

STRATIFIED REDUCTION OF MANY-BODY DYNAMICAL SYSTEMS

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Abstract. The center-of-mass system for many bodies in \mathbb{R}^3 admits a natural action of the rotation group $SO(3)$. According to the orbit types for the $SO(3)$ action, the center-of-mass system M is stratified into strata. A quantum Hamiltonian system and a classical Lagrangian system are defined on $L^2(M)$ and on $T(M)$, respectively. These systems are also stratified according to the stratification of M , and then reduced by the rotational symmetry, respectively.

1. Introduction

Consider a smooth manifold M on which acts a compact Lie group G . According to the orbit types of the group action, the manifold is stratified into different strata. Mechanics will be set up on each stratum and then reduced by symmetry. We apply this idea, taking M and G as the center-of-mass system for N bodies and the rotation group $SO(3)$, respectively. The center-of-mass system M will be stratified into $M = \dot{M} \cup M_1 \cup M_0$, where \dot{M} and M_1 are the set of non-singular configurations or non-linear molecules, and the set of collinear configurations or linear molecules, respectively, and M_0 is a singleton which denotes the simultaneous collision configuration. We have no need to discuss mechanics on M_0 . A quantum Hamiltonian system is defined on $L^2(M)$, and stratified into those on $L^2(\dot{M})$ and $L^2(M_1)$, which are reduced to quantum systems on vector bundles over $\dot{M}/SO(3)$ and $M_1/SO(3)$, respectively. A classical Lagrangian system is defined on $T(M)$, and stratified into those on $T(\dot{M})$ and $T(M_1)$, which are reduced to classical systems on vector bundles over $\dot{M}/SO(3)$ and $M_1/SO(3)$, respectively.

2. The Center-of-mass System

Let $\mathbf{x}_j, j = 1, \dots, N$, be position vectors of particles in \mathbb{R}^3 and m_j the masses of particles. The center-of-mass system is defined to be

$$M = \{x = (\mathbf{x}_1, \dots, \mathbf{x}_N); \mathbf{x}_j \in \mathbb{R}^3, \sum_{j=1}^N m_j \mathbf{x}_j = \mathbf{0}\}.$$

Let

$$F_x = \text{span}\{\mathbf{x}_1, \dots, \mathbf{x}_N\}.$$

Then M is broken up into four parts,

$$M = \bigcup_{k=0}^3 M_k, \quad M_k := \{x \in M; \dim F_x = k\}.$$

The rotation group $SO(3)$ acts on M in the natural manner,

$$x \mapsto gx = (g\mathbf{x}_1, \dots, g\mathbf{x}_N).$$

According to the dimensionality of F_x , the orbits \mathcal{O}_x are classified into three types

$$\mathcal{O}_x \cong \begin{cases} SO(3) & \text{for } x \in M_2 \cup M_3 \\ S^2 & \text{for } x \in M_1 \\ \{0\} & \text{for } x \in M_0. \end{cases}$$

We call the configuration $x \in M_2 \cup M_3$ non-singular and $x \in M_0 \cup M_1$ singular, respectively. With respect to the orbit types, M is stratified into

$$M = M_0 \cup M_1 \cup \dot{M}, \quad \dot{M} := M_2 \cup M_3.$$

The $SO(3)$ action defines an equivalence relation on M . The orbit space $M/SO(3)$ is called a shape space, the space of shapes of configurations. The projection map $M \rightarrow M/SO(3)$ is also stratified into

$$\begin{cases} \dot{M} \longrightarrow \dot{M}/SO(3) \\ M_1 \longrightarrow M_1/SO(3) \\ M_0 \longrightarrow M_0/SO(3) = \{0\} \end{cases}$$

among which the principal stratum \dot{M} is made into an $SO(3)$ bundle.

The Jacobi vectors are defined by the formulae

$$\mathbf{r}_j = \left(\frac{1}{\mu_j} + \frac{1}{m_{j+1}} \right)^{-1/2} \left(\mathbf{x}_{j+1} - \frac{1}{\mu_j} \sum_{i=1}^j m_i \mathbf{x}_i \right), \quad \mu_j := \sum_{i=1}^j m_i.$$

Then, the center-of-mass system M can be viewed as the set of the Jacobi vectors

$$M \cong \{(\mathbf{r}_1, \dots, \mathbf{r}_{N-1}); \mathbf{r}_j \in \mathbb{R}^3, j = 1, \dots, N-1\}.$$

3. Fourier Analysis of Wave Functions

Before discussing the group action on wave functions, we make a brief review of Fourier analysis [2]. We introduce the Euler angles through $g = e^{\phi R(e_3)} e^{\theta R(e_2)} \times e^{\psi R(e_3)}$, where $R(e_k)$ are defined through $R(e_k)\mathbf{a} = e_k \times \mathbf{a}$. Let $(D^\ell, \mathcal{H}^\ell)$ be unitary irreducible representations for $SO(3)$, $\ell = 0, 1, 2, \dots$, where \mathcal{H}^ℓ is the representation space with an orthonormal basis e_m^ℓ , $|m| \leq \ell$. We denote by $D_{mn}^\ell(g)$ the matrix elements of D^ℓ with respect to e_m^ℓ , and by $d\mu(g) = \sin \theta d\theta d\phi d\psi$ the invariant volume element on $SO(3)$.

For $f \in L^2(M)$, the function $f(gx)$ can be expanded into the Fourier series,

$$f(gx) = \sum_{\ell=0}^{\infty} \sum_{|m|, |n| \leq \ell} D_{mn}^\ell(g) (P_{nm}^\ell f)(x)$$

where the Fourier coefficients are defined by

$$(P_{nm}^\ell f)(x) := \frac{2\ell + 1}{8\pi^2} \int_{SO(3)} \bar{D}_{mn}^\ell(h) f(hx) d\mu(h).$$

If we define the map $E_m^\ell : L^2(M) \rightarrow \mathcal{H}^\ell \otimes L^2(M)$ by

$$E_m^\ell f = \frac{1}{\sqrt{2\ell + 1}} \sum_{|n| \leq \ell} e_n^\ell \otimes P_{nm}^\ell f$$

one can check that E_m^ℓ satisfies the equivariance condition

$$(E_m^\ell f)(gx) = D^\ell(g)(E_m^\ell f)(x).$$

4. Non-singular Configurations, Quantum Theory

Let $\pi : \dot{M} \rightarrow \dot{M}/SO(3)$ be the $SO(3)$ fiber bundle. The tangent space to \dot{M} can be splitted into a direct sum

$$T_x(\dot{M}) = V_x \oplus H_x$$

where V_x and V_x^\perp are defined by

$$V_x := T_x(\mathcal{O}_x), \quad H_x := V_x^\perp$$

respectively, with respect to the metric

$$ds^2 = \sum_{j=1}^{N-1} d\mathbf{r}_j \cdot d\mathbf{r}_j.$$

This decomposition of $T(\dot{M})$ defines a connection on \dot{M} . In a dual manner, the connection is defined as follows: Through the inertia tensor $A_x : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ defined

by

$$A_x(\mathbf{v}) = \sum_{j=1}^{N-1} \mathbf{r}_j \times (\mathbf{v} \times \mathbf{r}_j), \quad x = (\mathbf{r}_1, \dots, \mathbf{r}_{N-1}), \quad x \in \dot{M}$$

the connection form is defined to be

$$\omega_x = R \left(A_x^{-1} \sum_{j=1}^{N-1} \mathbf{r}_j \times d\mathbf{r}_j \right).$$

We now consider the kinetic energy integral, from which the Laplacian is derived through integration by part

$$T = \frac{1}{2} \int_M \sum_{j=1}^{N-1} \frac{\partial \bar{f}}{\partial \mathbf{r}_j} \cdot \frac{\partial f}{\partial \mathbf{r}_j} dV = -\frac{1}{2} \int_M \bar{f} \Delta f dV,$$

where dV denotes the standard volume element on M . We wish to put the Laplacian in terms of local coordinates. Let $\sigma : U \rightarrow \dot{M}$ be a local section, where U is an open subset of \dot{M} . Then we can put $x \in \pi^{-1}(U)$ in the form $x = g\sigma(q)$, $q \in U$. We denote the local coordinates of q by (q^α) . By making intensive use of the connection form, we can break up the Laplacian Δ into

$$\Delta = \Delta_{\text{rot}} + \Delta_{\text{vib}}, \quad \begin{cases} \Delta_{\text{rot}} = \sum_{a,b=1}^3 A^{ab} K_a K_b \\ \Delta_{\text{vib}} = \sum_{\alpha,\beta=1}^{3N-6} \frac{1}{\rho(q)} \left(\frac{\partial}{\partial q^\alpha} \right)^* \left(a^{\alpha\beta} \rho(q) \left(\frac{\partial}{\partial q^\beta} \right)^* \right) \end{cases}$$

where K_a and $\left(\frac{\partial}{\partial q^\alpha} \right)^*$ denote the infinitesimal rotation and the infinitesimal vibration, which are defined, respectively, as follows:

$$K_a = \frac{d}{dt} g e^{tR(e_a)} \sigma(q) \Big|_{t=0},$$

$$\omega_{g\sigma(q)} \left(\left(\frac{\partial}{\partial q^\alpha} \right)^* \right) = 0, \quad \pi_* \left(\left(\frac{\partial}{\partial q^\alpha} \right)^* \right) = \frac{\partial}{\partial q^\alpha}.$$

The other quantities used to express Δ_{rot} and Δ_{vib} are defined as follows:

$$a_{\alpha\beta} = ds^2 \left(\left(\frac{\partial}{\partial q^\alpha} \right)^*, \left(\frac{\partial}{\partial q^\beta} \right)^* \right), \quad A_{ab} = ds^2(K_a, K_b), \\ (a^{\alpha\beta}) = (a_{\alpha\beta})^{-1}, \quad (A^{ab}) = (A_{ab})^{-1}, \quad \rho(q) = \sqrt{\det(A_{ab}) \det(a_{\alpha\beta})}.$$

Operating the equivariant \mathcal{H}^ℓ -valued function

$$(E_m^\ell f)(g\sigma(q)) = D^\ell(g)(E_m^\ell f)(\sigma(q))$$

with $(\partial/\partial q^\alpha)^*$ results in

$$\left(\frac{\partial}{\partial q^\alpha}\right)^* D^\ell(g)(E_m^\ell f)(\sigma(q)) = D^\ell(g)\nabla_\alpha(E_m^\ell f)(\sigma(q))$$

where ∇_α is the operator given by

$$\nabla_\alpha = I_{2\ell+1} \otimes \frac{\partial}{\partial q^\alpha} + i \sum_a \Lambda_\alpha^a(q) [\tilde{J}_a^{(\ell)}]$$

$[\tilde{J}_a^{(\ell)}]$ denoting the representation matrices for $so(3)$, and $\Lambda_\alpha^a(q)$ being given through

$$\omega_{\sigma(q)} = \sum_{a=1}^3 \sum_{\alpha=1}^{3N-6} \Lambda_\alpha^a(q) dq^\alpha R(e_a).$$

In the same manner, we can obtain the reduced Laplacian [1],

$$\Delta^{\text{red}} = \frac{1}{\rho(q)} \sum_{\alpha,\beta} \nabla_\alpha (a^{\alpha\beta} \rho(q) \nabla_\beta) - \sum_{a,b} A^{ab} [\tilde{J}_a^{(\ell)}] [\tilde{J}_b^{(\ell)}]$$

which acts on cross sections of $\dot{M} \times_{SO(3)} \mathcal{H}^\ell$, a complex vector bundle over $\dot{M}/SO(3)$.

5. Collinear Configurations, Quantum Theory

In this section, we take up M_1 , the space of collinear configurations. The tangent space to M_1 can be decomposed also into a direct sum,

$$T_x(M_1) = V_x^{(1)} \oplus H_x^{(1)}$$

where $V_x^{(1)}$ and $H_x^{(1)}$ are defined by

$$V_x^{(1)} := T_x(\mathcal{O}_x), \quad H_x^{(1)} := (V_x^{(1)})^\perp$$

respectively, with respect to the induced metric $ds^2|_{M_1}$ on M_1 . The inertia tensor A_x is singular at $x \in M_1$. In fact, for

$$x = (\zeta_1 \mathbf{u}_3, \dots, \zeta_{N-1} \mathbf{u}_3) \in M_1$$

one has $\ker A_x = \text{span}\{\mathbf{u}_3\}$, where $\mathbf{u}_a := ge_a$, $a = 1, 2, 3$, is the moving frame. However, one can define

$$(A_x^{(1)})^{-1} : \text{span}\{\mathbf{u}_1, \mathbf{u}_2\} \rightarrow \text{span}\{\mathbf{u}_1, \mathbf{u}_2\}$$

and further a (singular) connection form

$$\omega_x^{(1)} = R \left((A_x^{(1)})^{-1} \sum_{j=1}^{N-1} \mathbf{r}_j \times d\mathbf{r}_j \right).$$

Now we are going to express the kinetic operator for collinear configurations in terms of local coordinates. For $x = g\sigma_0(\zeta)$ with $\sigma_0(\zeta) = (\zeta_1 e_3, \dots, \zeta_{N-1} e_3)$, the induced metric on M_1 is given by

$$ds^{2(1)} = \sum_{j=1}^{N-1} \zeta_j^2 (d\theta^2 + \sin^2 \theta d\phi^2) + \sum_{j=1}^{N-1} d\zeta_j^2.$$

The kinetic energy integral is then put in the form

$$T^{(1)} = \frac{1}{2} \int_{M_1} \left(\frac{1}{\rho_1(\zeta)} \left(\left| \frac{\partial f}{\partial \theta} \right|^2 + \frac{1}{\sin^2 \theta} \left| \frac{\partial f}{\partial \phi} \right|^2 \right) + \sum_{j=1}^{N-1} \left| \frac{\partial f}{\partial \zeta_j} \right|^2 \right) dV^{(1)}$$

where $dV^{(1)}$ is the volume element formed from $ds^{2(1)}$, and $ds\rho_1(\zeta) = \sum_{j=1}^{N-1} \zeta_j^2$. Integration by part provides the Laplacian

$$\Delta^{(1)} = \frac{1}{\rho_1(\zeta)} \Lambda + \frac{1}{\rho_1(\zeta)} \sum_{j=1}^{N-1} \frac{\partial}{\partial \zeta_j} \left(\rho_1(\zeta) \frac{\partial}{\partial \zeta_j} \right)$$

where

$$\Lambda = \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2}.$$

Since $e^{tR(e_3)}\sigma_0(\zeta) = \sigma_0(\zeta)$, the equivariance condition

$$(E_m^\ell f)(\sigma_0(\zeta)) = D^\ell(e^{tR(e_3)})(E_m^\ell f)(\sigma_0(\zeta))$$

implies that

$$(E_m^\ell f)(g\sigma_0(q)) = \sqrt{4\pi} \sum_{|n| \leq \ell} e_n^\ell \otimes \bar{Y}_{\ell n}(ge_3) (P_{0m}^\ell f)(\sigma_0(q))$$

where $Y_{\ell n}$ denote the spherical harmonics on S^2 , being related with the D -functions by

$$Y_{\ell n}(ge_3) = \sqrt{\frac{2\ell+1}{4\pi}} \bar{D}_{n0}^\ell(g).$$

Operating $(E_m^\ell f)(g\sigma_0(q))$ with $\Delta^{(1)}$, one obtains the reduced Laplacian [1],

$$\Delta^{(1)\text{red}} = \frac{1}{\rho_1(\zeta)} \sum_{j=1}^{N-1} \frac{\partial}{\partial \zeta_j} \left(\rho_1(\zeta) \frac{\partial}{\partial \zeta_j} \right) - \frac{\ell(\ell+1)}{\rho_1(\zeta)}$$

which acts on cross sections of $M_1 \times_{SO(3)} \mathcal{H}^\ell$, a direct sum of complex line bundles over $M_1/SO(3)$.

6. Non-singular Configurations, Classical Theory

In this section, we treat non-singular configurations in Lagrangian mechanics. Let $\sigma : U \rightarrow M$ be a local section. Then one has $x = g\sigma(q)$, $q \in U$. We now take (q, g) as local coordinates in $\pi^{-1}(U)$, and (q, \dot{q}, g, \dot{g}) as local coordinates in $T(\pi^{-1}(U))$, respectively. In view of $\omega_{g\sigma(q)} = g(g^{-1}dg + \omega_{\sigma(q)})g^{-1}$, we introduce an $so(3)$ -valued variable

$$\Pi = \xi + \sum_{\alpha} \Lambda_{\alpha}(q) \dot{q}^{\alpha}$$

where

$$\xi = g^{-1}\dot{g}, \quad \Lambda_{\alpha}(q) = \sum_a \Lambda_{\alpha}^a(q) R(e_a).$$

Then, we may take (q, \dot{q}, g, Π) as local coordinates in $T(\pi^{-1}(U))$.

By the variational principle, we can show that the Euler-Lagrange equations for $L(q, \dot{q}, g, \Pi)$ are given by

$$\begin{aligned} \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}^{\alpha}} \right) - \frac{\partial L}{\partial q^{\alpha}} &= \left\langle \frac{\partial L}{\partial \Pi}, \sum_{\beta} K_{\alpha\beta} \dot{q}^{\beta} \right\rangle - \left\langle \frac{\partial L}{\partial \Pi}, [\Pi, \Lambda_{\alpha}] \right\rangle \\ &\quad - \frac{1}{2} \left\langle g^{-1} \frac{\partial L}{\partial g} - \left(\frac{\partial L}{\partial g} \right)^T g, \Lambda_{\alpha} \right\rangle \\ \frac{d}{dt} \frac{\partial L}{\partial \Pi} &= \left[\frac{\partial L}{\partial \Pi}, \Pi \right] - \sum_{\beta} \left[\frac{\partial L}{\partial \Pi}, \Lambda_{\beta} \right] \dot{q}^{\beta} + \frac{1}{2} \left(g^{-1} \frac{\partial L}{\partial g} - \left(\frac{\partial L}{\partial g} \right)^T g \right) \end{aligned}$$

where

$$\begin{aligned} \langle A, B \rangle &:= \text{trace}(A^T B) \\ K_{\alpha\beta} &:= \frac{\partial \Lambda_{\beta}}{\partial q^{\alpha}} - \frac{\partial \Lambda_{\alpha}}{\partial q^{\beta}} - [\Lambda_{\alpha}, \Lambda_{\beta}]. \end{aligned}$$

The $K_{\alpha\beta} \in so(3)$ are the components of the curvature form.

If L is rotationally invariant, one has a reduced Lagrangian $L^*(q, \dot{q}, \Pi)$ defined on

$$T(\dot{M})/SO(3) \cong T(\dot{M}/SO(3)) \oplus \tilde{\mathcal{G}}$$

where $\tilde{\mathcal{G}} = \dot{M} \times_{SO(3)} \mathcal{G}$ and $\mathcal{G} = so(3)$. For force-free non-singular configurations, L is rotationally invariant, and expressed as

$$L^* = \frac{1}{2} \sum_{\alpha, \beta} a_{\alpha\beta} \dot{q}^{\alpha} \dot{q}^{\beta} + \frac{1}{4} \langle \Pi, RAR^{-1}\Pi \rangle$$

where $R : \mathbb{R}^3 \rightarrow so(3)$ and $A = A_{\sigma(q)}$. The Euler-Lagrange equations then reduce to and are put in the vector form,

$$\sum_{\beta} a_{\alpha\beta} \left(\frac{d}{dt} \dot{q}^{\beta} + \sum_{\gamma,\delta} \left\{ \begin{matrix} \beta \\ \gamma\delta \end{matrix} \right\} \dot{q}^{\gamma} \dot{q}^{\delta} \right) = \sum_{\beta} A\pi \cdot \kappa_{\alpha\beta} \dot{q}^{\beta} + \pi \cdot \left(\frac{\partial}{\partial q^{\alpha}} - \Lambda_{\alpha} \right) (A\pi)$$

$$\frac{d}{dt} (A\pi) = A\pi \times \pi - \sum_{\beta} A\pi \times \lambda_{\beta} \dot{q}^{\beta}$$

where

$$\Pi = R(\pi), \quad \Lambda_{\beta} = R(\lambda_{\beta}), \quad K_{\alpha\beta} = R(\kappa_{\alpha\beta}).$$

Note here that $\partial/\partial q^{\alpha} - \Lambda_{\alpha}$ denotes the covariant derivation acting on local sections in $\tilde{\mathcal{G}}$. One can further show that the total angular momentum is conserved, i.e.

$$R^{-1} \left(g \frac{\partial L}{\partial \Pi} g^{-1} \right) = g A \pi.$$

7. Collinear Configurations, Classical Theory

In view of $x = (\zeta_1 g e_3, \dots, \zeta_{N-1} g e_3) \in M_1$ with $g = e^{\phi \hat{e}_3} e^{\theta \hat{e}_2}$, we take local coordinates $(\zeta, \dot{\zeta}, \mathbf{u}, \dot{\mathbf{u}})$ for $T(M_1)$ with $\mathbf{u} := g e_3$. On the variational principle, we can show that the Euler-Lagrange equations are given by

$$\frac{\partial L}{\partial \zeta_{\alpha}} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\zeta}_{\alpha}} \right) = 0$$

$$P \left(\frac{\partial L}{\partial \mathbf{u}} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\mathbf{u}}} \right) \right) = 0$$

where P is the projection operator given by

$$P = I - \mathbf{u} \mathbf{u}^T.$$

Since $\dot{\mathbf{u}} = g \xi e_3$ with $\xi = g^{-1} \dot{g}$, we can take $(\zeta, \dot{\zeta}, \mathbf{u}, \xi e_3)$ as local coordinates. If L is rotationally invariant, one has a reduced Lagrangian $L^*(\zeta, \dot{\zeta}, \xi e_3)$ defined on

$$T(M_1)/SO(3) \cong T(M_1/SO(3)) \oplus V$$

where V is a vector bundle over $M_1/SO(3)$. For force-free collinear configurations, L is rotationally invariant, and expressed as

$$L^* = \frac{1}{2} \sum_{\alpha} (\dot{\zeta}_{\alpha})^2 + \frac{1}{2} \rho_1(\zeta) |\boldsymbol{\Omega} \times \mathbf{e}_3|^2$$

where

$$\rho_1(\zeta) = \sum_{\alpha} (\zeta_{\alpha})^2, \quad \xi = R(\boldsymbol{\Omega}).$$

The Euler-Lagrange equations then reduce to

$$\frac{d}{dt}\dot{\zeta}_\alpha = \zeta_\alpha |Q(\boldsymbol{\Omega})|^2$$

$$\frac{d}{dt}(\rho(\zeta)\boldsymbol{\Omega} \times \mathbf{e}_3) = -Q(\boldsymbol{\Omega} \times (\rho(\zeta)\boldsymbol{\Omega} \times \mathbf{e}_3))$$

where Q is the projection operator given by

$$Q := I - \mathbf{e}_3 \mathbf{e}_3^T.$$

We can show again that the total angular momentum is also conserved, i.e.

$$g\rho(\zeta)Q(\boldsymbol{\Omega}).$$

References

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