7 Hamiltonian Formulation

7.1 Kinematics of Rods

An elastic rod consists of a curve in space, denoted $\boldsymbol{r}(s) : [0,1] \to \mathbb{R}^3$, and an orthonormal frame of *directors*, denoted $\{\boldsymbol{d}_i(s)\}_{i=1}^3$. The kinematic equations

$$\begin{aligned} \boldsymbol{r}' &= \boldsymbol{v}, && (7.125)\\ \boldsymbol{d}_i' &= \boldsymbol{u} \times \boldsymbol{d}_i, \quad i = 1,2,3, && (7.126) \end{aligned}$$

where $'$ indicates differentiation with respect to the independent variable s, define the vectors $\boldsymbol{v}$ and $\boldsymbol{u}$. The components $u_k(s) \equiv \boldsymbol{u}(s) \cdot \boldsymbol{d}_k(s)$ are the strains with respect to bending $(k = 1,2)$ and twisting $(k = 3)$. The components $v_k(s) \equiv \boldsymbol{v}(s) \cdot \boldsymbol{d}_k(s)$ are the strains associated with shear and stretching. We assume that the rod is unshearable ($v_1 = 0 = v_2$) and inextensible ($v_3 = 1$). Combining these assumptions with the kinematic equation (7.125) yields the equation $\boldsymbol{r}' = \boldsymbol{d}_3$, which relates the centerline $\boldsymbol{r}$ to the frame of directors $\{\boldsymbol{d}_i\}$.

7.2 Force and Moment Balance Laws

The stresses acting across each material normal cross-section are equivalent to a force and moment applied at the centroid of the cross-section at $\boldsymbol{r}(s)$; let $\boldsymbol{n}(s)$ and $\boldsymbol{m}(s)$ denote, respectively, this resultant force and moment (of the material on the side s^+ acting on the material on the side s^-). We will here assume that the only external loads are couples and forces applied at the ends of the rod. Then the force and moment balance laws are

$$\boldsymbol{n}'(s) = \boldsymbol{0}, \tag{7.127}$$

and

$$\boldsymbol{m}'(s) + \boldsymbol{r}'(s) \times \boldsymbol{n}(s) = \boldsymbol{0}. \tag{7.128}$$

7.3 Constitutive Relations

In order to complete the formulation of an elastic rod, constitutive relations between the strains u_i and the moments, $m_i \equiv \boldsymbol{m} \cdot \boldsymbol{d}_i$, must be presented. In particular, we consider hyperelastic rods; we assume that there exists a convex, strain energy density function $W(\mathsf{w})$, $\mathsf{w} = (w_1, w_2, w_3)$, such that $W_{\mathsf{w}}(0) = 0$ and

$$m_i = W_{w_i}(u_i - \hat{u}_i), \quad \text{for } i = 1,2,3, \tag{7.129}$$

where $\hat{\mathbf{u}}(s) = (\hat{u}_1(s), \hat{u}_2(s), \hat{u}_3(s))$ is the triplet of strains describing the curvature and twist of the unstressed rod.

W is taken to be quadratic in $u_i - \hat{u}_i$. The assumption of diagonal quadratic energy, namely,

$$W(\mathbf{u} - \hat{\mathbf{u}}) = \frac{1}{2}\sum_{i=1}^{3} K_i(u_i - \hat{u}_i)^2, \tag{7.130}$$

defines the linear constitutive relations,

$$m_i = K_i(u_i - \hat{u}_i) \tag{7.131}$$

via equation (7.129). The quadratic energy assumption (7.130) is equivalent to a linear elasticity assumption.

The positive functions $K_i(s)$ in equation (7.130) represent the bending and twisting stiffnesses of the rod.

7.4 Representation of Directors by Euler Parameters

Thus far we have not specified any particular parameterization of the directors $\{d_i(s)\}$. For three-dimensional equilibria, a parameterization of the directors $\{d_i(s)\}$ is equivalent to selecting a representation for the group of proper orthogonal transformations $SO(3)$. In mechanics there are several common choices for such a representation. Euler parameters can be used, which provides a global (i.e. singularity free), four parameter, two–to–one description of $SO(3)$.

The components of the orthonormal triad $\{d_i\}$ (with respect to the fixed space basis) in terms of a set of Euler parameters $q = (q_1, q_2, q_3, q_4)$ are given by:

$$d_1 = \begin{pmatrix} q_1^2 - q_2^2 - q_3^2 + q_4^2 \\ 2(q_1q_2 + q_3q_4) \\ 2(q_1q_3 - q_2q_4) \end{pmatrix}, \quad d_2 = \begin{pmatrix} 2(q_1q_2 - q_3q_4) \\ -q_1^2 + q_2^2 - q_3^2 + q_4^2 \\ 2(q_2q_3 + q_1q_4) \end{pmatrix}, \tag{7.132}$$

$$d_3 = \begin{pmatrix} 2(q_1q_3 + q_2q_4) \\ 2(q_2q_3 - q_1q_4) \\ -q_1^2 - q_2^2 + q_3^2 + q_4^2 \end{pmatrix}. \tag{7.133}$$

The parametrization of the directors by quaternions involves the normalization factor $|\boldsymbol{q}|^2 = 1$.

The strains $\boldsymbol{u_i}$ appearing in equations (7.130) are given in terms of the Euler parameters by

$$\boldsymbol{u_i = 2q' \cdot B_i q}\,, \qquad \boldsymbol{i = 1,\ 2,\ 3.} \tag{7.134}$$

Here the $\boldsymbol{B_i}$ are $\mathbf{4} \times \mathbf{4}$ skew–symmetric matrices:

$$\boldsymbol{B_1} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{B_2} = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

$$\boldsymbol{B_3} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

For any set of Euler parameters the vectors $\{\boldsymbol{B_i q}\}$, together with $\boldsymbol{q}$, form an orthonormal basis for $\mathbb{R}^4$. Geometrically, the vector $\boldsymbol{B_i q}$ acts as the infinitesimal generator of rotation about the $\boldsymbol{i}$th director $\mathbf{d}_i$.

7.5 Variational Formulations

The energy functional of the elastic rod is

$$\int_0^1 \boldsymbol{W(u_1, u_2, u_3, \hat{u}_1, \hat{u}_2, \hat{u}_3, s)\ ds}, \tag{7.135}$$

where $\boldsymbol{W}$ is chosen to be quadratic in the strains as seen in Equation (7.130). As the strains, denoted $\boldsymbol{u_i}$, can be written as functions of the Euler parameters $\boldsymbol{q}$ and their derivatives $\boldsymbol{q'}$; thus $\boldsymbol{W}$ is a function of the Euler parameters $\boldsymbol{q}$ and their derivative $\boldsymbol{q'}$

Using equation (7.134) to eliminate the strains, the strain energy density function can be written in terms of the Euler parameters and their derivatives

$$\boldsymbol{W}(\mathbf{u} - \hat{\mathbf{u}},\ \boldsymbol{s}) = \boldsymbol{W}\left(\boldsymbol{2q' \cdot B_i q - \hat{u}_i,\ s}\right). \tag{7.136}$$

The equilibrium configurations can then be characterized as constrained critical points of the energy functional

$$\int_0^1 W\left(2q' \cdot B_i q - \hat{u}_i,\ s\right)\ ds\ , \tag{7.137}$$

subject to the constraints,

$$r'(s) = d_3(q(s)) \qquad \text{and} \qquad q(s) \cdot q'(s) = 0\,, \tag{7.138}$$

and appropriate boundary conditions, including the requirement that the Euler parameters have unit norm at one end point. Here $\mathbf{d_3}(q(s))$ denotes the vector of quadratic functions of q_i. By introducing Lagrange multiplier functions $\lambda(s) \in \mathbb{R}^3$ and $\mu(s) \in \mathbb{R}$ associated with the pointwise constraints (7.138), the equilibrium configurations can be characterized as unconstrained critical points of the Lagrangian

$$\mathcal{L}(q, q', r', \lambda, \mu, s) = W\left(2q' \cdot B_i q - \hat{u}_i,\ s\right) + \lambda \cdot (r' - d_3) + \mu\, q \cdot q'\,. \tag{7.139}$$

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A necessary condition for the energy to have a minimum at (r_0, q_0) is that minimum satisfy the Euler-Lagrange equations.

The Euler-Lagrange derivative with respect to r yields the force balance law $\lambda' = 0$ where λ represents the force n in Equation (7.127). Since λ is constant, the term $\lambda \cdot \int_0^1 (r' - d_3)\ ds$ can be integrated to yield

$$\begin{aligned}\lambda \cdot \int_0^1 (r' - d_3)\ ds &= \lambda \cdot \left(r(1) - r(0) - \int_0^1 d_3\ ds\right), &(7.140)\\ &= -\lambda \cdot \int_0^1 d_3\ ds. &(7.141)\end{aligned}$$

The four Euler-Lagrange equations with respect to q are

$$2m_i' B_i q = m_i \left[-\left(4B_i q'\right) - 2u_i \frac{q}{|q|^2}\right] - \left[\frac{\partial(d_3 \cdot \lambda)}{\partial q}\right]^T - \mu' q. \tag{7.142}$$

In order to recover the moment balance laws, we project Equation (7.142) onto $B_j q$. Taking the inner product of (7.142) with $B_j q$, yields

$$2m_j' = -2m_i u_k \epsilon_{ijk} - \left[\frac{\partial(d_3 \cdot \lambda)}{\partial q}\right]^T \cdot B_j q, \tag{7.143}$$

where ϵ_{ikj} is the standard permutation symbol. The last term can be rewritten as

$$\begin{aligned}\left[\frac{\partial(d_3\cdot\lambda)}{\partial q}\right]^T\cdot B_j q &= \left[\frac{\partial d_3}{\partial q}\right]^T\lambda\cdot B_j q = \frac{\partial d_3}{\partial q}B_j q\cdot\lambda \\ &= 2\epsilon_{j3k}d_k\cdot\lambda = 2\epsilon_{j3k}\lambda_k\end{aligned}$$

so that the equilibrium equations become

$$m_j' = -m_i u_k \epsilon_{ijk} - \epsilon_{j3k}\lambda_k. \tag{7.144}$$

Explicitly, Equation (7.144) reduces to the moment balance laws

$$m_1' = -u_2 m_3 + u_3 m_2 + d_2\cdot\lambda, \tag{7.145}$$

$$m_2' = u_1 m_3 - u_3 m_1 - d_1\cdot\lambda, \tag{7.146}$$

$$m_3' = -u_1 m_2 + u_2 m_1, \tag{7.147}$$

which are equivalent to (7.128), the balance laws in the fixed frame.

The value of the derivative of the Lagrange multiplier μ is determined by taking the inner product of (7.142) with q

$$\begin{aligned}0 &= m_i\left[-(4q\cdot B_i q') - 2u_i\right] - \frac{\partial(d_3\cdot\lambda)}{\partial q}\cdot q - \mu' \\ &= -\frac{\partial(d_3\cdot\lambda)}{\partial q}\cdot q - \mu' = -2\lambda d_3 - \mu'.\end{aligned}$$

7.6 Hamiltonian Formulations

The Hamiltonian system involves the (standard) Legendre transform $W^*(\mathsf{v},\, s)$ of the constitutive function $W(\mathsf{w},\, s)$. We assume that

$$\frac{\partial W}{\partial \mathsf{w}}(0) = 0, \tag{7.148}$$

and that W is a strictly convex function of w. Then the variables v conjugate to w are defined by

$$\mathsf{v} = \frac{\partial W}{\partial \mathsf{w}}(\mathsf{w})\,. \tag{7.149}$$

By the strict convexity assumption we can invert to solve for w, to get

$$\mathsf{w} = \phi(\mathsf{v})\,. \tag{7.150}$$

The Legendre transform is then defined to be

$$W^*(\mathbf{v}) = \mathbf{v} \cdot \phi(\mathbf{v}) - W(\phi(\mathbf{v})). \tag{7.151}$$

In the special case of a pure quadratic W,

$$W(\mathbf{w}) = \frac{1}{2} \sum_i K_i\, w_i^2\,, \tag{7.152}$$

the conjugate variables are $v_i = K_i\, w_i$, and the Legendre transform is

$$W^*(\mathbf{v}) = \frac{1}{2} \sum_i \frac{v_i^2}{K_i}. \tag{7.153}$$

We claim that the Hamiltonian leading to the equations governing the equilibria of an elastica can now be written in the form

$$H(r, q, n, \nu, s) = W^*(\mathbf{m}, s) + \mathbf{m} \cdot \hat{\mathbf{u}}(s) + n \cdot d_3. \tag{7.154}$$

The phase space variables in this Hamiltonian formulation are the axis r, the force n which is conjugate to r, the Euler parameters q, and their conjugate variable, namely ν. The right hand side of (7.154) can be written in terms of the phase variables by substituting the expression (7.133) for $d_3(q)$ and by using the relations

$$m_i = \frac{1}{2}\nu \cdot B_i q \,(= W_{u_i}(\mathbf{u} - \hat{\mathbf{u}})) \quad i = 1, 2, 3, \tag{7.155}$$

which follow from the hyper-elastic constitutive relation and the components of the definition of ν in the directions $B_i q$. The second equation in (7.155) can itself be further inverted using the implicitly defined inverse function ϕ introduced in equations (7.150) and (7.151), leading to the expression

$$\mathbf{u} = \hat{\mathbf{u}} + \phi\left(\frac{\nu \cdot B_1 \mathbf{q}}{2}, \frac{\nu \cdot B_2 q}{2}, \frac{\nu \cdot B_3 q}{2}\right) \tag{7.156}$$

for the strains. In the particular case of linear elasticity, (7.156) simplifies to

$$u_i = \hat{u}_i + \frac{\nu \cdot B_i q}{2\, K_i}, \qquad i = 1,\ 2,\ 3, \tag{7.157}$$

and the Hamiltonian takes the explicit form

$$H(r, q, \mathrm{n}, \nu) = \sum_{i=1}^{3} \left(\frac{m_i^2}{2\, K_i} + \hat{u}_i m_i\right) + n \cdot d_3. \tag{7.158}$$

The Hamiltonian system of equations governing equilibria is of the form

$$\begin{cases} \mathbf{r}' = \dfrac{\partial H}{\partial \mathbf{n}} = \mathbf{d}_3, \\ \mathbf{q}' = \dfrac{\partial H}{\partial \nu} = \dfrac{1}{2} \displaystyle\sum_{i=1}^{3} u_i \, \mathbf{B}_i \mathbf{q}, \\ \mathbf{n}' = -\dfrac{\partial H}{\partial \mathbf{r}} = 0, \\ \nu' = -\dfrac{\partial H}{\partial \mathbf{q}} = \dfrac{1}{2} \displaystyle\sum_{i=1}^{3} u_i \, \mathbf{B}_i \nu - \dfrac{\partial \mathbf{d}_3}{\partial \mathbf{q}}^T \mathbf{n}, \end{cases} \tag{7.159}$$

where again $d_3(q)$ is defined by the formula (7.133), so that

$$\frac{\partial d_3}{\partial \mathbf{q}} = 2 \begin{pmatrix} q_3 & q_4 & q_1 & q_2 \\ -q_4 & q_3 & q_2 & -q_1 \\ -q_1 & -q_2 & q_3 & q_4 \end{pmatrix},$$

and the u_i are written in terms of the phase variables q and ν using relation (7.156), or in the case of linear elasticity the explicit form (7.157).

7.7 Discussion of the Hamiltonian Formulations

The equilibrium equations (7.159) are a set of fourteen ordinary differential equations with boundary conditions. By construction, this system yields to the balance laws and to the different constraints given respectively in (7.127),(7.128) and (7.138).

The first equation of (7.159) is the constraint $r'(s) = d_3(q(s))$. The projection of the second equation onto q yields to

$$q(s) \cdot q'(s) = \frac{1}{2} \sum_{i=1}^{3} u_i \mathbf{q} \mathbf{B}_i \mathbf{q} = 0,$$

and the projection of this same equation onto $\mathbf{B}_k \mathbf{q}$ yields to the kinematics relation

$$u_k = 2q' \cdot B_k q.$$

The moment balance law is derived from the expression of q' and the projection of ν' onto $\mathbf{B}_k \mathbf{q}$.

7.8 Analysis of Integrals and Symmetries

We next detail the integrals or conserved quantities of the Hamiltonian system (7.159), i.e., functions of the phase variables that are independent of arc–length s.

Six integrals are obtained immediately from equations (7.127),(7.128). The three components of force $\mathbf{n}$ are constant due to the translational symmetry of the Hamiltonian system in space. Similarly the three components of $\mathbf{m} + \mathbf{r} \times \mathbf{n}$ are invariant as a consequence of rotational symmetry about the three inertial axes. To see that these expressions provide integrals of (7.159), we merely need to write them as functions of the phase variables. Components of $\mathbf{n}$ and $\mathbf{r}$ with respect to the fixed basis are trivially phase variables, and it can be verified that the components $\overline{m}_i$ of $\mathbf{m}$ with respect to the fixed space basis can be written as

$$\overline{m}_i = \frac{1}{2}\nu \cdot \mathbf{F}_i \mathbf{q}, \qquad i = 1,\ 2,\ 3, \tag{7.160}$$

where

$$\mathbf{F}_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{F}_2 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix},$$

$$\mathbf{F}_3 = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}.$$

In addition to the integrals listed above which have physical interpretations, there are two integrals which arise from the representation of $SO(3)$ by the four Euler parameters, rather than by a three parameter description. By construction, the second equation of (7.159) implies

$$\mathbf{q} \cdot \mathbf{q}' = \frac{1}{2} \sum_{i=1}^{3} u_i\, \mathbf{q} \cdot \mathbf{B}_i \mathbf{q} = 0,$$

so that $|\mathbf{q}|^2$ is a seventh integral.

Next consider the quantity $\boldsymbol{\nu}\cdot\mathbf{q}+2\mathbf{r}\cdot\mathbf{n}$. By virtue of (7.159), we find

$$\begin{aligned}\frac{d}{ds}(\boldsymbol{\nu}\cdot\mathbf{q}+2\mathbf{r}\cdot\mathbf{n}) = & -\mathbf{n}\cdot\frac{\partial\mathbf{d}_3}{\partial\mathbf{q}}\mathbf{q}+\frac{1}{2}\sum_{i=1}^{3}u_i\mathbf{q}\cdot\mathbf{B}_i\boldsymbol{\nu} \\ & +\frac{1}{2}\sum_{i=1}^{3}u_i\boldsymbol{\nu}\cdot\mathbf{B}_i\mathbf{q}+2\mathbf{d}_3\cdot\mathbf{n}.\end{aligned} \tag{7.161}$$

Euler's Theorem for homogeneous functions implies that $2\mathbf{d}_3 = \dfrac{\partial\mathbf{d}_3}{\partial\mathbf{q}}\mathbf{q}$. Moreover the matrices $\mathbf{B}_i$ are skew symmetric, so it follows that (7.161) vanishes and

$$\boldsymbol{\nu}\cdot\mathbf{q}+2\mathbf{r}\cdot\mathbf{n} \tag{7.162}$$

is an eighth integral of the system. The integral (7.162) is associated with invariance of the Hamiltonian under the (variational) symmetry in which $\mathbf{q}$ is replaced by $(1+\epsilon)\mathbf{q}$, $\boldsymbol{\nu}$ is replaced by $(1+\epsilon)^{-1}\boldsymbol{\nu}$, $\mathbf{r}$ is replaced by $(1+\epsilon)^2\mathbf{r}$ and $\mathbf{n}$ is replaced by $(1+\epsilon)^{-2}\mathbf{n}$. Specification of the value of the integral (7.162) merely eliminates the gauge freedom in $\boldsymbol{\nu}$.

The above integrals arise for all constitutive laws. There are two additional, constitutive dependent, integrals that arise in each of the cases of an *isotropic* rod, and a *uniform* rod. The tangential component of bending moment is

$$m_3(s)\equiv\mathbf{m}\cdot\mathbf{d}_3=\frac{\boldsymbol{\nu}\cdot\mathbf{B}_3\mathbf{q}}{2}$$

A straightforward computation, using (7.157), (7.159) and properties of the $\mathbf{B}_i$ matrices, reveals that

$$\begin{aligned}2\frac{d}{ds}m_3(s) &= (\boldsymbol{\nu}\cdot\mathbf{B}_3\mathbf{q}'+\boldsymbol{\nu}'\cdot\mathbf{B}_3\mathbf{q}) = -u_1\boldsymbol{\nu}\cdot\mathbf{B}_2\mathbf{q}+u_2\boldsymbol{\nu}\cdot\mathbf{B}_1\mathbf{q} \\ &= (\boldsymbol{\nu}\cdot\mathbf{B}_1\mathbf{q})(\boldsymbol{\nu}\cdot\mathbf{B}_2\mathbf{q})\left(\frac{1}{K_2}-\frac{1}{K_1}\right)-\hat{u}_1\boldsymbol{\nu}\cdot\mathbf{B}_2\mathbf{q}+\hat{u}_2\boldsymbol{\nu}\cdot\mathbf{B}_1\mathbf{q}\,.\end{aligned}$$

Accordingly, if $K_1(s)\equiv K_2(s)$ and $\hat{u}_1\equiv\hat{u}_2\equiv 0$, then $m_3(s)=\boldsymbol{\nu}\cdot\mathbf{B}_3\mathbf{q}/2$ provides a ninth integral. This case will be described as a *transversely isotropic* or just *isotropic* rod.

The second constitutive dependent symmetry is uniformity. If the constitutive function W has no explicit s dependence, which in the linearly elastic case means the stiffnesses K_i and the unstressed strains $\hat{u}_i$ are all constant, then the Hamiltonian H (7.154) has no explicit s dependence, and therefore represents a tenth integral of the system. The associated symmetry is translation in the arc-length s, or relabeling of the material point corresponding to $s = 0$.

In summary the Hamiltonian system always has at least eight integrals, namely $\mathbf{n}$, $|\mathbf{q}|^2$, $\mathbf{m}+\mathbf{r}\times\mathbf{n}$, and $\boldsymbol{\nu}\cdot\mathbf{q}+2\mathbf{r}\cdot\mathbf{n}$. If the rod is isotropic m_3 provides an additional integral, and if the rod is uniform then the Hamiltonian $\boldsymbol{H}$ (7.154) provides a tenth integral.