ defined by $h(\mu, \theta_g(a_{ref})) = H_{a_{ref}}(g^{-1}\mu)$.

(i) $\alpha(t) \in T^*_{g(t)}G$, solution of $X_{H_{a_{ref}}}$, $\alpha(0) = \mu_0 \in T^*_eG = \mathfrak{g}^*$. Then $(\mu(t), a(t)) := (g(t)^{-1}\alpha(t), \theta_{g(t)^{-1}}(a_{ref})) \in \mathfrak{s}^*$ solution of $X_h \in \mathfrak{X}\left(\mathcal{O}^{\sigma}_{(\mu_0,a_{ref})}, \omega^-\right)$, $(\mu(0), a(0)) = (\mu_0, a_0)$. Conversely, given $\mu_0 \in \mathfrak{g}^*$, the solution $\alpha(t)$ of $X_{H_{a_{ref}}}$ is reconstructed from the solution $(\mu(t), a(t))$ of $X_h \in \mathfrak{X}\left(\mathcal{O}^{\sigma}_{(\mu_0,a_{ref})}\right)$, $(\mu(0), a(0)) = (\mu_0, a_0)$ by setting $\alpha(t) = g(t)\mu(t)$, $g(t)$ is the solution of $\dot{g}(t) = g(t)\frac{\delta h}{\delta \mu(t)}$, $g(0) = e$.

(ii) Extend h arbitrarily to $\mathfrak{s}^*$. Hamilton's equations on $\left(\mathcal{O}^{\sigma}_{(\mu_0,a_{ref})}, \omega^-\right)$

$$\frac{\partial}{\partial t}(\mu, a) = \left(\mathrm{ad}^*_{\frac{\delta h}{\delta \mu}}\mu - \frac{\delta h}{\delta a} \diamond a + \mathbf{d}c^T\left(\frac{\delta h}{\delta a}\right), -\frac{\delta h}{\delta \mu}a - \mathbf{d}c\left(\frac{\delta h}{\delta \mu}\right)\right)$$

where $\mu(0) = \mu_0$ and $a(0) = g(0)^{-1}a_{ref} + c(g(0)^{-1})$.

h is not defined on the whole $\mathfrak{s}^*$. **(ii)** states that the equations of motion can be nevertheless computed from the usual formula of an affine Lie-Poisson vector field by arbitrarily extending h to $\mathfrak{s}^*$. The proof shows that the extension of h does not matter. $\delta h/\delta \mu \in \mathfrak{g}$, $\delta h/\delta a \in V$ make sense only if one thinks of h being defined on $\mathfrak{s}^*$.

G.) The charged strand equations

Lagrangian variables $(\Lambda, \boldsymbol{r}) : [0, L] \to SE(3)$

Convective variables

$$\Omega := \Lambda^{-1}\Lambda', \quad \omega := \Lambda^{-1}\dot{\Lambda} : [0, L] \to \mathfrak{so}(3)$$

$$\boldsymbol{\Gamma} := \Lambda^{-1}\boldsymbol{r}', \quad \boldsymbol{\gamma} := \Lambda^{-1}\dot{\boldsymbol{r}}, \quad \boldsymbol{\rho} := \Lambda^{-1}\boldsymbol{r} : [0, L] \to \mathbb{R}^3.$$

Generalization: $[0, L] \longleftrightarrow \mathcal{D}$, $SE(3) \longleftrightarrow S = \mathcal{O} \circledS E$, $\mathcal{O}$ a Lie group (order parameter) with a *left* representation E. For $\mathcal{D}$ manifold $G := \mathcal{F}(\mathcal{D}, S) \ni (\Lambda, r)$, $\Lambda : \mathcal{D} \to \mathcal{O}$, $r : \mathcal{D} \to E$, $V^* := \Omega^1(\mathcal{D}, \mathfrak{s}) \oplus \mathcal{F}(\mathcal{D}, E)$ $\ni (\Omega, \Gamma, \rho)$, $\Omega \in \Omega^1(\mathcal{D}, \mathfrak{o})$, $\Gamma \in \Omega^1(\mathcal{D}, E)$, $\rho : \mathcal{D} \to E$. V^* is dual of $V = \mathfrak{X}(\mathcal{D}, \mathfrak{s}^*) \oplus \mathcal{F}(\mathcal{D}, E^*)$, where $\mathfrak{X}(\mathcal{D}, \mathfrak{s})$, $\mathfrak{s}$-valued vector fields on $\mathcal{D}$. Representation $G \times V^* \to V^*$:

$$(\Lambda, r)(\Omega, \Gamma, \rho) = (\mathrm{Ad}_{(\Lambda, r)}(\Omega, \Gamma), \Lambda\rho).$$

V^*-valued group one-cocycle $c : S \to V^*$

$$c(\Lambda, r) := \left((\Lambda, r)\mathbf{d}(\Lambda, r)^{-1}, -r\right).$$

Since $\quad (u,w,f)\diamond(\Omega,\Gamma,\rho) = (\mathrm{ad}^*_\Omega u + w\diamond\Gamma + f\diamond\rho, -\Omega_i w),$

$\mathbf{d}c(\omega,\gamma) = (-\mathbf{d}\omega, -\mathbf{d}\gamma, -\gamma), \quad$ and $\quad \mathbf{d}c^{\mathsf{T}}(u,w,f) = (\mathrm{div}(u), \mathrm{div}(w) - f),$

the **affine Euler-Poincaré equations** become

$$\begin{cases} (\partial_t - \mathrm{ad}^*_\omega)\dfrac{\delta l}{\delta\omega} + (\mathrm{div} - \mathrm{ad}^*_\Omega)\dfrac{\delta l}{\delta\Omega} = \dfrac{\delta l}{\delta\gamma}\diamond\gamma + \dfrac{\delta l}{\delta\Gamma}\diamond\Gamma + \dfrac{\delta l}{\delta\rho}\diamond\rho \\ (\partial_t + \omega)\dfrac{\delta l}{\delta\gamma} + (\mathrm{div} + \Omega)\dfrac{\delta l}{\delta\Gamma} = \dfrac{\delta l}{\delta\rho} \end{cases}$$

and the **"advection equations"** are

$$\begin{cases} \partial_t\Omega + \mathrm{ad}_\omega\Omega = \mathbf{d}\omega \\ (\partial_t + \omega)\Gamma = (\mathbf{d} + \Omega)\gamma \\ \partial_t\rho + \omega\rho = \gamma. \end{cases}$$

We have assumed that the Lagrangian l given explicitly in terms of the variables $(\omega,\gamma,\Omega,\Gamma,\rho)$. Equivalently, l is induced by an affine left-invariant Lagrangian $L : TG \times V^* \to \mathbb{R}$. This does not hold if nonlocal terms are present!

Lagrangian of the charged strand has the expression

$$l(\boldsymbol{\omega},\gamma,\boldsymbol{\Omega},\boldsymbol{\kappa},\boldsymbol{\Gamma},\boldsymbol{\rho}) = l_{loc}(\boldsymbol{\omega},\gamma,\boldsymbol{\Omega},\boldsymbol{\Gamma},\boldsymbol{\rho}) + l_{np}(\xi,\boldsymbol{\kappa},\boldsymbol{\Gamma}), \qquad \text{for}$$
$$l_{loc}(\boldsymbol{\omega},\gamma,\boldsymbol{\Omega},\boldsymbol{\Gamma},\boldsymbol{\rho}) = K(\boldsymbol{\omega},\gamma) - E_{loc}(\boldsymbol{\Omega},\boldsymbol{\Gamma},\boldsymbol{\rho})$$
$$l_{np}(\xi,\boldsymbol{\kappa},\boldsymbol{\Gamma}) = \iint U\left(\xi(s,s'),\boldsymbol{\kappa}(s,s'),\boldsymbol{\Gamma}(s),\boldsymbol{\Gamma}(s')\right)\mathrm{d}s\,\mathrm{d}s'$$

$U : SE(3)\times\mathbb{R}^3\times\mathbb{R}^3 \to \mathbb{R}$ and $\left(\xi(s,s'),\boldsymbol{\kappa}(s,s')\right) := (\Lambda,\boldsymbol{r})^{-1}(s)(\Lambda,\boldsymbol{r})(s')$.

Crucial observations

(1) l_{np} is induced by a $SO(3)$-invariant potential $E_{np} = E_{np}(\Lambda,\boldsymbol{r})$. Thus the total Lagrangian l can be seen as being induced by the $SO(3)$-invariant Lagrangian $L_0 = L_0(\Lambda,\dot{\Lambda},\boldsymbol{r},\dot{\boldsymbol{r}})$ given by

$$L_0(\Lambda,\dot{\Lambda},\boldsymbol{r},\dot{\boldsymbol{r}}) = K(\Lambda,\dot{\Lambda},\boldsymbol{r},\dot{\boldsymbol{r}}) - E_{loc}\left(c\left((\Lambda,\boldsymbol{r})^{-1}\right)\right) - E_{np}(\Lambda,\boldsymbol{r}),$$

where K is the $\mathcal{F}(\mathcal{D},SE(3))$-left invariant extension of the kinetic energy K. We have replaced the dependence of E_{loc} on $(\boldsymbol{\Omega},\boldsymbol{\Gamma},\boldsymbol{\rho})$ by a dependence on $(\Lambda,\boldsymbol{r})$ through the cocycle c. The affine Euler-Poincaré dynamics yields the relation $(\boldsymbol{\Omega},\boldsymbol{\Gamma},\boldsymbol{\rho}) = c\left((\Lambda,\boldsymbol{r})^{-1}\right)$ which allows us to recover the dependence of the potential on $(\boldsymbol{\Omega},\boldsymbol{\Gamma},\boldsymbol{\rho})$.

(2) The group $SO(3)$ is precisely the isotropy group

$$G_0^c = \mathcal{F}(\mathcal{D}, SE(3))_0^c = \{(\Lambda, \boldsymbol{r}) \in G \mid c(\Lambda, \boldsymbol{r}) = 0\}$$

of the affine action at zero.

These two remarks allow us to obtain the dynamics of the molecular strand by the affine reduction at fixed parameter. Do it in general: $\mathcal{D}$ and $\mathcal{O} \circledS E$, applicable to any $\mathcal{O}$-invariant Lagrangian

$$L_0 = L_0(\Lambda, \dot{\Lambda}, r, \dot{r}) : T[\mathcal{F}(\mathcal{D}, \mathcal{O} \circledS E)] \to \mathbb{R}.$$

L_0 can be nonlocal and may depend on the derivatives of Λ and r. An important class of such Lagrangians is given by

$$L_0(\Lambda, \dot{\Lambda}, r, \dot{r}) = K(\Lambda, \dot{\Lambda}, r, \dot{r}) - P(\Lambda, r),$$

where K is the kinetic energy associated to an $\mathcal{O}$-invariant metric on $\mathcal{F}(\mathcal{D}, \mathcal{O} \circledS E)$ and the potential P is an $\mathcal{O}$-invariant function on $\mathcal{F}(\mathcal{D}, \mathcal{O} \circledS E)$; P can be nonlocal, or depend on derivatives of Λ and r. For the molecular strand, K is left-invariant and P is given by

$$P(\Lambda, r) = E_{loc}\left(c\left((\Lambda, r)^{-1}\right)\right) + E_{np}(\Lambda, r), \quad \text{where}$$

$$E_{np}(\Lambda, r) := \iint_{\mathcal{D}} U\left(\xi(s,s'), \kappa(s,s'), \Lambda^{-1}\mathbf{d}r(s), \Lambda^{-1}\mathbf{d}r(s')\right) \mathrm{d}s\, \mathrm{d}s'$$

$$\left(\xi(s,s'), \kappa(s,s')\right) := (\Lambda, r)^{-1}(s)(\Lambda, r)(s') \in \mathcal{O} \circledS E$$

and one readily sees that E_{np} is $\mathcal{O}$-invariant. Recall the cocycle

$$c\left((\Lambda, r)^{-1}\right) = \left(\Lambda^{-1}\mathbf{d}\Lambda, \Lambda^{-1}\mathbf{d}r, \Lambda^{-1}r\right).$$

A useful generalization of E_{np} is

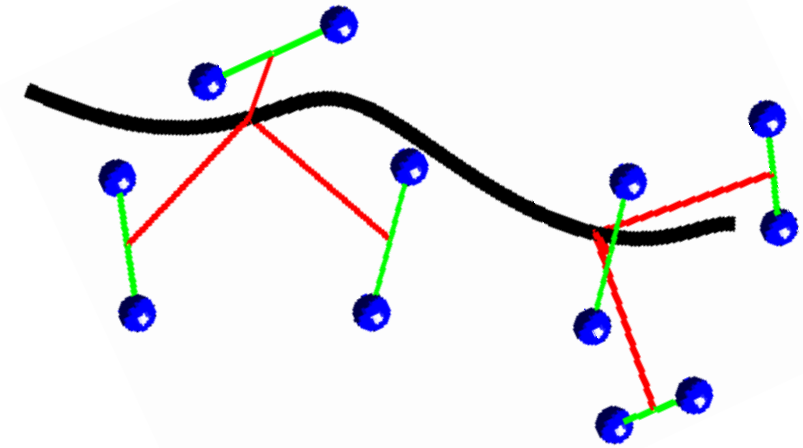
$$E_{np}(\Lambda, r) := \iint_{\mathcal{D}} U\Big(\xi(s,s'), \kappa(s,s'), c\left((\Lambda, r)^{-1}\right)(s), c\left((\Lambda, r)^{-1}\right)(s')\Big) \mathrm{d}s\, \mathrm{d}s'.$$

Apply the reduction theorems (Lagrangian or Hamiltonian)

$$\begin{cases} (\partial_t - \mathrm{ad}^*_\omega) \dfrac{\delta l}{\delta \omega} + (\mathrm{div} - \mathrm{ad}^*_\Omega) \dfrac{\delta l}{\delta \Omega} = \dfrac{\delta l}{\delta \gamma} \diamond \gamma + \dfrac{\delta l}{\delta \Gamma} \diamond \Gamma + \dfrac{\delta l}{\delta \rho} \diamond \rho, \\ \qquad + \displaystyle\int \left[\xi(s,s') \frac{\partial U}{\partial \xi}(s',s) - \frac{\partial U}{\partial \xi}(s,s') \xi(s',s) - \kappa(s,s') \diamond \frac{\partial U}{\partial \kappa}(s,s') \right] \mathrm{d}s' \\ (\partial_t + \omega) \dfrac{\delta l}{\delta \gamma} + (\mathrm{div} + \Omega) \dfrac{\delta l}{\delta \Gamma} = \dfrac{\delta l}{\delta \rho} + \displaystyle\int \left[\xi(s,s') \frac{\partial U}{\partial \kappa}(s',s) - \frac{\partial U}{\partial \kappa}(s,s') \right] \mathrm{d}s'. \end{cases}$$

The motion is Hamiltonian on affine coadjoint orbits.

DYNAMICS OF MULTIBOUQUETS



Rigid conformations of charges (red) are distributed along the centerline (solid black curve). At the end of each rigid branch, *another* rigid bouquet of charges is attached (two blue spheres on a rigid green rod). Orientations of the bouquets attached at the ends of different branches of the same dendrite (red bouquet) can be different. More bouquets can be attached to the blue spheres, etc. Elastic forces induced by deformations of the centerline and the relative deformation of bouquets, electrostatic and other nonlocal forces (e.g., Lennard-Jones) due to the interactions between each pair of charges.

Dendronized (dendritic) polymers are compound molecular structures formed by assembling multiple *dendrimers* (a low molecular weight unit to which a number of dendrons, or branches, is attached) that are each connected by its base to a long polymeric backbone. Known as *rod-shaped dendrimers*, the first patent for synthesizing them is in 1987 (Tomalia and Kirchhoff, US patent 4,694,064); description appeared in 1990 (Tomalia-Naylor-Goddard).

Spatio-temporal modeling of dynamical properties is not known. Reason: mathematical difficulties because of simultaneous forces coming from the elastic deformations of the polymer backbone and its attached dendrimers, and long-range interactions between the dendrimers through screened electrostatic and other forces.

Goal: Present a theory for arbitrary elastic and nonlocal interactions arising from charge distributions on branched structures.

Basic idea for modeling: Start with charged strand dynamics and add branching. Leads to iterated semidirect products with cocycles.

A.) Semidirect product of groups with cocycle

G_1, G_2 Lie groups. G_1 acts on G_2 by Lie group homomorphisms. Form $G_1 \circledS G_2$ with multiplication

$$(g_1, g_2)(\bar{g}_1, \bar{g}_2) := (g_1\bar{g}_1, g_2(g_1 \cdot \bar{g}_2)), \qquad g_1, \bar{g}_1 \in G_1, \quad g_2, \bar{g}_2 \in G_2,$$

$g_1 \cdot \bar{g}_2$ denotes the action of g_1 on $\bar{g}_2$; $(g_1, g_2)^{-1} = (g_1^{-1}, g_1^{-1} \cdot g_2^{-1})$.

The choice $G_1 = SE(3)$, $G_2 = SO(3)$, where the semidirect product $SE(3) \circledS SO(3)$ is defined by the action $(\Lambda_1, \boldsymbol{r}) \cdot \Lambda_2 := \Lambda_1\Lambda_2\Lambda_1^{-1}$, $(\Lambda_1, \boldsymbol{r}) \in SE(3)$, $\Lambda_2 \in SO(3)$, gives the two-level bouquets.

$G_1 \circledS G_2$ acts on a dual vector space V^* by an affine action

$$\theta_{(g_1,g_2)}a = (g_1, g_2)a + c(g_1, g_2), \quad a \in V^*$$

where $a \mapsto (g_1, g_2)a$ denotes a representation of $G_1 \circledS G_2$ on V^* and $c : G_1 \circledS G_2 \to V^*$ is a group one-cocycle, that is,

$$c((g_1, g_2)(\bar{g}_1, \bar{g}_2)) = (g_1, g_2)c(\bar{g}_1, \bar{g}_2) + c(g_1, g_2)$$

for all $(g_1, g_2), (\bar{g}_1, \bar{g}_2) \in G_1 \circledS G_2$.

B.) Lagrangian reduction and reduced variational principle

$L : T(G_1 \circledS G_2) \times V^* \to \mathbb{R}$ a G_1-invariant Lagrangian

$$(g_1, \dot{g}_1, g_2, \dot{g}_2, a_0) \mapsto (hg_1, h\dot{g}_1, h \cdot g_2, h \cdot \dot{g}_2, (h, e)a_0 + c(h, e)), \quad h \in G_1.$$

$$(T(G_1 \circledS G_2) \times V^*)\,/G_1 \cong \mathfrak{g}_1 \times TG_2 \times V^* \cong \mathfrak{g}_1 \times G_2 \times \mathfrak{g}_2 \times V^*$$

$$[g_1, \dot{g}_1, g_2, \dot{g}_2, a_0]_{G_1} \stackrel{\sim}{\longmapsto} \left(g_1^{-1}\dot{g}_1, g_1^{-1} \cdot g_2, g_1^{-1} \cdot (g_2^{-1}\dot{g}_2), \theta_{(g_1,g_2)^{-1}a_0}\right)$$

Special case of metamorphosis reduction in image registration.

Lagrangian $\ell : \mathfrak{g}_1 \times G_2 \times \mathfrak{g}_2 \times V^* \to \mathbb{R}$ defined by

$$\begin{aligned} L(g_1, \dot{g}_1, g_2, \dot{g}_2, a_0) &= \ell\left(g_1^{-1}\dot{g}_1, g_1^{-1} \cdot g_2, g_1^{-1} \cdot (g_2^{-1}\dot{g}_2), \theta_{(g_1,g_2)^{-1}a_0}\right) \\ &=: \ell(\omega_1, p, \omega_2, a), \end{aligned}$$

where we have introduced the reduced variables defined by

$$\omega_1 = g_1^{-1}\dot{g}_1 \in \mathfrak{g}_1, \qquad \omega_2 = g_1^{-1} \cdot g_2^{-1}\dot{g}_2 \in \mathfrak{g}_2$$
$$p = g_1^{-1} \cdot g_2 \in G_2 \qquad a = \theta_{(g_1,g_2)^{-1}a_0} = \theta_{(g_1,g_1\cdot p)^{-1}a_0} \in V^*.$$

The variations of these variables are:

$$\delta\omega_1 = \dot{\eta}_1 + [\omega_1, \eta_1] \in \mathfrak{g}_1, \qquad \text{where} \qquad \eta_1 = g_1^{-1}\delta g_1 \in \mathfrak{g}_1$$
$$\delta p = p\eta_2 - \eta_1 \cdot p \in TG_2, \qquad \text{where} \qquad \eta_2 = g_1^{-1} \cdot g_2^{-1}\delta g_2 \in \mathfrak{g}_2$$
$$\delta\omega_2 = \dot{\eta}_2 + [\omega_2, \eta_2] + \omega_1 \cdot \eta_2 - \eta_1 \cdot \omega_2 \in \mathfrak{g}_2$$
$$\delta a = -\eta_1 a - \eta_2 a - \partial_1 c(\eta_1) - \partial_2 c(\eta_2) \in V^*,$$

η_i are curves in $\mathfrak{g}_i$ vanishing at the endpoints and $\partial_i c : \mathfrak{g}_i \to V^*$, $i = 1, 2$, are the partial derivatives of c, that is,

$$\partial_1 c(\xi_1) := \frac{d}{dt}\Big|_{t=0} c(\exp(t\xi_1), e), \qquad \partial_2 c(\xi_2) := \frac{d}{dt}\Big|_{t=0} c(e, \exp(t\xi_2)).$$

The dots $(\cdot)$ appearing in the above expression denote the operations naturally induced by the action of G_1 on G_2:

$$g_1 \cdot \omega_2 = \frac{d}{dt}\Big|_{t=0} g_1 \cdot \exp(t\omega_2), \qquad \omega_1 \cdot \omega_2 = \frac{d}{dt}\Big|_{t=0} \exp(t\omega_1) \cdot \omega_2,$$

where $g_1 \in G_1$, $\omega_1 \in \mathfrak{g}_1$, $\omega_2 \in \mathfrak{g}_2$. Finally, $\eta_1 \cdot p \in TG_2$ is the infinitesimal generator of the G_1-action on G_2 evaluated at $p \in G_2$.

Need *diamond operations*: For representation of $G_1 \circledS G_2$ on V^*:

$$\diamond_i : V \times V^* \to \mathfrak{g}_i^*, \quad \langle v \diamond_i a, \eta_i \rangle = -\langle \eta_i a, v \rangle = \langle a, \eta_i v \rangle ;$$

for the representation of G_1 on $\mathfrak{g}_2$:

$$\diamond_{12} : \mathfrak{g}_2 \times \mathfrak{g}_2^* \to \mathfrak{g}_1^*, \quad \langle \xi_2 \diamond_{12} \mu_2, \eta_1 \rangle = \langle \mu_2, \eta_1 \cdot \xi_2 \rangle .$$

Using the above constrained variations,

$$\delta \int_{t_1}^{t_2} \ell(\omega_1, p, \omega_2, a) dt = 0,$$

is equivalent to the reduced Euler-Lagrange equations,

$$\begin{cases} \dfrac{d}{dt}\dfrac{\delta \ell}{\delta \omega_1} = \mathrm{ad}^*_{\omega_1} \dfrac{\delta \ell}{\delta \omega_1} - \mathbf{J}_{12}\left(\dfrac{\delta \ell}{\delta p}\right) - \omega_2 \diamond_{12} \dfrac{\delta \ell}{\delta \omega_2} + \dfrac{\delta \ell}{\delta a} \diamond_1 a - \partial_1 c^{\mathsf{T}}\left(\dfrac{\delta \ell}{\delta a}\right), \\ \dfrac{d}{dt}\dfrac{\delta \ell}{\delta \omega_2} = \mathrm{ad}^*_{\omega_2} \dfrac{\delta \ell}{\delta \omega_2} + p^{-1}\dfrac{\delta \ell}{\delta p} - \omega_1 \cdot \dfrac{\delta \ell}{\delta \omega_2} + \dfrac{\delta \ell}{\delta a} \diamond_2 a - \partial_2 c^{\mathsf{T}}\left(\dfrac{\delta \ell}{\delta a}\right), \end{cases}$$

to which we add the two "advection equations"

$$\dot{p} = p\omega_2 - \omega_1 \cdot p \quad \text{and} \quad \dot{a} + \omega_1 a + \omega_2 a + \partial_1 c(\omega_1) + \partial_2 c(\omega_2) = 0.$$

$\mathbf{J}_{12} : T^*G_2 \to \mathfrak{g}_1^*$ is the momentum map of the cotangent lift

$$\langle \mathbf{J}_{12}(\alpha_{g_2}), \xi_1 \rangle = \langle \alpha_{g_2}, \xi_1 \cdot g_2 \rangle , \quad \alpha_{g_2} \in T^*_{g_2} G_2, \quad \xi_1 \in \mathfrak{g}_1.$$

C.) Hamiltonian reduction and Poisson bracket

$H : T^*(G_1 \circledS G_2) \times V^* \to \mathbb{R}$, a G_1-invariant Hamiltonian. E.g., H is obtained from L by a Legendre transformation, the variable in V^* is a parameter. $T^*(G_1 \circledS G_2) \times V^*$ has product Poisson structure with V^* trivial. Hence, Hamilton's equations for H are equivalent to the canonical Hamilton equations for H_{a_0} together with the equation $\dot{a}_0 = 0$. As on the Lagrangian side, define $H_{a_0}(\alpha_{g_1}, \alpha_{g_2}) := H(\alpha_{g_1}, \alpha_{g_2}, a_0)$.

The G_1-quotient map $T^*(G_1 \circledS G_2) \times V^* \to \mathfrak{g}_1^* \times G_2 \times \mathfrak{g}_2^* \times V^*$

$$(\alpha_{g_1}, \alpha_{g_2}, a_0) \mapsto (\mu_1, p, \mu_2, a) := \left(g_1^{-1}\alpha_{g_1}, g_1^{-1} \cdot g_2, g_1^{-1} \cdot (g_2^{-1}\alpha_{g_2}), \theta_{(g_1,g_2)^{-1}}(a_0)\right)$$

defines the reduced Hamiltonian $h(\mu_1, p, \mu_2, a)$ on $\mathfrak{g}_1^* \times G_2 \times \mathfrak{g}_2 \times V^*$. If H comes from a Lagrangian L by Legendre transformation, h is also obtained from ℓ by the reduced Legendre transformation,

$$h(\mu_1, p, \mu_2, a) = \langle \mu_1, \omega_1 \rangle + \langle \mu_2, \omega_2 \rangle - \ell(\omega_1, p, \omega_2, a), \qquad \frac{\delta \ell}{\delta \omega_i} = \mu_i.$$

Reduced Poisson bracket on $\mathfrak{g}_1^* \times G_2 \times \mathfrak{g}_2^* \times V^*$

$$
\begin{aligned}
\{f,h\} = &-\left\langle \mu_1, \left[\frac{\delta f}{\delta \mu_1}, \frac{\delta h}{\delta \mu_1}\right]\right\rangle - \left\langle \mu_2, \left[\frac{\delta f}{\delta \mu_2}, \frac{\delta h}{\delta \mu_2}\right]\right\rangle \\
&- \left\langle \mu_2, \frac{\delta f}{\delta \mu_1}\cdot\frac{\delta h}{\delta \mu_2} - \frac{\delta h}{\delta \mu_1}\cdot\frac{\delta f}{\delta \mu_2}\right\rangle \\
&- \left\langle a, \frac{\delta f}{\delta \mu_1}\frac{\delta h}{\delta a} + \frac{\delta f}{\delta \mu_2}\frac{\delta h}{\delta a} - \frac{\delta h}{\delta \mu_1}\frac{\delta f}{\delta a} - \frac{\delta h}{\delta \mu_2}\frac{\delta f}{\delta a}\right\rangle \\
&+ \left\langle \partial_1 c\left(\frac{\delta f}{\delta \mu_1}\right) + \partial_2 c\left(\frac{\delta f}{\delta \mu_2}\right), \frac{\delta h}{\delta a}\right\rangle - \left\langle \partial_1 c\left(\frac{\delta h}{\delta \mu_1}\right) + \partial_2 c\left(\frac{\delta h}{\delta \mu_2}\right), \frac{\delta f}{\delta a}\right\rangle \\
&+ \left\langle \frac{\delta f}{\delta \mu_1}, \mathbf{J}_{12}\left(\frac{\delta h}{\delta p}\right)\right\rangle + \left\langle \frac{\delta f}{\delta p}, p\frac{\delta h}{\delta \mu_2}\right\rangle \\
&- \left\langle \frac{\delta h}{\delta \mu_1}, \mathbf{J}_{12}\left(\frac{\delta h}{\delta p}\right)\right\rangle - \left\langle \frac{\delta h}{\delta p}, p\frac{\delta f}{\delta \mu_2}\right\rangle .
\end{aligned}
$$

First three lines: Lie-Poisson bracket on $((\mathfrak{g}_1 \circledS \mathfrak{g}_2) \circledS V)^*$; fourth line is due to the presence of the affine term; last two lines are new and arise because reduction is carried out for the subgroup $G_1 \subset G_1 \circledS G_2$ and not the whole semidirect product.

The Hamiltonian equations associated to this Poisson bracket are

$$\begin{cases} \dfrac{d}{dt}\mu_1 = \mathrm{ad}^*_{\frac{\delta h}{\delta \mu_1}}\,\mu_1 + \mathbf{J}_{12}\left(\dfrac{\delta h}{\delta p}\right) - \dfrac{\delta h}{\delta \mu_2}\diamond_{12}\,\mu_2 - \dfrac{\delta h}{\delta a}\diamond_1 a + \partial_1 c^{\mathsf{T}}\left(\dfrac{\delta h}{\delta a}\right), \\ \dfrac{d}{dt}\mu_2 = \mathrm{ad}^*_{\frac{\delta h}{\delta \mu_2}}\,\mu_2 - p^{-1}\dfrac{\delta h}{\delta p} - \dfrac{\delta h}{\delta \mu_1}\cdot\mu_2 - \dfrac{\delta h}{\delta a}\diamond_2 a + \partial_2 c^{\mathsf{T}}\left(\dfrac{\delta \ell}{\delta a}\right), \\ \dfrac{d}{dt}p = p\dfrac{\delta h}{\delta \mu_2} - \dfrac{\delta h}{\delta \mu_1}\cdot p, \\ \dfrac{d}{dt}a = -\dfrac{\delta h}{\delta \mu_1}a - \dfrac{\delta h}{\delta \mu_2}a - \partial_1 c\left(\dfrac{\delta h}{\delta \mu_1}\right) - \partial_2 c\left(\dfrac{\delta h}{\delta \mu_2}\right). \end{cases}$$

If h is obtained from a Lagrangian ℓ by the reduced Legendre transformation, these equations can be obtained by substituting the relations

$$\frac{\delta h}{\delta \mu_i} = \omega_i, \qquad \frac{\delta h}{\delta p} = -\frac{\delta \ell}{\delta p}, \qquad \frac{\delta h}{\delta a} = -\frac{\delta \ell}{\delta a},$$

into the reduced Euler-Lagrange equations.

Generalization to N groups via iterated semidirect products.

D.) Affine reduction at fixed parameter

Unfortunately, in many applications, $L_{a_0} : T(G_1 \circledS G_2) \to \mathbb{R}$ is known only for a fixed value $a_0 \in V^*$; so theory does not apply because ℓ is not the reduction of a G_1-invariant function on $T(G_1 \circledS G_2) \times V^*$. There is a way out: assume that L_{a_0} is $(G_1)^c_{a_0}$-invariant, where

$$(G_1)^c_{a_0} := \{g_1 \in G_1 \mid \theta_{(g_1,e)} a_0 = a_0\}.$$

Often it happens (e.g., for the bouquets) that ℓ cannot be explicitly expressed as a function of the variables ξ_1, p, ξ_2, a but it has the form $\ell(\xi_1, p, \xi_2, a, g_1)$, where $g_1 \in G_1$ is such that $c(g_1^{-1}, p^{-1}) = a$.

If ℓ is $(G_1)^c_{a_0}$-invariant, i.e., $\ell(\xi_1, p, \xi_2, a, hg_1) = \ell(\xi_1, p, \xi_2, a, g)$ for all $h \in (G_1)^c_{a_0}$, then $\ell(\xi_1, p, \xi_2, a, g)$ is a well defined function of (ξ_1, p, ξ_2, a). Then, the equations of motion above are still valid, where one computes the functional derivatives as if g_1 were expressed explicitly in terms of ξ_1, p, ξ_2, a. Although this may not be possible, the derivatives may still have explicit expressions.

E.) Dynamics of multibouquets

We will work only with two level polymers for simplicity.

$\boldsymbol{r}(s,t)$ is position of the base line; s parameter of position, t time.
$\Lambda_1(s) \in SO(3)$ rotation of the first level of the rigid bouquet (red) measured relative to a fixed coordinate system.
$\Lambda_2(s) \in SO(3)$ rotation of the second bouquet level (green) measured relative to a frame attached to the previous bouquet. Depends also on the numbered vertex to which it is attached: say vertex k_1 for s and m_1 for s'.
Position of a given charge (blue) depends on the number of the charge in the second bouquet (called k_2 for s and m_2 for s'), on the orientations $\Lambda_1(s)$ and $\Lambda_2(s)$ and on the position of the base $\boldsymbol{r}(s)$:

$$\boldsymbol{c}_{k_1k_2}(s) = \boldsymbol{r}(s) + \Lambda_1(s)\boldsymbol{\eta}_{k_1}(s) + \Lambda_2(s)\Lambda_1(s)\boldsymbol{\eta}_{k_2}(s),$$
$$\boldsymbol{c}_{m_1m_2}(s') = \boldsymbol{r}(s') + \Lambda_1(s')\boldsymbol{\eta}_{m_1}(s') + \Lambda_2(s')\Lambda_1(s')\boldsymbol{\eta}_{m_2}(s').$$

Undisturbed state for the k_i-th charge: $\boldsymbol{r}(s) + \boldsymbol{\eta}_{k_i}(s)$, $\boldsymbol{\eta}_{k_i}(s)$ is a vector of constant length that determines the position of the k_i-th charge relative to $\boldsymbol{r}(s)$ along the curve in its reference configuration.

Setup

$\mathcal{F}(I, SE(3) \circledS SO(3)) \ni (\Lambda_1, \boldsymbol{r}, \Lambda_2)$ configuration space

So $G_1 = \mathcal{F}(I, SE(3)) \ni (\Lambda_1, \boldsymbol{r})$, $G_2 = \mathcal{F}(I, SO(3)) \ni \Lambda_2$,
G_1-action on G_2 by group homomorphisms is $(\Lambda_1, \boldsymbol{r}) \cdot \Lambda_2 := \Lambda_1 \Lambda_2 \Lambda_1^{-1}$,
$V \cong_{L^2} V^* = \mathcal{F}(I, \mathbb{R}^3)^4 \ni (\boldsymbol{\Omega}_1, \boldsymbol{\Gamma}, \boldsymbol{\Omega}_2, \boldsymbol{\rho})$
$\mathcal{F}(I, SE(3)) \circledS \mathcal{F}(I, SO(3))$-representation on $\mathcal{F}(I, \mathbb{R}^3)^4$

$$
\begin{aligned}
&(\Lambda_1, \boldsymbol{r}, \Lambda_2)(\boldsymbol{\Omega}_1, \boldsymbol{\Gamma}, \boldsymbol{\Omega}_2, \boldsymbol{\rho}) \\
&\qquad = (\Lambda_1 \boldsymbol{\Omega}_1, \Lambda_1 \boldsymbol{\Gamma} - \Lambda_1 \boldsymbol{\Omega}_1 \times \boldsymbol{r}, \Lambda_2 \Lambda_1 (\boldsymbol{\Omega}_1 + \boldsymbol{\Omega}_2) - \Lambda_1 \boldsymbol{\Omega}_1, \Lambda_1 \boldsymbol{\rho})
\end{aligned}
$$

$\mathcal{F}(I, SE(3)) \circledS \mathcal{F}(I, SO(3))$-group one-cocycle

$$
c(\Lambda_1, \boldsymbol{r}, \Lambda_2) := \left((\Lambda_1, \boldsymbol{r}, \Lambda_2) \partial_s (\Lambda_1, \boldsymbol{r}, \Lambda_2)^{-1}, -\boldsymbol{r} \right);
$$

motivated by a convenient expression of the reduced variables.

$(G_1)_0^c = SO(3) \subset \mathcal{F}(I, SE(3))$

Reduced convective variables

$$\begin{aligned} \omega_1 &= \Lambda_1^{-1}\dot{\Lambda}_1 \in \mathfrak{so}(3) & \Omega_1 &= \Lambda_1^{-1}\Lambda_1' \in \mathfrak{so}(3) \\ \gamma &= \Lambda_1^{-1}\dot{\boldsymbol{r}} \in \mathbb{R}^3 & \boldsymbol{\Gamma} &= \Lambda_1^{-1}\boldsymbol{r}' \in \mathbb{R}^3 \\ \omega_2 &= \Lambda_1^{-1}\Lambda_2^{-1}\dot{\Lambda}_2\Lambda_1 \in \mathfrak{so}(3) & \Omega_2 &= \Lambda_1^{-1}\Lambda_2^{-1}\Lambda_2'\Lambda_1 \in \mathfrak{so}(3) \\ p &= \Lambda_1^{-1}\Lambda_2\Lambda_1 \in \mathbb{R}^3 & \boldsymbol{\rho} &= \Lambda_1^{-1}\boldsymbol{r} \in \mathbb{R}^3 \end{aligned}$$

ω_i are angular rotations of each bouquet

ω_1 measured with respect to the base coordinate system

ω_2 measured with respect to Λ_1

Ω_1 describes infinitesimal twist of the base

$\boldsymbol{\Gamma}$ describes infinitesimal stretching of the base; there is no $\boldsymbol{\Gamma}_2$ as there is no stretching associated with the second bouquet

Ω_2 describes the infinitesimal twist of the second bouquet in the coordinate frame connected with the first bouquet

p is orientation of the second bouquet seen from the coordinate frame of the first bouquet.

Lagrangian

Material Lagrangian $L_0 : T\mathcal{F}(I, SE(3) \circledS SO(3)) \times \mathcal{F}(I, \mathbb{R}^3)^4 \to \mathbb{R}$

$$L_{(a_0=0)} = L(\Lambda_1, \dot{\Lambda}_1, \boldsymbol{r}, \dot{\boldsymbol{r}}, \Lambda_2, \dot{\Lambda}_2); \qquad 0 \in \mathcal{F}(I, \mathbb{R}^3)^4,$$

is $(G_1)_0^c$-invariant. After symmetry reduction it has the form

$$\ell = \ell_{loc}(\boldsymbol{\omega}_1, \boldsymbol{\gamma}, \boldsymbol{\omega}_2, p, \boldsymbol{\Omega}_1, \boldsymbol{\Gamma}, \boldsymbol{\Omega}_2, \boldsymbol{\rho}) + \ell_{np}(\boldsymbol{\omega}_1, \boldsymbol{\gamma}, \boldsymbol{\omega}_2, p, \boldsymbol{\Omega}_1, \boldsymbol{\Gamma}, \boldsymbol{\Omega}_2, \boldsymbol{\rho}, (\Lambda_1, \boldsymbol{r})),$$

ℓ_{np} has still a dependence on $(\Lambda_1, \boldsymbol{r})$, where $(\Lambda_1, \boldsymbol{r})$ are such that $c((\Lambda_1, \boldsymbol{r})^{-1}, p^{-1}) = (\boldsymbol{\Omega}_1, \boldsymbol{\Gamma}, \boldsymbol{\Omega}_2, \boldsymbol{\rho})$. ℓ_{np} has the nonlocal expression

$$\ell_{np} = \iint U\Big(\xi(s, s'), \boldsymbol{\kappa}(s, s'), p(s), p(s'), \boldsymbol{\Gamma}(s), \boldsymbol{\Gamma}(s')\Big) \mathrm{d}s \mathrm{d}s',$$

where $U : SO(3) \times (\mathbb{R}^3)^5 \to \mathbb{R}$ is a given function and

$$\boldsymbol{\kappa}(s, s') := -\Lambda_1^{-1}(s)\Big(\boldsymbol{r}(s) - \boldsymbol{r}(s')\Big) \in \mathbb{R}^3,$$

$$\xi(s, s') := \Lambda_1^{-1}(s)\Lambda_1(s') \in \mathfrak{so}(3).$$

This general expression of ℓ_{np} allows the treatment of a potential depending on the Euclidean distance between two charges. The position of a charge is given by

$$\boldsymbol{c}_{k_1 k_2}(s) = \boldsymbol{r}(s) + \Lambda_1(s)\boldsymbol{\eta}_{k_1}(s) + \Lambda_2(s)\Lambda_1(s)\boldsymbol{\eta}_{k_2}(s),$$

and so the distance between two charges is found to be

$$d_{k_1k_2m_1m_2}(s,s') = \left|\boldsymbol{c}_{k_1k_2}(s) - \boldsymbol{c}_{k_1k_2}(s')\right|$$
$$= \left|-\boldsymbol{\kappa}(s,s') + \boldsymbol{\eta}_{k_1}(s) + p(s)\boldsymbol{\eta}_{k_2}(s) - \xi(s,s')\boldsymbol{\eta}_{m_1}(s') - \xi(s,s')p(s')\boldsymbol{\eta}_{m_2}(s')\right|.$$

This expression shows that the distance between two charges can be expressed solely in terms of the variables $\xi(s,s'), \boldsymbol{\kappa}(s,s'), p(s), p(s')$. ℓ_{np} is invariant under the $(G_1)_0^c = SO(3)$-action

$$(\Lambda_1(s), \boldsymbol{r}(s), \Lambda_2(s)) \mapsto (h\Lambda_1(s), h\boldsymbol{r}(s), h\Lambda_2(s)h^{-1}), \quad h \in SO(3).$$

Hence, the general theory applies.

Equations of motion

Affine representation θ of the group $G = \mathcal{F}(I, SE(3) \circledS SO(3))$ on $V^* = \Omega^1(I, \mathfrak{se}(3) \circledS \mathfrak{so}(3)) \times \mathcal{F}(I, \mathbb{R}^3)$:

$$\theta_{(\Lambda_1,\boldsymbol{r},\Lambda_2)}(\boldsymbol{\Omega}_1, \boldsymbol{\Gamma}, \boldsymbol{\Omega}_2, \boldsymbol{\rho}) = (\Lambda_1, \boldsymbol{r}, \Lambda_2)\,(\boldsymbol{\Omega}_1, \boldsymbol{\Gamma}, \boldsymbol{\Omega}_2, \boldsymbol{\rho}) + c(\Lambda_1, \boldsymbol{r}, \Lambda_2)$$
$$= (\Lambda_1\boldsymbol{\Omega}_1, \Lambda_1\boldsymbol{\Gamma} - \Lambda_1\boldsymbol{\Omega}_1 \times \boldsymbol{r}, \Lambda_2\Lambda_1(\boldsymbol{\Omega}_1 + \boldsymbol{\Omega}_2) - \Lambda_1\boldsymbol{\Omega}_1, \Lambda_1\boldsymbol{\rho})$$
$$+ \Big((\Lambda_1, \boldsymbol{r}, \Lambda_2)\partial_s(\Lambda_1, \boldsymbol{r}, \Lambda_2)^{-1}, -\boldsymbol{r}\Big)$$

$$
\begin{cases}
\Big(\partial_t + \boldsymbol{\omega}_1 \times \Big)\dfrac{\delta \ell_{loc}}{\delta \boldsymbol{\omega}_1} + \Big(\partial_s + \boldsymbol{\Omega}_1 \times \Big)\dfrac{\delta \ell_{loc}}{\delta \boldsymbol{\Omega}_1} + \boldsymbol{\rho} \times \dfrac{\delta \ell_{loc}}{\delta \boldsymbol{\rho}} + \boldsymbol{\Gamma} \times \dfrac{\delta(\ell_{loc} + \ell_{np})}{\delta \boldsymbol{\Gamma}} \\
\qquad + \boldsymbol{\gamma} \times \dfrac{\delta \ell_{loc}}{\delta \boldsymbol{\gamma}} + \boldsymbol{\omega}_2 \times \dfrac{\delta \ell_{loc}}{\delta \boldsymbol{\omega}_2} + \boldsymbol{\Omega}_2 \times \dfrac{\delta \ell_{loc}}{\delta \boldsymbol{\Omega}_2} + \dfrac{\delta \ell_{loc}}{\delta p} p^{-1} - p^{-1} \dfrac{\delta \ell_{loc}}{\delta p} \\
\qquad + \displaystyle\int \left(\frac{\partial U}{\partial p_1}(s, s') p(s)^{-1} - p(s)^{-1} \frac{\partial U}{\partial p_1}(s, s') \right) \mathrm{d}s' \\
\qquad + \displaystyle\int \left(\frac{\partial U}{\partial p_2}(s', s) p(s)^{-1} - p(s)^{-1} \frac{\partial U}{\partial p_2}(s', s) \right) \mathrm{d}s' \\
\qquad - \displaystyle\int \left(\frac{\partial U}{\partial \boldsymbol{\kappa}}(s, s') \times \boldsymbol{\kappa}(s, s') + \mathbf{Z}(s, s') \right) \mathrm{d}s' = 0, \\
\Big(\partial_t + \boldsymbol{\omega}_1 \times \Big)\dfrac{\delta \ell_{loc}}{\delta \boldsymbol{\gamma}} + \Big(\partial_s + \boldsymbol{\Omega}_1 \times \Big)\dfrac{\delta(\ell_{loc} + \ell_{np})}{\delta \boldsymbol{\Gamma}} - \dfrac{\delta \ell_{loc}}{\delta \boldsymbol{\rho}} \\
\qquad - \displaystyle\int \left(\xi(s, s') \frac{\partial U}{\partial \boldsymbol{\kappa}}(s', s) - \frac{\partial U}{\partial \boldsymbol{\kappa}}(s, s') \right) \mathrm{d}s' = 0, \\
\Big(\partial_t + \boldsymbol{\omega}_2 \times \Big)\dfrac{\delta \ell_{loc}}{\delta \boldsymbol{\omega}_2} + \Big(\partial_s + \boldsymbol{\Omega}_2 \times \Big)\dfrac{\delta \ell_{loc}}{\delta \boldsymbol{\Omega}_2} + \boldsymbol{\omega}_1 \times \dfrac{\delta \ell_{loc}}{\delta \boldsymbol{\omega}_2} + \boldsymbol{\Omega}_1 \times \dfrac{\delta \ell_{loc}}{\delta \boldsymbol{\Omega}_2} \\
\qquad - \displaystyle\int \left(p(s)^{-1} \frac{\partial U}{\partial p_1}(s, s') + p(s)^{-1} \frac{\partial U}{\partial p_2}(s', s) \right) \mathrm{d}s' = 0,
\end{cases}
$$

$$\widehat{\mathbf{Z}}(s,s') = \xi(s,s')\frac{\partial U}{\partial \xi}(s',s) - \frac{\partial U}{\partial \xi}(s,s')\xi^{\mathsf{T}}(s,s') \in \mathfrak{so}(3).$$

$\partial U/\partial \xi \in T_\xi SO(3)$, $\partial U/\partial p_i \in T_{p_i} SO(3)$, $\partial U/\partial \boldsymbol{\kappa} \in \mathbb{R}^3$, are the partial derivatives of $U(\xi, \boldsymbol{\kappa}, p_1, p_2)$ on $SO(3) \times \mathbb{R}^3 \times SO(3) \times SO(3)$.

To these equations add the kinematic equations

$$\begin{cases} \dot{p} = p\boldsymbol{\omega}_2 - \boldsymbol{\omega}_1 p + p\boldsymbol{\omega}_1 \\ (\partial_t + \boldsymbol{\omega}_1\times)\boldsymbol{\Omega}_1 = \partial_s \boldsymbol{\omega}_1 \\ (\partial_t + \boldsymbol{\omega}_1\times)\boldsymbol{\Gamma} = (\partial_s + \boldsymbol{\Omega}_1\times)\boldsymbol{\gamma} \\ (\partial_t + (\boldsymbol{\omega}_1 + \boldsymbol{\omega}_2)\times)\boldsymbol{\Omega}_2 = (\partial_s + \boldsymbol{\Omega}_1\times)\boldsymbol{\omega}_2 \\ (\partial_t + \boldsymbol{\omega}_1\times)\boldsymbol{\rho} = \boldsymbol{\gamma}. \end{cases}$$

Note that the terms involving ξ and $\boldsymbol{\kappa}$ do not enter the angular momentum for the second bouquet. This is because there is no term analogous to ξ involving Λ_2.

Poisson brackets for the Hamiltonian evolution of two-bouquets is obtained from the general formula.

The derivatives of the nonlocal term can be computed.

$$\mathbf{d}_{k_1k_2m_1m_2}(s,s') =$$
$$-\boldsymbol{\kappa}(s,s') + \boldsymbol{\eta}_{k_1}(s) + p(s)\boldsymbol{\eta}_{k_2}(s) - \xi(s,s')\boldsymbol{\eta}_{m_1}(s') - \xi(s,s')p(s')\boldsymbol{\eta}_{m_2}(s')$$

$$d_{k_1k_2m_1m_2}(s,s') = \left|\mathbf{d}_{k_1k_2m_1m_2}(s,s')\right| .$$

Often, the potential energy U is a function of $d_{k_1k_2m_1m_2}(s,s')$ and

$$\ell_{np} = \sum_{k_1,k_2,m_1,m_2} \int U\Big(d_{k_1k_2m_1m_2}(s,s')\Big)\,|\boldsymbol{\Gamma}(s)|\,\Big|\boldsymbol{\Gamma}(s')\Big|\,\mathrm{d}s\,\mathrm{d}s' .$$

For example,

$$\frac{\partial U}{\partial \xi}(s,s')\xi^{-1}(s,s') =$$
$$\sum_{k_1,k_2,m_1,m_2} \frac{U'\Big(d_{k_1k_2m_1m_2}(s,s')\Big)}{d_{k_1k_2m_1m_2}(s,s')}\Big(\mathbf{d}_{k_1k_2m_1m_2} \times \xi\left(\boldsymbol{\eta}_{m_1}(s') + p(s')\boldsymbol{\eta}_{m_2}(s')\right)\Big)\widehat{\ }$$

$$\xi(s,s')\frac{\partial U}{\partial \xi}(s',s) =$$

$$\sum_{k_1,k_2,m_1,m_2} \frac{U'\Big(d_{k_1k_2m_1m_2}(s',s)\Big)}{d_{k_1k_2m_1m_2}(s',s)}\Big(- \mathbf{d}_{m_1m_2k_1k_2} \times \Big(\boldsymbol{\eta}_{m_1}(s) + p(s)\boldsymbol{\eta}_{m_2}(s)\Big)\Big)\widehat{\ }.$$

$$p^{-1}(s)\frac{\partial U}{\partial p(s)}(s,s') =$$

$$\sum_{k_1,k_2,m_1,m_2} \frac{U'\Big(d_{k_1k_2m_1m_2}(s,s')\Big)}{d_{k_1k_2m_1m_2}(s,s')}\Big(p^{-1}(s)\mathbf{d}_{k_1k_2m_1m_2}(s,s') \times \boldsymbol{\eta}_{k_2}(s)\Big)\widehat{\ }$$

$$p^{-1}(s)\frac{\partial U}{\partial p(s')}(s',s) =$$

$$\sum_{k_1,k_2,m_1,m_2} \frac{U'\Big(d_{k_1k_2m_1m_2}(s,s')\Big)}{d_{k_1k_2m_1m_2}(s,s')}\Big(- p^{-1}(s)\mathbf{d}_{m_1m_2k_1k_2}(s,s') \times \boldsymbol{\eta}_{m_2}(s)\Big)\widehat{\ }.$$

This is generalized to N bouquets.