

Holonomy reduced dynamics of triatomic molecular systems

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September 6, 2010

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Abstract

Whereas it is easy to reduce the translational symmetry of a molecular system by using, e.g., Jacobi coordinates the situation is much more involved for the rotational symmetry. In this paper we address the latter problem using *holonomy reduction*. We suggest that the configuration space may be considered as the reduced holonomy bundle with a connection induced by the mechanical connection. Using the fact that for the special case of the three-body problem, the holonomy group is $SO(2)$ (as opposed to $SO(3)$ like in systems with more than three bodies) we obtain a holonomy reduced configuration space of topology $\mathbf{R}_+^3 \times S^1$. The dynamics then takes place on the cotangent bundle over the holonomy reduced configuration space. On this phase space there is an S^1 symmetry action coming from the conserved reduced angular momentum which can be reduced using the standard symplectic reduction method. Using a theorem by Arnold it follows that the resulting symmetry reduced phase space is again a natural mechanical phase space, i.e. a cotangent bundle. This is different from what is obtained from the usual approach where symplectic reduction is used from the outset. This difference is discussed in some detail, and a connection between the reduced dynamics of a triatomic molecule and the motion of a charged particle in a magnetic field is established.

PACS numbers: 45.50.Jf, 02.40.-k, 45.20.Jj

AMS classification numbers: 70F07, 70G65, 53C80

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1 Introduction

In molecular dynamics which is the subject of this paper and generally in dynamical systems theory the reduction of the number of degrees of freedom is of central importance for both computational and conceptual reasons. A molecular system is a many body system consisting of the nuclei and electrons of the constituting atoms. The electronic degrees of freedom are typically dealt with in a Born-Oppenheimer approximation. Since the nuclear masses are a few thousands times bigger than the mass of an electron one assumes that the nuclei adiabatically interact via the forces obtained from a potential energy surface that is obtained from the electronic ground state energy as a function of the nuclear configurations. The computation of such potential energy surfaces is based on density functional theory and other methods and is an art in physical chemistry. For several molecular systems such potential energy surfaces are tabulated in the chemistry literature. Given such a potential energy surface a molecular system reduces to an N -body system which only involves the degrees of freedom of the N nuclei in the system. This N -body system can then be treated classically or quantum mechanically. In particular for light atoms (respectively nuclei) like hydrogen quantum effects might play an important role which make a quantum mechanical treatment necessary. We note that state of the art quantum computations for, e.g., reactive scattering are even today only feasible for three or maximally four atoms. For this reason and also conceptual reasons one desires to get rid of as many degrees as possible. A reduction of the number of ‘effective’ degrees of freedom of a molecular N -body system can be achieved by exploiting the symmetries of the system. These symmetries consist of overall translations and rotations. The reduction of translational degrees of freedom is simple and can be achieved by using Jacobi coordinates or changing to a centre of mass coordinate system. For rotations, the situation is much more involved as a clear distinction between rotational degrees of freedom and (internal) vibrational degrees of freedom only exists in an approximate sense in the vicinity of an equilibrium position. Here the distinction between vibrations and rotations can be achieved from the so called *Eckart frame* [1] that is widely used in applications [2]. This approximation is however only of local validity since large amplitude vibrations may produce rotations. A major step towards a geometric understanding of why a separation of rotations and vibrations cannot be achieved globally goes back to the work of Guichardet [3] who used the differential geometry framework of principal bundles to give a mathematically rigorous definition of vibrational motions. He showed that the translational reduced configuration space is a principal bundle with structure group given by the special orthogonal group, and introduced a connection which naturally relates to molecular motions. The inseparability of rotations and vibrations then follows from the nonvanishing curvature of this so called *mechanical connection*. Iwai and Tachibana [4, 5] used Guichardet’s approach to study in great detail both the classical and the quantum mechanical dynamics of N -body molecular systems. Using the setting of principle bundles Iwai[6] in particular showed that the Eckart frame can also be defined for general configurations (i.e., no necessarily equilibrium configurations) of a molecule. However, this frame is then not unique and therefore not suitable for studying large amplitude vibrational motions of a molecule. Iwai moreover applied the Marsden-Weinstein-Meyer symplectic reduction procedure [7, 8] to reduce the constant angular momentum motion of an N -body system. He showed that for nonvanishing angular momentum the reduced phase space is then no longer a natural mechanical

system in the sense that it is no longer given as the cotangent bundle over a (reduced) configuration space. A gauge theoretical interpretation of the reduction of symmetries and the related choice of a reference frame in N -body systems was introduced in [9, 10]. In their constructive and instructive paper Littlejohn and Reinsch[10] used Lagrangian reduction instead of symplectic reduction mentioned above. For more related work we mention the refer to [11, 12, 13, 14, 15, 16].

In this paper we use modern tools from the geometric description of molecular motion described above to introduce a new way to reduce the symmetry specifically of triatomic molecular system. We obtain a reduced configuration space and deduce the reduced dynamics for a triatomic molecule in a way which can be summarized as follows. Consider three atoms (or nuclei) in \mathbf{R}^3 . Using Jacobi coordinates the translational symmetry in the absence of external forces can be used to reduce the nine-dimensional configuration space $\mathbf{R}^3 \times \mathbf{R}^3 \times \mathbf{R}^3$ of the triatomic system to the six-dimensional space $\mathbf{R}^3 \times \mathbf{R}^3$. Excluding collinear (and hence also collisional) configurations from $\mathbf{R}^3 \times \mathbf{R}^3$ gives the translation reduced configuration space P on which the special orthogonal group $SO(3)$ acts freely. The space P is a principal bundle with base space given by the positive half space \mathbf{R}_+^3 [11]. Kinetic energy gives a metric on P , and a connection can be obtained by defining horizontal spaces as orthogonal complements of the tangent spaces of orbits of the $SO(3)$ action. As known [3, 10] the connection on P has a nontrivial holonomy group which is $SO(2)$. This enables us to use the holonomy reduction theorem [19] to reduce P to the holonomy bundle which we denote by Q . Since P is a trivial bundle [11], Q is also trivial and hence topologically $\mathbf{R}_+^3 \times SO(2)$, or equivalently $\mathbf{R}_+^3 \times S^1$. The reduced phase space is then given by the cotangent bundle T^*Q . We explicitly derive the Hamiltonian on T^*Q and deduce the reduced dynamics on T^*Q . In the final step we then use the conservation of the reduced angular momentum related to an S^1 action on T^*Q to apply the symplectic reduction procedure. Using a theorem in [17] we find that the reduced phase space is then a natural mechanical system, namely the cotangent bundle over Q/S^1 .

We note that there is no natural way to generalize these results to systems of four or more atoms. The reason is that triatomic systems are in many respects special. For example, the holonomy group of a system of four or more atoms is $SO(3)$, and the translation reduced space is not a trivial bundle [10].

2 Reduced configuration space

2.1 Principle bundle picture

Consider a molecular system of three atoms. Let $\mathbf{x}_i \in \mathbf{R}$, $i = 1, 2, 3$, be the position vectors of these atoms. Suppose that there are no external forces. Then the mass-weighted Jacobi vectors

$$\begin{aligned} \mathbf{r} &= \sqrt{\frac{m_1 m_2}{m_1 + m_2}} (\mathbf{x}_1 - \mathbf{x}_3), \\ \mathbf{s} &= \sqrt{\frac{m_2 (m_1 + m_2)}{m_1 + m_2 + m_3}} \left(\mathbf{x}_2 - \frac{m_1 \mathbf{x}_1 + m_3 \mathbf{x}_3}{m_1 + m_3} \right), \end{aligned}$$

can be chosen to reduce the symmetry of overall translations. (For different choices of Jacobi vectors see B.) Excluding collinear (and hence also collisional) configurations we obtain the six-dimensional translation reduced configuration space

$$P = \{x = (\mathbf{r}, \mathbf{s}) : \lambda \mathbf{r} + \mu \mathbf{s} \neq 0 \text{ for all } (\lambda, \mu) \in \mathbf{R}^2 \setminus \{0\}\} \subset \mathbf{R}^3 \times \mathbf{R}^3.$$

Proper rotations $g \in SO(3)$ act on P in the natural way

$$g(\mathbf{r}, \mathbf{s}) = (g\mathbf{r}, g\mathbf{s}).$$

On P this action is free and it thus follows from standard results that

$$M := P/SO(3)$$

has a manifold structure. The space M is usually referred to as *shape space* or *internal space*. Furthermore, the canonical projection $\pi : P \rightarrow M$ defines a principal bundle with structure group $SO(3)$ [3]. This means that P consists of smoothly glued copies of $SO(3)$, i.e., locally, P is diffeomorphic to $M \times SO(3)$. Topologically, this local decomposition also holds globally which following Iwai [11] can be seen as follows. Using Jacobi coordinates

$$r = \sqrt{\langle \mathbf{r}, \mathbf{r} \rangle}, \quad s = \sqrt{\langle \mathbf{s}, \mathbf{s} \rangle}, \quad \phi = \cos^{-1}(\langle \mathbf{r}, \mathbf{s} \rangle / rs),$$

where $\langle \cdot, \cdot \rangle$ is the usual dot product on \mathbf{R}^3 , and introducing coordinates

$$w_1 = r^2 - s^2, \quad w_2 = 2rs \cos \phi, \quad w_3 = 2rs \sin \phi > 0$$

one sees that $M \cong \mathbf{R}_+^3 = \{(w_1, w_2, w_3) : w_3 > 0\}$. As pointed out in [11], P is a trivial bundle as M is contractible to a single point. So, topologically, $P \cong \mathbf{R}_+^3 \times SO(3)$.

2.2 Nontrivial holonomy

Turning back to the action of $SO(3)$ on P one can see that the *fundamental vector field* \tilde{A} associated with an element A in the Lie algebra $so(3)$ is given by

$$\tilde{A}|_x = \left. \frac{d}{dt} \right|_{t=0} (e^{tA}x), \quad (1)$$

or equivalently,

$$\tilde{A}|_x = (A\mathbf{r}, A\mathbf{s}) = (\mathbf{w} \times \mathbf{r}, \mathbf{w} \times \mathbf{s}), \quad (2)$$

where $\mathbf{w} \in \mathbf{R}^3$ is the unique vector corresponding to A by the isomorphism

$$R^{-1} : so(3) \rightarrow \mathbf{R}^3, \quad \begin{pmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{pmatrix} \mapsto \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}. \quad (3)$$

Let N be an orbit of the $SO(3)$ action, say $N = SO(3)x$ for a point $x \in P$, then $T_x N = \{\tilde{A}|_x : A \in so(3)\}$. Consider the orthogonal complement H_x of $T_x N$ in $T_x P$ with respect to the Euclidean dot product on P given by

$$dx^2 = \langle \mathbf{r}, \mathbf{r} \rangle + \langle \mathbf{s}, \mathbf{s} \rangle. \quad (4)$$

Clearly the distribution $x \mapsto H_x$, which we call the *horizontal distribution*, defines a connection [11] $\omega : TP \rightarrow so(3)$ on P which is a special case of the *mechanical connection* defined in [18]. A vector field X^* with $X^*|_x \in H_x$ for all $x \in P$ is called *horizontal*. The *horizontal lift* of a vector field X on M is accordingly the unique horizontal vector field X^* on P such that $d\pi(X^*) = X$. We have $\omega(X^*) = 0$ for every horizontal vector field X^* and $\omega(\tilde{A}) = A$ for every fundamental vector field \tilde{A} . In order to compute the horizontal lifts of the coordinate vector fields $\partial_r, \partial_s, \partial_\phi$ on M we give an explicit expression for the metric dx^2 in (4). To this end we follow [10, 13] and introduce a frame $\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3$ in \mathbf{R}^3 according to

$$\begin{aligned}\mathbf{r} &= r \mathbf{u}_1, \\ \mathbf{s} &= s \cos \phi \mathbf{u}_1 + s \sin \phi \mathbf{u}_2, \\ \mathbf{u}_3 &= \mathbf{u}_1 \times \mathbf{u}_2.\end{aligned}$$

If Euler angles (α, β, γ) on $SO(3)$ are chosen via

$$g = e^{R(\alpha \mathbf{e}_1)} e^{R(\beta \mathbf{e}_2)} e^{R(\gamma \mathbf{e}_3)}, \quad 0 \leq \alpha, \gamma \leq 2\pi, \quad 0 \leq \beta \leq \pi,$$

where $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ is the standard basis of \mathbf{R}^3 , R is defined in (3) and $g\mathbf{e}_i = \mathbf{u}_i$, $i = 1, 2, 3$, then with

$$\begin{aligned}\Theta_1 &= \sin \gamma d\beta - \sin \beta \cos \gamma d\alpha, \\ \Theta_2 &= \cos \gamma d\beta + \sin \beta \sin \gamma d\alpha, \\ \Theta_3 &= \cos \beta d\alpha + d\gamma,\end{aligned}$$

one obtains [13]

$$\begin{aligned}d\mathbf{r} &= dr \mathbf{u}_1 + r\Theta_3 \mathbf{u}_2 - r\Theta_2 \mathbf{u}_3, \\ ds &= \eta_1 \mathbf{u}_1 + \eta_2 \mathbf{u}_2 + \eta_3 \mathbf{u}_3,\end{aligned}$$

where

$$\begin{aligned}\eta_1 &= ds \cos \phi - s \sin \phi d\phi - s \sin \phi \Theta_3, \\ \eta_2 &= ds \sin \phi + s \cos \phi d\phi + s \cos \phi \Theta_3, \\ \eta_3 &= s \sin \phi \Theta_1 - s \cos \phi \Theta_2.\end{aligned}$$

In local coordinates the metric $d\mathbf{x}^2$ then assumes the form

$$d\mathbf{x}^2 = dr^2 + r^2(\Theta_2^2 + \Theta_3^2) + \eta_1^2 + \eta_2^2 + \eta_3^2.$$

This expression can be used to locally compute the horizontal lift X^* of a vector field X on M : X^* is orthogonal to $\partial_\alpha, \partial_\beta, \partial_\gamma$, and $d\pi(X^*) = X$. It follows that

$$\partial_r^* = \partial_r, \quad \partial_s^* = \partial_s, \quad \partial_\phi^* = \partial_\phi - \frac{r^2}{r^2 + s^2} \partial_\gamma. \quad (5)$$

In gauge theory the factor $\frac{r^2}{r^2 + s^2}$ is referred to as a component of a *Yang-Mills potential* [5].

2.3 Holonomy reduction

By Equation (5) we have arrived at the well-known phenomena of inseparability of rotations and vibrations [3, 6]. Namely from (5) we see that the distribution spanned by $\partial_r^*, \partial_s^*, \partial_\phi^*$ is not integrable, and hence, if these vector fields are considered as infinitesimal vibrational motions one can say that vibrations generate rotations. This is why the internal space M is not a submanifold of P [5]. On the other hand $\partial_r^*, \partial_s^*, \partial_\phi^*, \partial_\gamma$ do span an involutive and hence integrable distribution. The maximal integral manifold Q_x of that distribution at a point $x \in P$ is a good candidate for being the reduced configuration space because vibrational motions through x live in that space. In fact we will obtain the reduced dynamics of a triatomic molecule on the cotangent bundle over Q_x by employing the holonomy reduction of principle bundles: A curve on P is called horizontal if its tangents are horizontal. Fix a point $x \in P$ and denote by $P(x)$ the set of all points in P which can be joined to x by horizontal curves. It is known that [3, 10] the holonomy group of ω is $SO(2)$ (see also A), and since M is connected and paracompact the holonomy reduction theorem [19] implies that $P(x)$ is a reduced bundle with structure group $SO(2)$, which is in fact Q_x . Furthermore, Q_x is a trivial bundle as it has the same base space as P . These observations suggest that the reduced configuration space of a triatomic molecular system is topologically $\mathbf{R}_+^3 \times SO(2)$. The induced metric on Q_x is thus

$$dq^2 = dr^2 + ds^2 + \frac{r^2 s^2}{r^2 + s^2} d\phi^2 + \frac{1}{r^2 + s^2} \zeta^2, \quad (6)$$

where

$$\zeta = s^2 d\phi + (r^2 + s^2) d\gamma. \quad (7)$$

3 Reduced dynamics

3.1 Angular momentum

In the following we want to put our derivation above into the context of some well known results. It is known [1] that in the case of small vibrations one can separate vibrations and rotations in the vicinity of an equilibrium point. In the present situation if one chooses $d\gamma = 0$ in (6) the well-known Eckart kinetic energy is obtained. This is the gauge dependent internal metric $h_{\mu\nu}$ in [10]. Thus one can conclude that in case of small vibrations the internal motions of molecule live in the integral manifolds of the distribution spanned by $\partial_r, \partial_s, \partial_\phi$, called the *Eckart space*. Next, consider the angular momentum

$$\mathbf{J} = R(\mathbf{r} \times d\mathbf{r} + \mathbf{s} \times d\mathbf{s})$$

on P which is computed locally to be

$$\mathbf{J} = R((r^2 \Theta_2 - s \cos \phi \eta_3) \mathbf{u}_2 + (r^2 \Theta_3 + s \cos \phi \eta_2 - s \sin \phi \eta_1 + s \sin \phi \eta_3) \mathbf{u}_3).$$

So, its restriction to Q_x is

$$\mathbf{J}|_{Q_x} = R(\zeta \mathbf{u}_3).$$

If the angular momentum of the system is identically zero, then $\zeta = 0$, and hence

$$dq^2 = dr^2 + ds^2 + \frac{r^2 s^2}{r^2 + s^2} d\phi^2.$$

3.2 Holonomy reduced Hamiltonian

In the case of vanishing angular momentum the Hamiltonian is obtained to be

$$H = \frac{1}{2}p_r^2 + \frac{1}{2}p_s^2 + \frac{1}{2}\left(\frac{1}{r^2} + \frac{1}{s^2}\right)p_\phi^2 + V(r, s, \phi), \quad (8)$$

where p_r, p_s, p_ϕ are the conjugate momenta and $V(r, s, \phi)$ is the potential energy which is assumed to be rotationally invariant. This Hamiltonian is widely used in applications. By (7) we observe that vibrational motions live in the integral manifold of the distribution spanned by $\partial_r^*, \partial_s^*, \partial_\gamma$. That space may be called *zero-angular momentum space*.

If the reduced angular momentum $\mathbf{J}|_{Q_x}$ is a non-zero constant, we have $\zeta = \text{const.} \neq 0$. Then, equivalently, ∂_ϕ^* is a non-zero constant and hence the vibrational motions remain in a three-dimensional affine space which is parallel to the zero-angular momentum space.

Taking into account the contribution of ζ in the induced metric dq on Q_x in (6) the Hamiltonian in (8) changes to the general *holonomy reduced Hamiltonian*

$$H = \frac{1}{2}p_r^2 + \frac{1}{2}p_s^2 + \frac{1}{2}\left(\frac{1}{r^2} + \frac{1}{s^2}\right)p_\phi^2 - \frac{1}{r^2}p_\phi p_\gamma + \frac{1}{2r^2}p_\gamma^2 + V(r, s, \phi).$$

The corresponding Hamiltonian vector field is given by

$$\begin{aligned} X = & p_r \partial_r + p_s \partial_s + \left(\left(\frac{1}{r^2} + \frac{1}{s^2} \right) p_\phi - \frac{1}{r^2} p_\gamma \right) \partial_\phi + \frac{1}{r^2} (p_\gamma - p_\phi) \partial_\gamma + \\ & \left(\frac{1}{r^3} (p_\gamma - p_\phi)^2 - \frac{\partial V}{\partial r} \right) \partial_{p_r} + \left(\frac{1}{s^3} p_\phi^2 - \frac{\partial V}{\partial s} \right) \partial_{p_s} - \frac{\partial V}{\partial \phi} \partial_{p_\phi}. \end{aligned}$$

Since γ is cyclic the conjugate momentum p_γ is conserved. To put it another way $\mathbf{J}|_{Q_x}$ is an S^1 -equivariant momentum and the standard symplectic reduction theorem can be applied. Using a theorem by Arnold (see [17], page 378) the resulting reduced phase space is again a natural mechanical system, i.e. a cotangent bundle.

4 Comments on related work

4.1 The relation between the motions of a triatomic molecule and a charged particle in a magnetic field

In [20, 21] the idea is introduced to describe the motion of a charged particle in a magnetic field by extending the configuration space \mathbf{R}^3 to $\mathbf{R}^3 \times S^1$ such that the angle corresponding to S^1 is cyclic and its conserved conjugate momentum gives the charge of the particle in the magnetic field. Since the holonomy reduced configuration space is $\mathbf{R}_+^3 \times S^1$ we can identify the motion of a triatomic molecule to that of a charged particle in a magnetic field

as follows. Let \mathbf{q} denote a point in M with coordinates (r, s, ϕ) . If \mathbf{A} denote the one-form $(r^2 + s^2)^{-1}\zeta = \frac{s^2}{(r^2 + s^2)}d\phi + d\gamma$ on \mathbf{R}_+^3 , then by the metric (6) the kinetic energy can be written as

$$L_K = \frac{1}{2} \|\dot{\mathbf{q}}\|^2 + \frac{1}{2}(\mathbf{A} \cdot \dot{\mathbf{q}} + \dot{\gamma})^2$$

which is reminiscent of the so called *Kaluza-Klein Lagrangian* [21]. The conjugate momenta are then

$$\mathbf{p} = \frac{\partial L_K}{\partial \dot{\mathbf{q}}} = \dot{\mathbf{q}} + (\mathbf{A} \cdot \dot{\mathbf{q}} + \dot{\gamma})\mathbf{A}$$

and

$$p_\gamma = \frac{\partial L_K}{\partial \dot{\gamma}} = \mathbf{A} \cdot \dot{\mathbf{q}} + \dot{\gamma}.$$

The one-form \mathbf{A} plays the role of a vector potential for the magnetic field. The conserved momentum p_γ is the charge $e = cp_\gamma$ (with c denoting the speed of light) [21].

4.2 Relation to symplectic and dimensional reduction

In [6] the symplectic reduction procedure [7, 8] is applied to the N -body problem. The cotangent bundle over the translation reduced configuration space P is a symplectic manifold with the canonical two-form, and the angular momentum $J : T^*P \rightarrow so(3)$ is an equivariant momentum map. For a $\mu \neq 0$, it is shown that $J^{-1}(\mu)$ is a principal bundle with structure group $SO(2)$ whereas the zero momentum space $J^{-1}(0)$ is a principal bundle with structure group $SO(3)$. Furthermore $J^{-1}(0)/SO(3)$ is shown to be diffeomorphic to $T^*(P/SO(3))$, but $J^{-1}(\mu)/SO(2)$ is no more a cotangent bundle because of dimensionality. As pointed out in [6] the procedure for the latter when applied to for three-bodies is in fact the *elimination of nodes*.

In contrast to the symplectic reduction procedure the first step in this paper was to pass from the translation reduced configuration space P of a triatomic molecule to a subbundle Q (the holonomy reduced bundle) which is a principle bundle with structure group $SO(2)$. Afterwards the angular momentum is then restricted to T^*Q , and finally the symplectic reduction procedure is applied. The reduced space is then always a cotangent bundle as follows from a theorem by Arnold (see [17], page 378).

We note that the method used in the present work is strongly related to dimensional reduction [22, 23], a method developed for symmetries of gauge fields. More precisely, in the case of spherical symmetry in 6 dimensions applied to an $SU(3)$ gauge theory, the 2 extra dimensions describing a sphere of radius R . One solution, with the largest set of Higgs fields, reduces to the 4-dimensional Weinberg-Salam model without fermions [22].

5 Conclusions

In this paper we used the geometric theory of molecular mechanics [3, 11, 10] to reduce the number of degrees of freedom in the molecular three-body problem. We followed the principal bundle setting of Guichardet[3] on the translation reduced configuration space, and using the holonomy reduction theorem [19] it was possible to reduce to a principle subbundle. This

may be interpreted as separating two rotational degrees of freedom from the maximal space that includes vibrational motions. It was then possible to induce the angular momentum and apply the very symplectic reduction procedure (to be precise, we used it in the form of the Noether's theorem here). This way, the remaining momentum space which is of 6 dimensions and also a phase space was obtained. The computations were local for the purpose illustration but the method is intrinsic. In some sense, the resulting space which is of 3 dimensions can be seen as a rotationless space. For the case of zero angular momentum this is a known earlier result. In the present paper it was generalized to the case of non-zero angular momentum. In particular we used our approach to rephrase the well known fact [20] that a triatomic molecular system behaves as a single particle in a magnetic field.

A A lemma by Guichardet

For completeness, we give a brief proof of the fact in that a vibrational motion of a triatomic molecule, which is defined as a curve with horizontal tangents, remains in a fixed plane as originally formulated by Guichardet [3]: Let $x(t) = (\mathbf{r}(t), \mathbf{s}(t))$ be a horizontal curve on P . We show that $F_{x(t)} := \text{span} \{\mathbf{r}(t), \mathbf{s}(t)\}$ is fixed. Indeed, since $x(t)$ is horizontal it is orthogonal to all fundamental vector fields which are given in (2), and hence $\mathbf{r}(t) \times \dot{\mathbf{r}}(t) + \mathbf{s}(t) \times \dot{\mathbf{s}}(t) = 0$. Let $\mathbf{y}(t)$ be a curve in \mathbf{R}^3 with $\langle \mathbf{y}(t), \mathbf{y}(t) \rangle = 1$ which is orthogonal to $F_{x(t)}$. So, $\dot{\mathbf{y}}(t)$ is orthogonal to $F_{x(t)}$. Hence $\langle \mathbf{y}(t), \mathbf{r}(t) \rangle = \langle \mathbf{y}(t), \mathbf{s}(t) \rangle = 0$ so $\langle \dot{\mathbf{y}}(t), \mathbf{r}(t) \rangle = \langle \dot{\mathbf{y}}(t), \mathbf{s}(t) \rangle = 0$ which implies $\dot{\mathbf{y}}$ is zero.

As a conclusion of the above fact it is observed [10] that during vibrational motions or shape deformations the Jacobi vectors remain in a fixed plane, and hence the Jacobi vectors before and after the vibrational motion can be transformed to one another by a plane rotation, i.e. the holonomy group is $SO(2)$.

B The kinematic group

Different clusterings of position vectors give rise to different choices of mass-weighted Jacobi vectors. These different choices are related to each other by transformations which are called *democracy transformations* [10]. The set of all democracy transformations forms a subgroup of the symmetry group $SO(3)$ called *democracy* or *kinematic group*. For the three-body problem the kinematic group is $SO(2)$. This is another special feature of the three-body problem.

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