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Hamiltonian and multi-symplectic structure of a rod model using quaternions.

by

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We study a new Hamiltonian formulation of a well known elastic rod model and obtain also a multi-symplectic fomulation of the equations.

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Abstract

The geometrically exact model of an elastic rod, formulated in [20] has been investigated. We present a constrained Hamiltonian formulation of the elastic rod model as well as a constrained multi-symplectic formulation of the model. In both formulations, quaternions are used to represent the group of rotations. The resulting Hamiltonian PDE and multi-symplectic formulation have simple looking formats involving constant structure matrices.

1 Introduction

In this paper we consider an elastic rod model first formulated in [20]. This model is a variant of the classical Kirchoff-Love model [16], when allowing for finite extension and shearing effects. Internal stress forces in the body depend linearly on the stress measures, and the material therefore possesses a hyperelastic behavior. The equations of motion are a system of partial differential equations (PDEs) on a manifold, and, in many respects, they resemble the Euler equations of rigid body dynamics. The first numerical discretization methods designed and applied to this model, aimed at obtaining numerical approximations lying on the configuration manifold, see [22] (static case) and [23] (dynamical case). An energy-momentum method was later presented in [11]. One of the main motivations for developing the energy-momentum method was the disappointing performance of conventional methods in long time simulations. Even methods usually regarded as very stable exhibited unacceptable numerical instability [11]. Numerical approximations for the model have later been studied by many authors, in particular energy-conserving and dissipative schemes based on finite element strategies, see for example [6, 7, 1, 2].

One important issue in the numerical simulation of this model is the choice of coordinates used to describe the configuration manifold, consisting of a cartesian product of the vector space $\mathbb{R}^3$ and the group of rotations, $SO(3)$. In [22], and in many papers later on, rotation matrices were used, while in [2] the authors choose directors reducing the amount of computations and the memory requirements: a rotation can be identified by two orthonormal vectors of $\mathbb{R}^3$ and represented by 6

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parameters satisfying two length constraints and one orthogonality constraint. In [6], [15] instead the kinematic constraints are imposed via appropriate algebraic equations and Lagrange multipliers.

In the recent paper [12] this model is employed for modeling pipe-lay offshore operations and the rod equations are coupled to a controlled rigid body (representing the vessel conducting the pipe-lay operations). In the same paper the configuration manifold is described using Euler angles and the choice of appropriate *conventions* (coordinate charts) is very important for the performance of the method. A robust implementation of this approach should allow for changes of chart when necessary.

The main contribution of the present work is the derivation of a Hamiltonian and a multi-symplectic formulation of the model in quaternions. We choose to represent rotations as unit quaternions (Euler parameters), we realize unit quaternions as vectors of $\mathbb{R}^4$ subjected to one length constraint. Compared to Euler angles, which give a local coordinatization of $SO(3)$ and allow to represent rotations with a minimal number of coordinates, unit quaternions use just one extra coordinate. The advantage is that we avoid the difficulties of local coordinatizations and changing of charts, see for example [13], [4] for a discussion of local vs global formulations of Hamiltonian systems and their symplectic integration.

The resulting Hamiltonian PDE has a simple looking format involving the canonical (constant) structure matrix typical of finite dimensional Hamiltonian systems, and it is subjected to kinematic constraints.

The new formulation has the advantage that strightforward finite-difference/ finite-element discretizations in space lead to canonical Hamiltonian semi-discretized ODE systems with constraints. The semi-discrete Hamiltonian system is obtained by first discretizing the Hamiltonian function in space, using a consistent approximation. The obtained discrete energy function is then used for defining a finite dimensional canonical Hamiltonian system, approximating the problem.

Multi-symplecticity is a generalization of classical symplecticity for finite-dimensional Hamiltonian systems to the infinite-dimensional case. Besides global preservation of energy and momentum, the multi-symplectic formulation of a Hamiltonian PDE implies local energy and momentum conservation properties. Following a procedure described in [10], from the Hamiltonian formulation we derive a multi-symplectic formulation of our problem by defining a new Hamiltonian function via a Legendre transform. For more details on multi-symplectic PDE's and multi-symplectic integrators, see e.g. [8, 9, 14].

2 Background

2.1 The elastic rod model

Here we give a short review of the elastic rod model formulated in [20]. For a given configuration of the elastic rod, the set occupied in $\mathbb{R}^3$ by its body $\mathcal{B} \subset \mathbb{R}^3$ is described by

$$\mathcal{B} = \{X(S,\xi_2,\xi_3) = \boldsymbol{\varphi}(S) + \xi_2 \boldsymbol{t}_2(S) + \xi_3 \boldsymbol{t}_3(S) \in \mathbb{R}^3 \mid (S,\xi_2,\xi_3) \in [0,L] \times A\},$$

where $[0,L] \times A = \mathcal{R} \in \mathbb{R}^3$ is the reference body, A is the cross section area, L its reference length and $\boldsymbol{t}_2(S)$, $\boldsymbol{t}_3(S)$ are mutually orthonormal vectors lying in the rod cross section plane at $\boldsymbol{\varphi}(S)$. Hence, the rod is fully described by the curve of

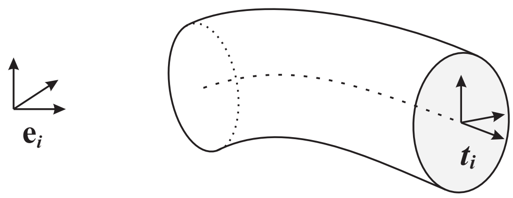

Figure 1: The body frame $\boldsymbol{t}_i(S)$, $i = 1, \ldots, 3$, relative to the spatial frame for a given rod configuration.

centroids $\boldsymbol{\varphi}(S)$ and the orientation of its cross sections, defined by the orthonormal frame $\boldsymbol{t}_i$, $i = 1, 2, 3$,

$$\boldsymbol{t}_i = \boldsymbol{\Lambda}\mathbf{e}_i, \quad \boldsymbol{\Lambda} \in \mathrm{SO}(3),$$

attached to each point of the curve of centroids, where $\boldsymbol{t}_1(S)$ is normal to the plane cross section at $\boldsymbol{\varphi}(S)$, see figure 1. The configuration space $\mathcal{C}$ of the elastic rod, letting the normal to the cross section be $\boldsymbol{t}_1 = \boldsymbol{\Lambda}\mathbf{e}_1$, is given by the set of functions

$$\mathcal{C} = \{(\boldsymbol{\varphi}, \boldsymbol{\Lambda}) \,:\, S \in [0, L] \to \mathbb{R}^3 \times \mathrm{SO}(3) \,|\, \langle \boldsymbol{\varphi}'(S), \boldsymbol{\Lambda}\mathbf{e}_1\rangle > 0\} = \mathbb{R}^3 \times \mathrm{SO}(3). \tag{1}$$

As reference configuration, $(\boldsymbol{\varphi_r}, \boldsymbol{\Lambda_r}) \in \mathcal{C}$ we assume that the rod is aligned along the spatial basis axis $\mathbf{e}_1$ such that

$$\boldsymbol{\varphi_r}(S) = S\mathbf{e}_1, \quad \boldsymbol{\Lambda_r}(S) = \mathbb{1},$$

where $\mathbb{1}$ is the 3×3 identity matrix [20] (letting the rod reference configuration be aligned along $\mathbf{e}_1$ instead of $\mathbf{e}_3$).

Following the notation by Simo et al. [22], the *material* coordinate vectors given in material basis $\boldsymbol{t}_i$ will be denoted by upper-case letters, while lower case letters are used to denote the vectors in the *spatial* basis $\mathbf{e}_i$. Let $\boldsymbol{W}$ be the body angular velocity, $\boldsymbol{\Omega}$ be the bending and torsional strain in body frame. Hence, the spatial vectors will be related to their material vectors by the expression

$$\boldsymbol{\omega} = \boldsymbol{\Lambda}\boldsymbol{\Omega}, \quad \mathbf{w} = \boldsymbol{\Lambda}\boldsymbol{W}.$$

This will give us the kinematics for the orientation of the cross sections along the line of centroids $\boldsymbol{\varphi}(S, t)$, $(S, t) \in [0, L] \times \mathbb{R}_+$,

$$\partial_S \boldsymbol{\Lambda}(S, t) = \widehat{\boldsymbol{\omega}}\boldsymbol{\Lambda} = \boldsymbol{\Lambda}\widehat{\boldsymbol{\Omega}}, \tag{2}$$

$$\partial_t \boldsymbol{\Lambda}(S, t) = \widehat{\mathbf{w}}\boldsymbol{\Lambda} = \boldsymbol{\Lambda}\widehat{\boldsymbol{W}}, \tag{3}$$

where the hat map $\widehat{\ }: \mathbb{R}^3 \to \mathfrak{so}(3)$, sends the axial vector $\boldsymbol{v}$ to its associated skew-symmetric matrix $\widehat{\boldsymbol{v}}$, i.e.

$$\boldsymbol{v} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}, \quad \widehat{\boldsymbol{v}} = \begin{bmatrix} 0 & -v_3 & v_2 \\ v_3 & 0 & -v_1 \\ -v_2 & v_1 & 0 \end{bmatrix}.$$

The assumption of an hyperelastic material behavior, corresponds to allowing for a bilinear quadratic energy function $\boldsymbol{\Psi}(\boldsymbol{\gamma}, \boldsymbol{\omega})$,

$$\boldsymbol{\Psi}(\boldsymbol{\gamma}, \boldsymbol{\omega}) = \frac{1}{2}\left[\langle \boldsymbol{\gamma}, \boldsymbol{D}_N \boldsymbol{\gamma}\rangle + \langle \boldsymbol{\omega}, \boldsymbol{D}_M \boldsymbol{\omega}\rangle\right],$$

$$\boldsymbol{D}_N = \boldsymbol{\Lambda} \boldsymbol{C}_N \boldsymbol{\Lambda}^T, \quad \boldsymbol{D}_M = \boldsymbol{\Lambda} \boldsymbol{C}_M \boldsymbol{\Lambda}^T, \tag{4}$$

and

$$\boldsymbol{C}_N = \mathrm{diag}([EA, GA_1, GA_2]), \quad \boldsymbol{C}_M = \mathrm{diag}([GJ, EI_1, EI_2]), \tag{5}$$

where

$$\boldsymbol{\gamma} = \partial_S \boldsymbol{\varphi}(S,t) - \boldsymbol{t}_1 = \partial_S \boldsymbol{\varphi}(S,t) - \boldsymbol{\Lambda}(S,t)\mathbf{e}_1, \tag{6}$$

is the strain measure for extension and shearing, and $\boldsymbol{\omega}$ gives the measure for twisting and bending.

The constants E and G are interpreted as the Young's modulus and the shear modulus, A is the cross-sectional area of the rod, A_2 and A_3 are the effective shear areas, I_2 and I_3 the polar moments of inertia of the cross section plane relative to the principal axes, and J is the Saint Venant torsional modulus.

The internal stress resultant $\boldsymbol{n}$ and stress couple $\boldsymbol{m}$ are obtained by differentiation from the bilinear quadratic energy function $\boldsymbol{\Psi}(\boldsymbol{\gamma}, \boldsymbol{\omega})$,

$$\boldsymbol{n} = \frac{\partial}{\partial \boldsymbol{\gamma}} \boldsymbol{\Psi} = \boldsymbol{D}_N \boldsymbol{\gamma}, \tag{7}$$

$$\boldsymbol{m} = \frac{\partial}{\partial \boldsymbol{\omega}} \boldsymbol{\Psi} = \boldsymbol{D}_M \boldsymbol{\omega}. \tag{8}$$

Stress forces in material form are given in upper-case letters,

$$\begin{aligned} \boldsymbol{N} &= \boldsymbol{\Lambda}^T \boldsymbol{n} = \boldsymbol{C}_N \boldsymbol{\Gamma}, \qquad \boldsymbol{\Gamma} = \boldsymbol{\Lambda}^T \boldsymbol{\gamma} = \boldsymbol{\Lambda}^T \partial_S \boldsymbol{\varphi} - \mathbf{e}_1, \\ \boldsymbol{M} &= \boldsymbol{\Lambda}^T \boldsymbol{m} = \boldsymbol{C}_M \boldsymbol{\Omega}. \end{aligned}$$

The spatial form of the local, linear and angular, momentum balance equations are written, see e.g. [20, 23],

$$\rho_A \partial_{tt} \boldsymbol{\varphi} = \partial_S \boldsymbol{n} + \tilde{\boldsymbol{n}}, \tag{9}$$

$$\boldsymbol{I}_\rho \partial_t \mathbf{w} + \mathbf{w} \times (\boldsymbol{I}_\rho \mathbf{w}) = \partial_S \boldsymbol{m} + (\partial_S \boldsymbol{\varphi}) \times \boldsymbol{n} + \tilde{\boldsymbol{m}}, \tag{10}$$

for $(\boldsymbol{\varphi}(S,t), \boldsymbol{\Lambda}(S,t)) \in \mathcal{C}$ and external forces $\tilde{\boldsymbol{n}}$, $\tilde{\boldsymbol{m}}$. Here $\rho_A(S)$ is the mass per unit length of the rod in reference length, and $\boldsymbol{I}_\rho(S,t)$ is the time dependent inertia tensor in spatial basis

$$\boldsymbol{I}_\rho = \boldsymbol{\Lambda} \boldsymbol{J}_\rho \boldsymbol{\Lambda}^T, \quad \boldsymbol{J}_\rho = \mathrm{diag}([J_1, J_2, J_3]), \tag{11}$$

where $\boldsymbol{J}_\rho$ is the constant inertia tensor for the cross section in the reference configuration.

In the absence of external forces $\tilde{\boldsymbol{n}}$ and $\tilde{\boldsymbol{m}}$, we assume pure displacement boundary conditions, such that $\boldsymbol{\varphi}$ and $\boldsymbol{\Lambda}$ are described at the boundaries $S = 0$ and $S = L$. Then the total energy E (Hamiltonian) [21, 11] of the problem (9)–(10) is given by

$$E = T + U = \frac{1}{2} \int_0^L \langle \dot{\boldsymbol{\varphi}}, \rho_A \dot{\boldsymbol{\varphi}} \rangle + \langle \mathbf{w}, \boldsymbol{I}_\rho \mathbf{w} \rangle \, dS + \frac{1}{2} \int_0^L \langle \boldsymbol{\gamma}, \boldsymbol{D}_N \boldsymbol{\gamma} \rangle + \langle \boldsymbol{\omega}, \boldsymbol{D}_M \boldsymbol{\omega} \rangle \, dS, \tag{12}$$

where the first integral in the sum is the kinetic energy T and the second is the potential energy U.

2.2 Quaternions

We here review briefly the main properties of quaternions and introduce some notations that will be used throughout this paper, more information on this subject is found in e.g. [19]. The quaternions,

$$\mathbb{H} := \{\mathbb{q} = (q_0, \boldsymbol{q}) \in \mathbb{R} \times \mathbb{R}^3,\ \boldsymbol{q} = (q_1, q_2, q_3)^T\} \cong \mathbb{R}^4,$$

is a strictly skew field [3]. Addition and multiplication of two quaternions, $\mathbb{p} = (p_0, \boldsymbol{p})$, $\mathbb{q} = (q_0, \boldsymbol{q}) \in \mathbb{H}$, are defined by

$$\mathbb{p} + \mathbb{q} = (p_0 + q_0, \boldsymbol{p} + \boldsymbol{q})$$

and

$$\mathbb{p}\mathbb{q} = (p_0 q_0 - \boldsymbol{p}^T \boldsymbol{q}, p_0 \boldsymbol{q} + q_0 \boldsymbol{p} + \boldsymbol{p} \times \boldsymbol{q}), \tag{13}$$

respectively. For $\mathbb{q} \neq (0, \mathbf{0})$ there exist an inverse

$$\mathbb{q}^{-1} = \mathbb{q}^c / \|\mathbb{q}\|^2, \quad \|\mathbb{q}\| = \sqrt{q_0^2 + \|\boldsymbol{q}\|_2^2},$$

where $\mathbb{q}^c = (q_0, -\boldsymbol{q})$ is the conjugate of $\mathbb{q}$, such that $\mathbb{q}\mathbb{q}^{-1} = \mathbb{q}^{-1}\mathbb{q} = \mathbb{e} = (1, \mathbf{0})$. In the sequel we will consider $\mathbb{q} \in \mathbb{H}$ as a vector $\mathbb{q} = (q_0, q_1, q_2, q_3)^T \in \mathbb{R}^4$. The multiplication rule (13) can then be expressed by means of a matrix-vector product in $\mathbb{R}^4$. Namely, $\mathbb{p}\mathbb{q} = L(\mathbb{p})\mathbb{q} = R(\mathbb{q})\mathbb{p}$, where

$$L(\mathbb{p}) = \begin{bmatrix} p_0 & -\boldsymbol{p}^T \\ \boldsymbol{p} & (p_0 \mathbb{1} + \widehat{\boldsymbol{p}}) \end{bmatrix}, \quad R(\mathbb{q}) = \begin{bmatrix} q_0 & -\boldsymbol{q}^T \\ \boldsymbol{q} & (q_0 \mathbb{1} - \widehat{\boldsymbol{q}}) \end{bmatrix} \tag{14}$$

and $\mathbb{1}$ is the 3×3 identity matrix. Note that $R(\mathbb{q})$ and $L(\mathbb{p})$ commutes, i.e. $R(\mathbb{q})L(\mathbb{p}) = L(\mathbb{p})R(\mathbb{q})$.

Three-dimensional rotations in space can be represented by unit quaternions, sometimes referred to as Euler parameters,

$$\mathbb{S}^3 = \{\mathbb{q} \in \mathbb{H} \mid \|\mathbb{q}\| = 1\}.$$

$\mathbb{S}^3$ with the quaternion product is a Lie group, and $\mathbb{q}^{-1} = \mathbb{q}^c$ while $\mathbb{e} = (1, \mathbf{0})$ is the identity. There is a (surjective $2:1$) group homomorphism (the Euler-Rodriguez map) $\mathcal{E} : \mathbb{S}^3 \to SO(3)$, defined by

$$\mathcal{E}(\mathbb{q}) = \mathbb{1} + 2q_0 \widehat{\boldsymbol{q}} + 2\widehat{\boldsymbol{q}}^2,$$

and therefore $\mathbb{S}^3$ is a double-covering of $SO(3)$. The Euler-Rodriguez map can be explicitly written as

$$\mathcal{E}(\mathbb{q}) = \begin{bmatrix} 1 - 2(q_2^2 + q_3^2) & 2(q_1 q_2 - q_0 q_3) & 2(q_0 q_2 + q_1 q_3) \\ 2(q_0 q_3 + q_1 q_2) & 1 - 2(q_1^2 + q_3^2) & 2(q_2 q_3 - q_0 q_1) \\ 2(q_1 q_3 - q_0 q_2) & 2(q_0 q_1 + q_2 q_3) & 1 - 2(q_1^2 + q_2^2) \end{bmatrix}. \tag{15}$$

A rotation in $\mathbb{R}^3$,

$$\mathbf{w} = Q\mathbf{v}, \quad Q \in SO(3), \quad \mathbf{v}, \mathbf{w} \in \mathbb{R}^3,$$

can, for some $\mathbb{q} \in \mathbb{S}^3$, be expressed in quaternionic form as

$$W = L(\mathbb{q})R(\mathbb{q}^c)V = R(\mathbb{q}^c)L(\mathbb{q})V, \quad V = (0, \mathbf{v}),\ W = (0, \mathbf{w}) \in \mathbb{H}_{\mathcal{P}}, \tag{16}$$

where $\mathbb{H}_{\mathcal{P}} = \{\mathbb{q} \in \mathbb{H} \,|\, q_0 = 0\} \cong \mathbb{R}^3$ is the set of so called pure quaternions. It also follows from straightforward computations that

$$L(\mathbb{q})R(\mathbb{q}^c) = R(\mathbb{q}^c)L(\mathbb{q}) = \begin{bmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & \mathcal{E}(\mathbb{q}) \end{bmatrix}, \quad \mathbf{0} = (0,0,0)^T \in \mathbb{R}^3.$$

It is also evident that $\forall\ \mathbb{q} \in \mathbb{S}^3,\ L(\mathbb{q}), R(\mathbb{q}) \in O(4)$ are orthogonal matrices, such that $L(\mathbb{q})L(\mathbb{q})^T = L(\mathbb{q})L(\mathbb{q}^c) = \mathbb{1}_{4\times 4},\ R(\mathbb{q})R(\mathbb{q})^T = R(\mathbb{q})R(\mathbb{q}^c) = \mathbb{1}_{4\times 4}$.

2.2.1 The Lie algebra $\mathfrak{s}^3$

If $\mathbb{q} \in \mathbb{S}^3$, it follows from $\mathbb{q}\mathbb{q}^c = \mathbb{e}$ that

$$\mathfrak{s}^3 := T_{\mathbb{e}}\mathbb{S}^3 = \mathbb{H}_{\mathcal{P}}.$$

The Lie algebra $\mathfrak{s}^3$, associated to $\mathbb{S}^3$, is equipped with a Lie bracket $[\,\cdot\,,\cdot\,]_{\mathfrak{s}} : \mathfrak{s}^3 \times \mathfrak{s}^3 \to \mathfrak{s}^3$,

$$[\,V\,, W\,]_{\mathfrak{s}} := [L(V)W - L(W)V] = (0, 2\mathbf{v} \times \mathbf{w}) \in \mathfrak{s}^3,$$

where $V = (0, \mathbf{v})$, $W = (0, \mathbf{w}) \in \mathfrak{s}^3$.

The derivative map of $\mathcal{E}$ is $\mathcal{E}_* = T_{\mathbb{e}}\mathcal{E} : \mathfrak{s}^3 \to \mathfrak{so}(3)$ is given by

$$\mathcal{E}_*(V) = 2\widehat{\mathbf{v}}, \quad V = (0, \mathbf{v}) \in \mathfrak{s}^3, \tag{17}$$

and it is a Lie algebra isomorphism. Assume now that $\mathbb{q} \in \mathbb{S}^3$ is such that $\mathcal{E}(\mathbb{q}(S,t)) = \mathbf{\Lambda}(S,t)$, then $L(\mathbb{q}^c)\dot{\mathbb{q}} \in \mathfrak{s}^3$, $\mathbf{\Lambda}^T\dot{\mathbf{\Lambda}} \in \mathfrak{so}(3)$ and

$$\mathcal{E}_*(L(\mathbb{q}^c)\dot{\mathbb{q}}) = \mathbf{\Lambda}^T\dot{\mathbf{\Lambda}}. \tag{18}$$

Further, it can be shown that

$$\mathcal{E}_*(L(\mathbb{q})R(\mathbb{q}^c)V) = 2\widehat{\mathcal{E}(\mathbb{q})\mathbf{v}} \qquad \forall\, \mathbb{q} \in \mathbb{S}^3,\ V = (0, \mathbf{v}) \in \mathfrak{s}^3, \tag{19}$$

and as a consequence of (18) and (19) the kinematics of the cross sections (2) and (3) can be formulated in unit quaternions $\mathbb{S}^3$ as

$$\dot{\mathbb{q}} = \frac{1}{2}L(\mathbb{q})W = \frac{1}{2}R(\mathbb{q})\mathrm{w}, \quad \mathbb{q}' = \frac{1}{2}L(\mathbb{q})\Omega = \frac{1}{2}R(\mathbb{q})\omega, \tag{20}$$

$$W = 2L(\mathbb{q}^c)\dot{\mathbb{q}}, \quad \Omega = 2L(\mathbb{q}^c)\mathbb{q}', \quad \mathrm{w} = 2R(\mathbb{q}^c)\dot{\mathbb{q}}, \quad \omega = 2R(\mathbb{q}^c)\mathbb{q}', \tag{21}$$

where $W = (0, \boldsymbol{W}),\ \mathrm{w} = (0, \mathbf{w}),\ \Omega = (0, \mathbf{\Omega}),\ \omega = (0, \boldsymbol{\omega}) \in \mathfrak{s}$.

2.3 Hamiltonian formulation of the free rigid body

Following [17] we write an Hamiltonian formulation of the free rigid body motion in unit quaternions $\mathbb{S}^3$, see also [5] for constrained formulation of the rigid body in quaternions.

Having in mind the expression for the angular velocity in unit quaternions (21), the kinetic energy (total energy) is defined by,

$$L = \frac{1}{2}\langle \mathrm{W}, \widetilde{\boldsymbol{J}}\mathrm{W}\rangle = 2\langle \dot{\mathbb{q}}, L(\mathbb{q})\widetilde{\boldsymbol{J}}L(\mathbb{q}^c)\dot{\mathbb{q}}\rangle,$$

where

$$\widetilde{\boldsymbol{J}} = \begin{bmatrix} \alpha & \mathbf{0}^T \\ \mathbf{0} & \boldsymbol{J} \end{bmatrix}, \quad \alpha \in \mathbb{R}, \tag{22}$$

is the constant inertia matrix $\boldsymbol{J} = \mathrm{diag}([J_1, J_2, J_3])$ extended to $\mathbb{R}^{4\times 4}$. From the Legendre transformation one obtains the conjugate momenta

$$\mathbb{p} := \frac{\partial \mathcal{L}}{\partial \dot{\mathbb{q}}} = 4L(\mathbb{q})\widetilde{\boldsymbol{J}}L(\mathbb{q}^c)\dot{\mathbb{q}} \in T^*_{\mathbb{q}}\mathbb{S}^3, \tag{23}$$

and the map $T_{\mathbb{q}}\mathbb{S}^3 \to T^*_{\mathbb{q}}\mathbb{S}^3$ (23) is invertible for any α. Infact, $\mathbb{q} \in \mathbb{S}^3$ implies $\langle \mathbb{q}, \dot{\mathbb{q}} \rangle = 0$ and $L(\mathbb{q}^c)\dot{\mathbb{q}} \in \mathbb{H}_{\mathcal{P}}$. Consequently, α has no significance when $\mathbb{q} \in \mathbb{S}^3$. Taking $\alpha \neq 0$ we can write the Hamiltonian formulation of the free rigid body

$$\begin{aligned} \mathbb{p} &= \frac{1}{4}L(\mathbb{p})\widetilde{\boldsymbol{J}}L(\mathbb{q}^c)\dot{\mathbb{q}}, \\ \dot{\mathbb{q}} &= \frac{1}{4}L(\mathbb{q})\widetilde{\boldsymbol{J}}^{-1}L(\mathbb{q}^c)\mathbb{p}. \end{aligned}$$

This motivates a similar extension of the matrices $\boldsymbol{J}_\rho$ and $\boldsymbol{C}_M$ in the sections that follow.

3 Formulation of the Hamiltonian in quaternions

We will obtain the augmented Hamiltonian formulation on the cotangent bundle of $\mathbb{R}^3 \times \mathbb{H}$ with the holonomic constraint $g(\mathbb{q}) := \|\mathbb{q}\|^2 - 1 = 0$, from the augmented Lagrangian

$$\mathcal{L}(\boldsymbol{u}, \boldsymbol{u}_t, \boldsymbol{u}_S) = T - U - \lambda(\|\mathbb{q}\|^2 - 1), \quad \boldsymbol{u} = (\boldsymbol{\varphi}, \mathbb{q})^T \in \mathbb{R}^3 \times \mathbb{H}. \tag{24}$$

We extend for convenience the inertia tensor $\boldsymbol{J}_\rho \in \mathbb{R}^{3\times 3}$ to $\widetilde{\boldsymbol{J}}_\rho \in \mathbb{R}^{4\times 4}$, and analogously $\boldsymbol{C}_M \in \mathbb{R}^{3\times 3}$ to $\widetilde{\boldsymbol{C}}_M \in \mathbb{R}^{4\times 4}$ invertible 4×4-matrices, so that the new Lagrangian becomes regular on $T(\mathbb{R}^3 \times \mathbb{H})$. In particular

$$\widetilde{\boldsymbol{J}}_\rho = \begin{bmatrix} \alpha & \mathbf{0}^T \\ \mathbf{0} & \boldsymbol{J}_\rho \end{bmatrix}, \quad \widetilde{\boldsymbol{C}}_M = \begin{bmatrix} \alpha & \mathbf{0}^T \\ \mathbf{0} & \boldsymbol{C}_M \end{bmatrix}, \quad \alpha \neq 0,$$

and accordingly

$$\widetilde{\boldsymbol{I}}_\rho = L(\mathbb{q})R(\mathbb{q}^c)\widetilde{\boldsymbol{J}}_\rho L(\mathbb{q}^c)R(\mathbb{q}), \quad \widetilde{\boldsymbol{D}}_M = L(\mathbb{q})R(\mathbb{q}^c)\widetilde{\boldsymbol{C}}_M L(\mathbb{q}^c)R(\mathbb{q}). \tag{25}$$

This is convinient for the actual inversion of the Legendre transform when constructing the augmented Hamiltonian and multi-symplectic Hamiltonian, respectively. See [18] for general framework of constrained multi-symplectic theory.

The kinetic- and potential energy density functions, (12), are expressed in quaternions by

$$T = \frac{1}{2}\left[\langle \dot{\boldsymbol{\varphi}}, \rho_A \dot{\boldsymbol{\varphi}} \rangle + 4\langle \dot{\mathbb{q}}, R(\mathbb{q})\widetilde{\boldsymbol{I}}_\rho R(\mathbb{q}^c)\dot{\mathbb{q}} \rangle\right], \tag{26}$$

$$U = \frac{1}{2}\left[\langle \boldsymbol{\gamma}, \boldsymbol{D}_N \boldsymbol{\gamma} \rangle + 4\langle \mathbb{q}', R(\mathbb{q})\widetilde{\boldsymbol{D}}_M R(\mathbb{q}^c)\mathbb{q}' \rangle\right], \tag{27}$$

see also [21, 11, 23]. Here w, $\omega \in \mathbb{H}_{\mathcal{P}}$ are defined as in (21) and

$$\boldsymbol{\gamma} = \boldsymbol{\varphi}' - \mathcal{E}(\mathbb{q})\mathbf{e}_1.$$

We now introduce the conjugate variables, $\boldsymbol{p}_\varphi$ and $\mathbb{p}$, via the Legendre transform

$$\boldsymbol{p}_\varphi := \frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{\varphi}}} = \rho_A \dot{\boldsymbol{\varphi}}, \tag{28}$$

$$\mathbb{p} := \frac{\partial \mathcal{L}}{\partial \dot{\mathbb{q}}} = 4L(\mathbb{q})\widetilde{\boldsymbol{J}}_\rho L(\mathbb{q}^c)\dot{\mathbb{q}} = 4R(\mathbb{q})\widetilde{\boldsymbol{I}}_\rho R(\mathbb{q}^c)\dot{\mathbb{q}} \ \in T^*\mathbb{H}, \tag{29}$$

and finally obtain the augmented Hamiltonian

$$\mathcal{H} = \int_0^L h(\boldsymbol{u}, \boldsymbol{p}, \boldsymbol{u}_S)\, dS, \quad \boldsymbol{p} = (\boldsymbol{p}_\varphi, \mathbb{p}), \tag{30}$$

where h is the energy density function,

$$\begin{aligned} h(\boldsymbol{u}, \boldsymbol{p}, \boldsymbol{u}_S) &= \langle \boldsymbol{p}_\varphi, \dot{\boldsymbol{\varphi}}(\boldsymbol{p}_\varphi)\rangle + \langle \mathbb{p}, \dot{\mathbb{q}}(\mathbb{q}, \mathbb{p})\rangle - \mathcal{L}(\boldsymbol{u}, \boldsymbol{u}_t(\boldsymbol{u}, \boldsymbol{p}), \boldsymbol{u}_S) \\ &= \frac{1}{2}\left[\langle \boldsymbol{p}_\varphi, \rho_A^{-1}\boldsymbol{p}_\varphi\rangle + \frac{1}{4}\langle \mathbb{p}, R(\mathbb{q})\widetilde{\boldsymbol{I}}_\rho^{-1} R(\mathbb{q}^c)\mathbb{p}\rangle\right] \\ &\quad + \frac{1}{2}\left[\langle \boldsymbol{\gamma}, \boldsymbol{D}_N\boldsymbol{\gamma}\rangle + 4\langle \mathbb{q}', R(\mathbb{q})\widetilde{\boldsymbol{D}}_M R(\mathbb{q}^c)\mathbb{q}'\rangle\right] + \lambda(\|\mathbb{q}\|^2 - 1), \end{aligned} \tag{31}$$

and

$$\dot{\boldsymbol{\varphi}}(\boldsymbol{p}_\varphi) = \rho_A^{-1}\boldsymbol{p}_\varphi, \quad \dot{\mathbb{q}}(\mathbb{q}, \mathbb{p}) = \frac{1}{4}R(\mathbb{q})\widetilde{\boldsymbol{I}}_\rho^{-1} R(\mathbb{q}^c)\mathbb{p}. \tag{32}$$

The abstract form of the equation of motion for the constrained Hamiltonian problem is stated as

$$\partial_t \boldsymbol{x} = \mathcal{J}\frac{\delta \mathcal{H}}{\delta \boldsymbol{x}}, \qquad \mathcal{J} := \begin{bmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{bmatrix} \in \mathbb{R}^{14\times 14}, \tag{33}$$

$$g(\boldsymbol{x}) = 0, \qquad g(\boldsymbol{x}) := \|\mathbb{q}\|^2 - 1, \tag{34}$$

where $\mathbb{1}$ is the 7×7 identity matrix, $\boldsymbol{x} = (\boldsymbol{u}, \boldsymbol{p})^T \in \mathbb{R}^{14}$, $\boldsymbol{u} = (\boldsymbol{\varphi}, \mathbb{q})^T \in \mathbb{R}^7$ and $\boldsymbol{p} = (\boldsymbol{p}_\varphi, \mathbb{p})^T \in \mathbb{R}^7$. In other words, a constrained system of partial differential equations

$$\partial_t \boldsymbol{u} = \begin{bmatrix} \dot{\boldsymbol{\varphi}} \\ \dot{\mathbb{q}} \end{bmatrix} = \begin{bmatrix} \rho_A^{-1}\boldsymbol{p}_\varphi \\ (1/4)R(\mathbb{q})\widetilde{\boldsymbol{I}}_\rho^{-1} R(\mathbb{q}^c)\mathbb{p} \end{bmatrix}, \tag{35}$$

$$\partial_t \boldsymbol{p} = \begin{bmatrix} \dot{\boldsymbol{p}}_\varphi \\ \dot{\mathbb{p}} \end{bmatrix} = \begin{bmatrix} -\partial h/\partial \boldsymbol{\varphi} + \partial_S(\partial h/\partial \boldsymbol{\varphi}') \\ -\partial h/\partial \mathbb{q} + \partial_S(\partial h/\partial \mathbb{q}') \end{bmatrix}, \tag{36}$$

$$0 = \|\mathbb{q}\|^2 - 1. \tag{37}$$

Here, the equation for $\boldsymbol{p}_\varphi$ in (36) is

$$\dot{\boldsymbol{p}}_\varphi = [\boldsymbol{D}_N, \widehat{\boldsymbol{\omega}}]\,\boldsymbol{\gamma} - \boldsymbol{D}_N\boldsymbol{\gamma}', \tag{38}$$

where $[\,\cdot\,,\,\cdot\,]$ is the usual commutator for 3×3-matrices ($[A,B] = AB - BA$),

$$\boldsymbol{\gamma}' = \boldsymbol{\varphi}'' - \widehat{\boldsymbol{\omega}}\mathcal{E}(\mathbb{q})\mathbf{e}_1$$

and

$$\boldsymbol{\omega}(\mathbb{q}, \mathbb{q}') = 2(q_0\boldsymbol{q}' - q_0'\boldsymbol{q} + \widehat{\boldsymbol{q}}\boldsymbol{q}') = 2\left[-\boldsymbol{q} \quad (q_0\mathbb{1} - \widehat{\boldsymbol{q}})\right]\mathbb{q}'.$$

The equation for $\mathbb{p}$, (36), becomes

$$\begin{aligned}\dot{\mathbb{p}} = \frac{1}{4}R(\mathbb{q})L(\mathbb{p})L(\mathbb{q}^c)\widetilde{\boldsymbol{I}}_\rho^{-1}R(\mathbb{q}^c)\mathbb{p} + R(\mathbb{q})\Big[L(\varphi') - R(\varphi')\Big]\begin{bmatrix} 0 \\ \boldsymbol{D}_N\boldsymbol{\gamma}\end{bmatrix} \\ + 2R(\mathbb{q})\left[L(\omega)\widetilde{\boldsymbol{D}}_M\omega + \widetilde{\boldsymbol{D}}_M\omega'\right] + 2\langle(\mathcal{E}(\mathbb{q}) - \mathbb{1})\boldsymbol{\varphi}', \boldsymbol{D}_N\boldsymbol{\gamma}\rangle\mathbb{q} - 2\lambda\mathbb{q}. \qquad (39)\end{aligned}$$

Detailed calculations for the equations of motions can be found in the appendix 5.1.1–5.1.2, as well as the solution for the Lagrange multiplier (5.2),

$$\lambda = -\langle\omega, \widetilde{\boldsymbol{D}}_M\omega\rangle - \langle(\mathbb{1} - \mathcal{E}(\mathbb{q}))\boldsymbol{\varphi}', \boldsymbol{D}_N\boldsymbol{\gamma}\rangle.$$

Substituting the above expression for λ in (39) and multiplying with $(1/2)R(\mathbb{q}^c)$ from the left and using (29), one reproduces (10) (formulated in quaternions). Equation (9) is reproduced from (38) by using (28).

4 Multi-symplectic formulation

4.1 Review of multi-symplectic PDEs

A PDE is said to be multi-symplectic if it can be written as a linear system of first order equations of the type

$$M\boldsymbol{z}_t + K\boldsymbol{z}_x = \nabla_{\boldsymbol{z}}\mathcal{S}(\boldsymbol{z}), \qquad (40)$$

where $\boldsymbol{z} \in \mathbb{R}^d$, M and K are skew-symmetric $d \times d$-matrices and $\mathcal{S} : \mathbb{R}^d \to \mathbb{R}$ is a smooth function, see [8] and [9] for a comprehensive description. Defining the two-forms

$$\omega := \mathrm{d}\boldsymbol{z} \wedge M\mathrm{d}\boldsymbol{z}, \quad \kappa := \mathrm{d}\boldsymbol{z} \wedge K\mathrm{d}\boldsymbol{z}, \qquad (41)$$

any solution $\mathrm{d}\boldsymbol{z}$, of the variational equation associated with (40), will satisfy the multi-symplectic conservation law

$$\partial_t\omega + \partial_x\kappa = 0. \qquad (42)$$

The equation (40) also obeys the local energy and momentum conservation laws, i.e.

$$\partial_t e(z) + \partial_x f(z) = 0, \quad \text{and} \quad \partial_t i(z) + \partial_x g(z) = 0, \qquad (43)$$

where

$$e(z) = \mathcal{S}(z) - \frac{1}{2}z_x^T K^T z, \quad f(z) = \frac{1}{2}z_t^T K^T z, \qquad (44)$$

$$g(z) = \mathcal{S}(z) - \frac{1}{2}z_t^T M^T z, \quad i(z) = \frac{1}{2}z_x^T M^T z. \qquad (45)$$

Integrating the densities $f(z)$ and $i(z)$ over the spatial domain one obtains, for suitable boundary conditions, the global conservative quantities of energy $E(z)$ (12) and momentum $I(z)$,

$$E(z) = \int_0^L e(z)\,dx, \quad \text{and} \quad I(z) = \int_0^L i(z)\,dx, \qquad (46)$$

such that $(d/dt)E(z) = (d/dt)I(z) = 0$.

4.2 The multi-symplectic formulation $\mathcal{S}$

We construct the constrained multi-symplectic formulation in quaternions by defining

$$\mathcal{S}(\boldsymbol{u},\boldsymbol{p},\boldsymbol{v}) = \langle \boldsymbol{p}, \boldsymbol{u}_t(\boldsymbol{p})\rangle + \langle \boldsymbol{v}, \boldsymbol{u}_S(\boldsymbol{v})\rangle - \mathcal{L}(\boldsymbol{u}, \boldsymbol{u}_t(\boldsymbol{p}), \boldsymbol{u}_S(\boldsymbol{v})), \tag{47}$$

where $\mathcal{L}(\boldsymbol{u}, \boldsymbol{u}_t(\boldsymbol{p}), \boldsymbol{u}_S(\boldsymbol{v}))$ is the Lagrangian (24) defined in the previous section, $\boldsymbol{p} = (\boldsymbol{p}_\varphi, \mathbb{p})^T \in \mathbb{R}^7$ are given by the former Legendre transforms (28)–(29) and $\boldsymbol{v} = (\boldsymbol{v}_\varphi, \mathbb{v})^T \in \mathbb{R}^7$ are the second conjugate variables defined by

$$\boldsymbol{v}_\varphi := \frac{\partial \mathcal{L}}{\partial \boldsymbol{\varphi}'} = -\boldsymbol{D}_N \boldsymbol{\gamma} = -\boldsymbol{n}, \tag{48}$$

$$\mathbb{v} := \frac{\partial \mathcal{L}}{\partial \mathbb{q}'} = -4L(\mathbb{q})\widetilde{\boldsymbol{C}}_M L(\mathbb{q}^c)\mathbb{q}' = -4R(\mathbb{q})\widetilde{\boldsymbol{D}}_M R(\mathbb{q}^c)\mathbb{q}' \in T^*\mathbb{H} \tag{49}$$

such that

$$\boldsymbol{\varphi}'(\mathbb{q}, \boldsymbol{v}_\varphi) = -\boldsymbol{D}_N^{-1}\boldsymbol{v}_\varphi + \mathcal{E}(\mathbb{q})\mathbf{e}_1, \tag{50}$$

$$\mathbb{q}'(\mathbb{q}, \mathbb{v}) = -\frac{1}{4}R(\mathbb{q})\widetilde{\boldsymbol{D}}_M^{-1}R(\mathbb{q}^c)\mathbb{v}. \tag{51}$$

We can write the Lagrangian as a function of first and second conjugate variables $\boldsymbol{p}$ and $\boldsymbol{v}$,

$$\begin{aligned}\mathcal{L}(\boldsymbol{u}, \boldsymbol{u}_t(\boldsymbol{p}), \boldsymbol{u}_S(\boldsymbol{v})) = \frac{1}{2}&\left[\langle \boldsymbol{p}_\varphi, \rho_A^{-1}\boldsymbol{p}_\varphi\rangle + \frac{1}{4}\langle \mathbb{p}, R(\mathbb{q})\widetilde{\boldsymbol{I}}_\rho^{-1}R(\mathbb{q}^c)\mathbb{p}\rangle\right]\\ &- \frac{1}{2}\left[\langle \boldsymbol{v}_\varphi, \boldsymbol{D}_M^{-1}\boldsymbol{v}_\varphi\rangle + \frac{1}{4}\langle \mathbb{v}, R(\mathbb{q})\widetilde{\boldsymbol{D}}_M^{-1}R(\mathbb{q}^c)\mathbb{v}\rangle\right]\\ &- \lambda(\|\mathbb{q}\|^2 - 1),\end{aligned} \tag{52}$$

and consequently

$$\begin{aligned}\mathcal{S}(\boldsymbol{u},\boldsymbol{p},\boldsymbol{v}) = \frac{1}{2}&\left[\langle \boldsymbol{p}_\varphi, \rho_A^{-1}\boldsymbol{p}_\varphi\rangle + \frac{1}{4}\langle \mathbb{p}, R(\mathbb{q})\widetilde{\boldsymbol{I}}_\rho^{-1}R(\mathbb{q}^c)\mathbb{p}\rangle\right]\\ &- \frac{1}{2}\left[\langle \boldsymbol{v}_\varphi, \boldsymbol{D}_N^{-1}\boldsymbol{v}_\varphi - 2\mathcal{E}(\mathbb{q})\mathbf{e}_1\rangle + \frac{1}{4}\langle \mathbb{v}, R(\mathbb{q})\widetilde{\boldsymbol{D}}_M^{-1}R(\mathbb{q}^c)\mathbb{v}\rangle\right]\\ &+ \lambda(\|\mathbb{q}\|^2 - 1).\end{aligned} \tag{53}$$

Hence, the equations of motion are

$$\frac{\partial \mathcal{S}}{\partial \boldsymbol{u}} = -\partial_t \boldsymbol{p} - \partial_S \boldsymbol{v}, \tag{54}$$

$$\frac{\partial \mathcal{S}}{\partial \boldsymbol{p}} = \partial_t \boldsymbol{u}, \tag{55}$$

$$\frac{\partial \mathcal{S}}{\partial \boldsymbol{v}} = \partial_S \boldsymbol{u}, \tag{56}$$

$$0 = \|\mathbb{q}\|^2 - 1. \tag{57}$$

Let $\boldsymbol{z} = (\boldsymbol{u}, \boldsymbol{p}, \boldsymbol{v}, \lambda)^T \in \mathbb{R}^{22}$, then (54)–(57) can be written in the general multi-symplectic form (40) where

$$M = \begin{bmatrix} 0 & -\mathbb{1} & 0 & 0\\ \mathbb{1} & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{bmatrix}, \quad K = \begin{bmatrix} 0 & 0 & -\mathbb{1} & 0\\ 0 & 0 & 0 & 0\\ \mathbb{1} & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{bmatrix} \in \mathbb{R}^{22\times 22},$$

and $\mathbb{1}$ is the 7×7 identity matrix. The partial derivatives of S with respect to $\boldsymbol{\varphi}$ and $\mathbb{q}$ (54), respectively, are:

$$\frac{\partial \mathcal{S}}{\partial \boldsymbol{\varphi}} = 0, \tag{58}$$

and

$$\begin{aligned}\frac{\partial \mathcal{S}}{\partial \mathbb{q}} = &- \frac{1}{4} R(\mathbb{q}) L(\mathbb{p}) L(\mathbb{q}^c) \widetilde{\boldsymbol{I}}_\rho^{-1} R(\mathbb{q}^c)\mathbb{p} + \frac{1}{4} R(\mathbb{q}) L(\mathbb{v}) L(\mathbb{q}^c) \widetilde{\boldsymbol{D}}_M^{-1} R(\mathbb{q}^c)\mathbb{v} \\ &+ R(\mathbb{q}) \left[L(\boldsymbol{v}_\varphi) - R(\boldsymbol{v}_\varphi)\right] \begin{bmatrix} 0 \\ \boldsymbol{D}_N^{-1}\boldsymbol{v}_\varphi - \mathcal{E}(\mathbb{q})\mathbf{e}_1 \end{bmatrix} \\ &+ 2\langle (\mathcal{E}(\mathbb{q}) - \mathbb{1})\boldsymbol{v}_\varphi, \boldsymbol{D}_N^{-1}\boldsymbol{v}_\varphi - \mathcal{E}(\mathbb{q})\mathbf{e}_1\rangle \mathbb{q} + 2\lambda\mathbb{q}. \end{aligned} \tag{59}$$

Equations (55) and (56) are given by (32) and (50)–(51), respectively. Differentiating the constraint $g(\mathbb{q}) = 0$ twice, see appendix 5.3.1, yields

$$\lambda = -\langle (\mathcal{E}(\mathbb{q}) - \mathbb{1})\boldsymbol{v}_\varphi, \boldsymbol{D}_N^{-1}\boldsymbol{v}_\varphi - \mathcal{E}(\mathbb{q})\mathbf{e}_1\rangle.$$

Analogously to the Hamiltonian case, by a similar procedure as the one in the end of section 3, one can verify that the multi-symplectic formulation is reformulation of the original equations (9)–(10) in quaternions.

5 Appendix

5.1 Equations of motions: The Hamiltonian formulation

Detailed calculations for the variational derivative $\delta\mathcal{H}/\delta\boldsymbol{u}$ (33)

$$\frac{\delta \mathcal{H}}{\delta \boldsymbol{\varphi}} = \frac{\partial h}{\partial \boldsymbol{\varphi}} - \partial_S \frac{\partial h}{\partial \boldsymbol{\varphi}'}, \qquad \text{and} \qquad \frac{\delta \mathcal{H}}{\delta \mathbb{q}} = \frac{\partial h}{\partial \mathbb{q}} - \partial_S \frac{\partial h}{\partial \mathbb{q}'}. \tag{60}$$

5.1.1 Variational derivative with respect to $\boldsymbol{\delta\varphi}$

Straight forward computations give the second term in first equation of (60),

$$\frac{\partial h}{\partial \boldsymbol{\varphi}'} = \frac{\partial}{\partial \boldsymbol{\varphi}'}\left[\frac{1}{2}\langle \boldsymbol{\gamma}, \boldsymbol{D}_N\boldsymbol{\gamma}\rangle\right] = \boldsymbol{D}_N\boldsymbol{\gamma} = \boldsymbol{n}. \tag{61}$$

Since $\boldsymbol{\gamma} = \boldsymbol{\varphi}' - \mathcal{E}(\mathbb{q})\mathbf{e}_1$, we can compute the second term in the first equation (60)

$$\partial_S \frac{\partial h}{\partial \boldsymbol{\varphi}'} = \boldsymbol{D}_N'\boldsymbol{\gamma} + \boldsymbol{D}_N\boldsymbol{\gamma}' = \left[\widehat{\boldsymbol{\omega}}, \boldsymbol{D}_N\right]\boldsymbol{\gamma} + \boldsymbol{D}_N\boldsymbol{\gamma}' \tag{62}$$

where $[\,\cdot\,,\,\cdot\,]$ denotes the usual commutator for 3×3-matrices, $\boldsymbol{\gamma}' = \boldsymbol{\varphi}'' - \widehat{\boldsymbol{\omega}}\mathcal{E}(\mathbb{q})\mathbf{e}_1$ and

$$\boldsymbol{\omega}(\mathbb{q}, \mathbb{q}') = 2(q_0\boldsymbol{q}' - q_0'\boldsymbol{q} + \widehat{\boldsymbol{q}}\boldsymbol{q}') = 2\begin{bmatrix} q_0q_1' - q_0'q_1 - q_3q_2' + q_2q_3' \\ q_0q_2' - q_0'q_2 - q_1q_3' + q_3q_1' \\ q_0q_3' - q_0'q_3 - q_2q_1' + q_1q_2' \end{bmatrix}.$$

Finally $\partial h/\partial\boldsymbol{\varphi} = 0$, and the first equation of (60) follows

$$\frac{\delta \mathcal{H}}{\delta \boldsymbol{\varphi}} = \left[\widehat{\boldsymbol{\omega}}, \boldsymbol{D}_N\right]\boldsymbol{\gamma} + \boldsymbol{D}_N\boldsymbol{\gamma}'. \tag{63}$$

5.1.2 Variational derivative with respect to $\delta\mathbb{q}$

Differentiating the terms of the Hamiltonian density function h (31) with respect to $\mathbb{q}$. We have

$$\begin{aligned}\frac{\partial}{\partial\mathbb{q}}\langle\mathbb{p}, R(\mathbb{q})\widetilde{\boldsymbol{I}}_\rho^{-1}R(\mathbb{q}^c)\mathbb{p}\rangle =& \frac{\partial}{\partial\mathbb{q}}\langle L(\mathbb{q}^c)\mathbb{p}, \widetilde{\boldsymbol{J}}_\rho^{-1}L(\mathbb{q}^c)\mathbb{p}\rangle\\ =&\,2\left(\frac{\partial(L(\mathbb{q}^c)\mathbb{p})}{\partial\mathbb{q}}\right)^T\widetilde{\boldsymbol{J}}_\rho^{-1}L(\mathbb{q}^c)\mathbb{p}\\ =&-2R(\mathbb{q})L(\mathbb{p})L(\mathbb{q}^c)\widetilde{\boldsymbol{I}}_\rho^{-1}R(\mathbb{q}^c)\mathbb{p},\end{aligned}\tag{64}$$

and similarly

$$\begin{aligned}\frac{\partial}{\partial\mathbb{q}}\langle\mathbb{q}', R(\mathbb{q})\widetilde{\boldsymbol{D}}_M R(\mathbb{q}^c)\mathbb{q}'\rangle =& -2R(\mathbb{q})L(\mathbb{q}')L(\mathbb{q}^c)\widetilde{\boldsymbol{D}}_M R(\mathbb{q}^c)\mathbb{q}'\\ =& -\frac{1}{2}R(\mathbb{q})L(\omega)\widetilde{\boldsymbol{D}}_M\omega.\end{aligned}\tag{65}$$

Further, differentiation of $\langle\boldsymbol{\gamma}, \widetilde{\boldsymbol{D}}_N\boldsymbol{\gamma}\rangle = \langle\boldsymbol{\Gamma}, \widetilde{\boldsymbol{C}}_N\boldsymbol{\Gamma}\rangle$, where $\boldsymbol{\Gamma} = \mathcal{E}(\mathbb{q})^T\boldsymbol{\varphi}' - \mathbf{e}_1$, with respect to $\mathbb{q}$ gives

$$\begin{aligned}\frac{\partial}{\partial\mathbb{q}}\langle\boldsymbol{\gamma}, \widetilde{\boldsymbol{D}}_N\boldsymbol{\gamma}\rangle =&\,2\begin{bmatrix}\mathbf{0} & \left(\frac{\partial\boldsymbol{\Gamma}}{\partial\mathbb{q}}\right)^T\end{bmatrix}\begin{bmatrix}0\\ \boldsymbol{C}_N\boldsymbol{\Gamma}\end{bmatrix}\\ =&\,4\begin{bmatrix}0 & -(\boldsymbol{q}\times\boldsymbol{\varphi}')^T\\ \mathbf{0} & \widehat{\boldsymbol{q}\times\boldsymbol{\varphi}'} - q_0\widehat{\boldsymbol{\varphi}'} - \widehat{\boldsymbol{\varphi}'}\widehat{\boldsymbol{q}}\end{bmatrix}\begin{bmatrix}0\\ \boldsymbol{C}_N\boldsymbol{\Gamma}\end{bmatrix}.\end{aligned}\tag{66}$$

The above expression (66) can be simplified and written in a more convenient form

$$\begin{aligned}&4\begin{bmatrix}0 & -(\boldsymbol{q}\times\boldsymbol{\varphi}')^T\\ \mathbf{0} & \widehat{\boldsymbol{q}\times\boldsymbol{\varphi}'} - q_0\widehat{\boldsymbol{\varphi}'} - \widehat{\boldsymbol{\varphi}'}\widehat{\boldsymbol{q}}\end{bmatrix}\begin{bmatrix}0\\ \boldsymbol{C}_N\boldsymbol{\Gamma}\end{bmatrix} =\\ &\qquad 2R(\mathbb{q})\left[R(\varphi') - L(\varphi')\right]\begin{bmatrix}0\\ \boldsymbol{D}_N\boldsymbol{\gamma}\end{bmatrix} + 4\langle(\mathbb{1} - \mathcal{E}(\mathbb{q}))\boldsymbol{\varphi}', \boldsymbol{D}_N\boldsymbol{\gamma}\rangle\mathbb{q},\end{aligned}\tag{67}$$

where $\varphi' = (0, \boldsymbol{\varphi}') \in \mathbb{H}_{\mathcal{P}}$.

To find an explicit expression for the second term $\partial_S(\partial h/\partial\mathbb{q}')$ (60) we first have

$$\partial_S\left(L(\mathbb{q})R(\mathbb{q}^c)\right) = L(\mathbb{q}')R(\mathbb{q}^c) + L(\mathbb{q})R((\mathbb{q}^c)'),$$

and, since $L(\mathbb{q})L(\mathbb{q}^c) = R(\mathbb{q})R(\mathbb{q}^c) = \mathbb{1}_{4\times4}$, one has $L(\mathbb{q}')L(\mathbb{q}^c) = -L(\mathbb{q})L((\mathbb{q}^c)')$, $R(\mathbb{q}')R(\mathbb{q}^c) = -R(\mathbb{q})R((\mathbb{q}^c)')$. So, from $\omega = 2R(\mathbb{q}^c)\mathbb{q}'$, it follows

$$\partial_S\left(L(\mathbb{q})R(\mathbb{q}^c)\right) = \frac{1}{2}\left[L(\omega) - R(\omega)\right]L(\mathbb{q})R(\mathbb{q}^c).$$

The latter identity yields

$$\partial_S\widetilde{\boldsymbol{D}}_M = \frac{1}{2}\left[\left(L(\omega) - R(\omega)\right), \widetilde{\boldsymbol{D}}_M\right],\tag{68}$$

where $[\,\cdot\,,\,\cdot\,]$ is the usual commutator for 4×4-matrices. Thus, we have

$$\frac{\partial h}{\partial\mathbb{q}'} = \frac{\partial}{\partial\mathbb{q}'}\left[2\langle\mathbb{q}', R(\mathbb{q})\widetilde{\boldsymbol{D}}_M R(\mathbb{q}^c)\mathbb{q}'\rangle\right] = 4R(\mathbb{q})\widetilde{\boldsymbol{D}}_M R(\mathbb{q}^c)\mathbb{q}' = 2R(\mathbb{q})\widetilde{\boldsymbol{D}}_M\omega,\tag{69}$$

and using the identity (68)

$$\begin{aligned}\partial_S \frac{\partial h}{\partial \mathbb{q}'} &= 2R(\mathbb{q}')\widetilde{\boldsymbol{D}}_M\omega + R(\mathbb{q})\left[(L(\omega) - R(\omega)), \widetilde{\boldsymbol{D}}_M\right]\omega + 2R(\mathbb{q})\widetilde{\boldsymbol{D}}_M\omega' \\ &= R(\mathbb{q})\left(L(\omega)\widetilde{\boldsymbol{D}}_M\omega + 2\widetilde{\boldsymbol{D}}_M\omega'\right). \end{aligned} \tag{70}$$

Finally, with aid from the above results we obtain the equation for $\delta\mathcal{H}/\delta\mathbb{q} = \partial h/\partial\mathbb{q} - \partial_S(\partial h/\partial\mathbb{q}')$ (60), where h is the density function (31),

$$\begin{aligned}\frac{\delta\mathcal{H}}{\delta\mathbb{q}} = &-\frac{1}{4}R(\mathbb{q})L(\mathbb{p})L(\mathbb{q}^c)\widetilde{\boldsymbol{I}}_\rho^{-1}R(\mathbb{q}^c)\mathbb{p} - 2R(\mathbb{q})\left(L(\omega)\widetilde{\boldsymbol{D}}_M\omega + \widetilde{\boldsymbol{D}}_M\omega'\right) + 2\lambda\mathbb{q} \\ &+ R(\mathbb{q})\left[R(\varphi') - L(\varphi')\right]\begin{bmatrix} 0 \\ \boldsymbol{D}_N\boldsymbol{\gamma}\end{bmatrix} + 2\langle(\mathbb{1} - \mathcal{E}(\mathbb{q}))\boldsymbol{\varphi}', \boldsymbol{D}_N\boldsymbol{\gamma}\rangle\mathbb{q}. \end{aligned} \tag{71}$$

5.2 Solution of the Lagrange multiplier λ

Differentiating the constraint $g(\mathbb{q}) := \|\mathbb{q}\|^2 - 1 = 0$ with respect to t, $\partial_t g(\mathbb{q}) = 2\langle\dot{\mathbb{q}}, \mathbb{q}\rangle = 0$, inserting the expression for $\dot{\mathbb{q}} = (1/4)R(\mathbb{q})\widetilde{\boldsymbol{I}}_\rho^{-1}R(\mathbb{q}^c)\mathbb{p}$ (32),

$$\partial_t g(\mathbb{q}) = \frac{1}{2}\langle R(\mathbb{q})\widetilde{\boldsymbol{I}}_\rho^{-1}R(\mathbb{q}^c)\mathbb{p}, \mathbb{q}\rangle = \frac{1}{2}\langle\widetilde{\boldsymbol{I}}_\rho^{-1}R(\mathbb{q}^c)\mathbb{p}, \mathbb{e}\rangle = \frac{1}{2}\langle\mathbb{q}, \mathbb{p}\rangle,$$

gives the second constraint

$$\frac{1}{2}\langle\mathbb{q}, \mathbb{p}\rangle = 0. \tag{72}$$

Differentiating (72) once again,

$$\frac{1}{2}\left[\langle\dot{\mathbb{q}}, \mathbb{p}\rangle + \langle\mathbb{q}, \dot{\mathbb{p}}\rangle\right] = 0,$$

and plugging in the equations for $\dot{\mathbb{p}}$ and $\dot{\mathbb{q}}$,

$$\frac{1}{2}\left[\langle\dot{\mathbb{q}}, \mathbb{p}\rangle + \langle\mathbb{q}, \dot{\mathbb{p}}\rangle\right] = \frac{1}{2}\left[\langle\mathrm{w}, \widetilde{\boldsymbol{I}}_\rho\mathrm{w}\rangle - \langle\mathrm{w}, \widetilde{\boldsymbol{I}}_\rho\mathrm{w}\rangle\right] - \langle\omega, \widetilde{\boldsymbol{D}}_M\omega\rangle - \langle(\mathbb{1} - \mathcal{E}(\mathbb{q}))\boldsymbol{\varphi}', \boldsymbol{D}_N\boldsymbol{\gamma}\rangle - \lambda$$

gives the solution for the Lagrange multiplier λ

$$\lambda = -\langle\omega, \widetilde{\boldsymbol{D}}_M\omega\rangle - \langle(\mathbb{1} - \mathcal{E}(\mathbb{q}))\boldsymbol{\varphi}', \boldsymbol{D}_N\boldsymbol{\gamma}\rangle. \tag{73}$$

5.3 Equations for the rotation $\mathbb{q}$: The multi-symplectic formulation

The calculations are similar as for the Hamiltonian formulation. In particular, note that

$$\langle\boldsymbol{v}_\varphi, \boldsymbol{D}_N^{-1}\boldsymbol{v}_\varphi - 2\mathcal{E}(\mathbb{q})\mathbf{e}_1\rangle = \langle\mathcal{E}(\mathbb{q})^T\boldsymbol{v}_\varphi, \boldsymbol{C}_N^{-1}\mathcal{E}(\mathbb{q})^T\boldsymbol{v}_\varphi - 2\mathbf{e}_1\rangle$$

and

$$\begin{aligned}\frac{\partial}{\partial\mathbb{q}}\langle\boldsymbol{v}_\varphi, \boldsymbol{D}_N^{-1}\boldsymbol{v}_\varphi - 2\mathcal{E}(\mathbb{q})\mathbf{e}_1\rangle &= 2\begin{bmatrix}\mathbf{0} & \left(\dfrac{\partial(\mathcal{E}(\mathbb{q})^T\boldsymbol{v}_\varphi)}{\partial\mathbb{q}}\right)^T\end{bmatrix}\begin{bmatrix}0 \\ \boldsymbol{C}_N^{-1}\mathcal{E}(\mathbb{q})^T\boldsymbol{v}_\varphi - \mathbf{e}_1\end{bmatrix} \\ &= 4\begin{bmatrix}0 & -(\boldsymbol{q}\times\boldsymbol{v}_\varphi)^T \\ \mathbf{0} & \widehat{\boldsymbol{q}\times\boldsymbol{v}_\varphi} - q_0\widehat{\boldsymbol{v}_\varphi} - \widehat{\boldsymbol{v}_\varphi}\widehat{\boldsymbol{q}}\end{bmatrix}\begin{bmatrix}0 \\ \boldsymbol{C}_N^{-1}\mathcal{E}(\mathbb{q})^T\boldsymbol{v}_\varphi - \mathbf{e}_1\end{bmatrix}.\end{aligned}$$

Comparing with (67) in the Hamiltonian case, we see that the above expression can be rewritten,

$$\frac{\partial}{\partial \mathbb{q}}\langle \boldsymbol{v}_\varphi, \boldsymbol{D}_N^{-1}\boldsymbol{v}_\varphi - 2\mathcal{E}(\mathbb{q})\mathbf{e}_1\rangle = 2R(\mathbb{q})\Big[R(\boldsymbol{v}_\varphi) - L(\boldsymbol{v}_\varphi)\Big]\begin{bmatrix} 0 \\ \boldsymbol{D}_N^{-1}\boldsymbol{v}_\varphi - \mathcal{E}(\mathbb{q})\mathbf{e}_1 \end{bmatrix} + 4\langle(\mathbb{1} - \mathcal{E}(\mathbb{q}))\boldsymbol{v}_\varphi, \boldsymbol{D}_N^{-1}\boldsymbol{v}_\varphi - \mathcal{E}(\mathbb{q})\mathbf{e}_1\rangle \mathbb{q}.$$

5.3.1 Solution for the Lagrange multiplier in the multi-symplectic case

Differentiation of the constraint, $g(\mathbb{q}) := \|\mathbb{q}\|^2 - 1 = 0$, in time and space, respectively, gives two hidden constraints

$$\langle \mathbb{p}, \mathbb{q}\rangle = 0, \qquad \langle \mathbb{v}, \mathbb{q}\rangle = 0. \tag{74}$$

Differentiating twice yields

$$\begin{aligned}(\partial_t^2 + \partial_S^2)g(\mathbb{q}) &= \langle \mathbb{q}, \mathbb{v}' + \dot{\mathbb{p}}\rangle + \langle \mathbb{q}', \mathbb{v}\rangle + \langle \dot{\mathbb{q}}, \mathbb{p}\rangle \\ &= \langle(\mathcal{E}(\mathbb{q}) - \mathbb{1})\boldsymbol{v}_\varphi, \boldsymbol{D}_N^{-1}\boldsymbol{v}_\varphi - \mathcal{E}(\mathbb{q})\mathbf{e}_1\rangle + \lambda = 0.\end{aligned} \tag{75}$$

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