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The geometry and mechanics of multi-particle systems

by

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ABSTRACT. – This article deals with the geometry and mechanics for multi-particle systems. The center-of-mass system is viewed as a principal fibre bundle with structure group $SO(3)$, on which a natural connection is defined, and thereby rotational and vibrational vectors are defined strictly. A natural Riemannian structure and the connection on the center-of-mass system are put together to provide a geometric setting for the study of the geometry and mechanics for the multi-particle system. The equations of motion are discussed in keeping with the bundle structure of the center-of-mass system. Moreover, the reduction of the equations of motion is made along with a constant total angular momentum. In addition, variational equations are derived for the equations of motion with vanishing total angular momentum. In particular, at an equilibrium state, the variational equations reduces to the traditional equations of small vibrations. © Elsevier, Paris

RÉSUMÉ. – Ce travail traite de la géométrie et de la mécanique des systèmes de plusieurs corps. Le système du centre de masse est considéré comme un fibré principal de groupe structural $SO(3)$. Il est muni d'une connexion naturelle, qui permet de distinguer les vecteurs correspondant à des rotations de ceux correspondant à des vibrations. En combinant, sur le système du centre de masse, géométrie riemannienne et théorie de

connexions, on forme un cadre géométrique pour l'étude de la géométrie et de la mécanique des système à plusieurs corps. Les équations du mouvement sont étudiées en respectant la structure d'espace fibré du système du centre de masse. Des équations réduites sont formées pour une valeur constante fixée du moment cinétique total. Les équations des petites variations sont obtenues au voisinage de mouvements de moment cinétique total nul. En particulier, les équations des petits mouvements au voisinage d'une position d'équilibre se réduisent aux équations habituelles des petites vibrations. © Elsevier, Paris

1. INTRODUCTION

Multi-particle systems are looked upon as supermolecules, gigantic molecules, in which chemical reactions take place. The path along which the chemical reaction takes place can be viewed as a curve in the "internal" space, a space of molecule forms independent of its position or attitude. Local coordinates in the internal space are called internal coordinates. For example, configuration parameters such as bond lengths, valence angles are internal coordinates. Traditionally, in case of the small vibration of a molecule [1], one needs internal coordinates only in the vicinity of a stable equilibrium position. However, internal coordinates can be defined for configurations far from a stable equilibrium position.

In this article, the internal space is defined to be the quotient space of the center-of-mass system by the action of the rotation group $SO(3)$. An additional condition put on the center-of-mass system will be described in the following section. Then, the center-of-mass system is made into a principal fibre bundle with the structure group $SO(3)$, the base space of which is called the internal space. Further, a connection is defined naturally on this $SO(3)$ bundle, and thereby rotational and vibrational vectors are defined strictly. The connection was first introduced by A. Guichardet [2], who made effective use of it to show that rotational motions cannot be separated from vibrational motions; suppose a molecule starting from an initial position performs a continuous vibrational motion to get to a final position with the same shape or configuration as the initial one. Then the initial and final positions of the molecule are related by a pure rotation. This implies that vibrational motions give rise to

a rotation. Cats know this fact, who can fall on his legs when launched in the air.

On the other hand, the center-of-mass system is endowed with a flat Riemannian metric coming from the total kinetic energy. The Riemannian geometry and the connection theory for the center-of-mass system are put together to provide a geometric setting for the study of multi-particle systems. In performing the geometric study, "moving frames" on the center-of-mass system are of great use.

In this aspect, the geometric setting for multi-particle systems looks like Kaluza–Klein theory which is considered as Riemannian geometry of principal fibre bundles [3]. If a multi-particle system is replaced by a continuum, a similar geometric study will go through. Geometrical Cat's problem for deformable bodies has been treated by Montgomery [4], in which a gauge theoretical point of view is also taken. See also a book edited by Shapere and Wilczek [5], which is a collection of articles concerning Berry phases and deformable bodies. Quite recently, Littlejohn and Reinsch also study n-body systems from the gauge theoretical point of view [6]. The present authors started a geometric study of molecules in quantum chemistry [7], and one (T.I.) of authors has set up a geometric setting for three-body systems in two and three dimensions [8,9] and for n-body systems in two dimensions [10]. Classical mechanics in Hamiltonian formalism has been already discussed for n-body systems [11], rather in an abstract manner. A point to make in this article is to discuss n-body systems from the viewpoint of Kaluza–Klein geometry, and to write out equations of motion in an explicit manner.

This article is organized as follows: Section 2 deals with the center-of-mass system as a principal $SO(3)$ bundle, on which a natural connection is defined and thereby rotational and vibrational vectors are distinguished. The presence of non-vanishing curvature of this connection implies that rotational motions cannot be separated from vibrational motions. In Section 3, a moving frame associated with the bundle structure discussed in Section 2 plays a key role in studying the geometric structure of the center-of-mass system. A natural Riemannian metric and the bundle structure of the center-of-mass system are put together to determine the Riemannian geometry of the internal space. In particular, sectional curvatures of the internal space prove to be expressible in terms of the curvature discussed in Section 2. Section 4 is concerned with equations of motion in association with the bundle structure of the center-of-mass system. Then two sets of equations are obtained; one is concerned mainly

with angular variables, and the other mainly with internal coordinates. These sets of equation are, of course, coupled. In particular, if the multi-particle system is assumed to be rigid, the set of equations concerning angular variables becomes the Euler equation for a rigid body, and if the system consists of free particles with vanishing total angular momentum, the set of equations concerning the internal coordinates becomes the geodesic equation of the internal space. The reduction of the equations of motion is also discussed by use of the conservation of the total angular momentum. Section 5 deals with variational equations for the equations of motion obtained in Section 4. In the vicinity of an equilibrium state of the molecule, the variational equations reduce to those equations which have been discussed in the traditional theory of small vibrations. It is also shown that the sectional curvature of the internal space plays, in the variational equations, a role of an additive potential which is a positive semi-definite quadratic form in variation vectors. Section 6 deals with a three-particle system as an example.

2. CONNECTION THEORY

2.1. The internal space

In order to define the internal space and internal coordinates, it is strict and of great use to exploit notions from differential geometry (see [12–14], for example). Let X_0 be the space of all the ennuples $x = (x_1, \ldots, x_N)$ of the nucleus position vectors $x_\alpha \in \mathbb{R}^3$, $\alpha = 1, \ldots, N$. As is well-known, the translational degrees of freedom are gotten rid of from X_0 to give rise to the center-of-mass system

$$X = \left\{ x = (x_1, \ldots, x_N) \mid \sum_{\alpha=1}^{N} m_\alpha x_\alpha = 0 \right\}. \tag{2.1}$$

The rotation group $SO(3)$ acts on X in a natural manner,

$$\Phi_g : x \mapsto gx := (gx_1, \ldots, gx_N), \quad g \in SO(3),\ x \in X. \tag{2.2}$$

In what follows, we assume that the molecular configurations are not rectilinear. This means that the subspaces

$$F_x = \operatorname{span}\{x_1, x_2, \ldots, x_N\} \quad (N \geqslant 3) \tag{2.3}$$

are assumed to be of dimension greater than or equal to 2; $\dim F_x \geqslant 2$. Then, if $hx = x$ for $h \in SO(3)$ and for $x \in X$ with $\dim F_x \geqslant 2$, one has $h =$ identity. Thus the group $SO(3)$ acts freely on X, so that the quotient space $X/SO(3)$ becomes a manifold. For simplicity, we denote by the same letter X the subset of X with $\dim F_x \geqslant 2$. Now the X is made into a principal fibre bundle over the quotient space,

$$\pi : X \to M := X/SO(3), \tag{2.4}$$

where π is the natural projection. By definition of the quotient space, a point of M is an equivalence class of molecular configurations which are mutually connected by rotations, so that any molecular configuration of an equivalence class has the same form or shape. The M is referred to as the internal space, whose local coordinates are called internal coordinates. In [4,5], M is called the shape space. We notice also here that shape spaces were first introduced by D.G. Kendall [15] and are studied further in statistics [16].

To introduce a local coordinate system in X, we use the local triviality of the $SO(3)$ bundle (2.4),

$$\pi^{-1}(U) \cong U \times SO(3), \tag{2.5}$$

where U is an open subset of M. Then one has a local section σ in X, which is, by definition, a map of U to X satisfying $\pi \circ \sigma = \mathrm{id}_M$, id_M being the identity map of M. Hence, any point $x \in \pi^{-1}(U)$ is expressed as $x = g\sigma(q)$ along with $q \in U$ and $g \in SO(3)$. The local cross section σ is realized as follows: Fixing tentatively the form of the molecule by specifying a point $q \in U$, we lay the molecule in the space $\mathbb{R}^3$ in such a way that each particle, designated by α, is set as

$$\sigma_\alpha(q) = \sum_{a=1}^{3} C_\alpha^a(q) e_a, \quad \alpha = 1, \ldots, N, \tag{2.6}$$

where $C_\alpha^a(q)$ and e_a, $a = 1, 2, 3$, are functions of q and the standard basis of $\mathbb{R}^3$, respectively. Eqs. (2.6) define a local section σ. An example of how to lay the molecule in $\mathbb{R}^3$ will be given in Section 6. Then we rotate the molecule laid, to get each particle to take its position,

$$x_\alpha = \sum_{a=1}^{3} C_\alpha^a(q) g e_a, \quad g \in SO(3),\ \alpha = 1, \ldots, N, \tag{2.7}$$

which is a realization of $x = g\sigma(q)$. Thus we can describe molecule's configurations in terms of local coordinates $(q^i) \in U$ and $g \in SO(3)$, $i = 1, 2, \ldots, f = \dim M$.

2.2. Connection

In what follows, rotational and vibrational vectors are defined on X strictly according to [2,11]. To this end, a metric ds^2 and a connection form ω, which are closely related with the kinetic energy and the angular momentum of the molecule, respectively, play a key role; the metric is defined to be

$$ds^2 = \sum_{\alpha=1}^{N} m_\alpha (dx_\alpha | dx_\alpha), \quad x = (x_1, \ldots, x_N) \in X, \tag{2.8}$$

and the connection form to be

$$\omega = R\left(A_x^{-1} \sum_{\alpha=1}^{N} m_\alpha x_\alpha \times dx_\alpha \right), \tag{2.9}$$

where $(\,|\,)$ denotes the standard inner product in $\mathbb{R}^3$, and $R : \mathbb{R}^3 \to SO(3)$ is the vector space isomorphism defined by

$$R(w) = \begin{pmatrix} 0 & -w^3 & w^2 \\ w^3 & 0 & -w^1 \\ -w^2 & w^1 & 0 \end{pmatrix} \quad \text{for } w = (w^a) \in \mathbb{R}^3, \tag{2.10}$$

and $A_x : \mathbb{R}^3 \to \mathbb{R}^3$ is the inertia tensor defined at $x \in X$ for $w \in \mathbb{R}^3$ by

$$A_x(w) = \sum_{\alpha=1}^{N} m_\alpha x_\alpha \times (w \times x_\alpha). \tag{2.11}$$

We notice here that A_x is a symmetric positive-definite operator for x with $\dim F_x \geqslant 2$, so that A_x^{-1} exists. In fact, one has

$$(w | A_x(w)) = \sum_{\alpha=1}^{N} m_\alpha (w \times x_\alpha | w \times x_\alpha) \geqslant 0, \tag{2.12}$$

and thereby $(w|A_x(w)) = 0$ for some w, if and only if $w \times x_\alpha = 0$, $\alpha = 1, 2, \ldots, N$. If $w \neq 0$, the last condition implies that all the x_α

lay in the line determined by w, which contradicts our assumption that $\dim F_x \geqslant 2$. Thus $(w|A_x(w)) = 0$ if and only if $w = 0$.

Let us also be reminded of fundamental properties of R and A_x:

$$R(w)z = w \times z, \quad w, z \in \mathbb{R}^3, \tag{2.13}$$

$$R(gw) = gR(w)g^{-1}, \quad w \in \mathbb{R}^3,\ g \in SO(3), \tag{2.14}$$

$$A_{gx}(w) = gA_x(g^{-1}w) =: \mathrm{Ad}_g A_x(w), \quad w \in \mathbb{R}^3,\ g \in SO(3). \tag{2.15}$$

These are easy to prove by straightforward calculation. Note also that the Lie algebra $so(3)$ is endowed with a natural inner product defined by and equal to

$$R(u) \cdot R(w) := \tfrac{1}{2}\mathrm{tr}\big(R(u)^T R(w)\big) = (u|w) \quad \text{for } u,\ w \in \mathbb{R}^3. \tag{2.16}$$

On the above setting-up, we are to define rotational and vibrational vectors definitely. Rotational vectors are defined to be infinitesimal generators of the $SO(3)$ action, which turn out to be expressed as

$$\begin{aligned} &\frac{d}{dt}\big(\exp tR(w)x_1, \ldots, \exp tR(w)x_N\big)\Big|_{t=0} \\ &\quad = (w \times x_1, \ldots, w \times x_N) \quad \text{for } w \in \mathbb{R}^3. \end{aligned} \tag{2.17}$$

In terms of differential operators, the rotational vector (2.17) takes the form

$$\sum_{\alpha=1}^{N}\left(w \times x_\alpha \middle| \frac{\partial}{\partial x_\alpha}\right) = \left(w \middle| \sum_{\alpha=1}^{N} x_\alpha \times \frac{\partial}{\partial x_\alpha}\right) =: (w|J), \tag{2.18}$$

where J is the total angular momentum operator. A tangent vector $v = (v_1, \ldots, v_N)$ to X at x is called a vibrational vector, if it is orthogonal to any rotational vector at x with respect to the metric (2.8). Hence, the tangent vector $v = (v_1, \ldots, v_N)$ is shown to be a vibrational vector, if and only if

$$\sum_{\alpha=1}^{N} m_\alpha x_\alpha \times v_\alpha = 0. \tag{2.19}$$

This is also equivalent to

$$\omega(v) = R\left(A_x^{-1}\sum_{\alpha=1}^{N} m_\alpha x_\alpha \times v_\alpha\right) = 0. \tag{2.20}$$

Moreover, we have to point out that the ω satisfies, for rotational vectors,

$$\omega\left(\sum_{\alpha=1}^{N}\left(w \times x_\alpha \middle| \frac{\partial}{\partial x_\alpha}\right)\right) = R(w), \quad w \in \mathbb{R}^3, \tag{2.21}$$

and is subject to the transformation

$$\omega_{gx} = \mathrm{Ad}_g \omega_x, \quad g \in SO(3). \tag{2.22}$$

The proof can be carried out by using the definition (2.9) and the properties (2.13)–(2.15).

We proceed to describe rotational and vibrational vectors in local coordinates defined in (2.7). Let ω^a and J_a be the components of ω and of J with respect to the fixed frame e_a, respectively,

$$\omega = \sum_{a=1}^{3} R(e_a)\omega^a, \quad \omega \cdot R(e_a) = \omega^a, \tag{2.23}$$

$$J = \sum_{a=1}^{3} e_a J_a, \quad J_a = (e_a | J) = \sum_{\alpha=1}^{N}\left(e_a \times x_\alpha \middle| \frac{\partial}{\partial x_\alpha}\right). \tag{2.24}$$

We note here that from (2.22) the components of the connection form, ω^a, transform according to

$$\omega^a_{gx} = \sum_{b=1}^{3} g_{ab}\omega^b_x, \quad g = (g_{ab}) \in SO(3). \tag{2.25}$$

Now, from (2.21) it follows that $\omega(J_a) = R(e_a)$, which implies that ω^a are dual to J_a. The forms ω^a together with dq^i constitute a local basis of the space of one-forms on X, which satisfy

$$\omega^a(J_b) = \delta^a_b, \qquad dq^i(J_b) = 0, \quad i, j = 1, \ldots, f = \dim M. \tag{2.26}$$

To be strict in notation, we have to use $\pi^* dq^i$ for dq^i, which is the pull-back of dq^i, but we use dq^i for notational simplicity. By using ω^a and dq^i, we can determine vector fields ξ_j through

$$\omega^a(\xi_j) = 0, \qquad dq^i(\xi_j) = \delta^i_j. \tag{2.27}$$

The ξ_j and J_a are put together to form a local basis of tangent vector fields on X. We note here that from (2.27) and (2.20) it follows that the vector field ξ_j is vibrational.

For local expression of ω^a, we are to write out (2.9) in the local coordinates given by (2.7). Writing out dx_α, we have the expression

$$\sum_{\alpha=1}^{N} m_\alpha x_\alpha \times dx_\alpha = \sum_{\alpha=1}^{N} m_\alpha x_\alpha \times dgg^{-1}x_\alpha + \sum_{\alpha=1}^{N} m_\alpha x_\alpha \times \sum_{i=1}^{f} \frac{\partial x_\alpha}{\partial q^i} dq^i. \tag{2.28}$$

We here denote the components of the Maure–Cartan form dgg^{-1} by Θ^a;

$$dgg^{-1} = \sum_{a=1}^{3} \Theta^a R(e_a), \tag{2.29}$$

and set

$$\beta_i^a := \left(A_x^{-1} \sum_{\alpha=1}^{N} m_\alpha x_\alpha \times \frac{\partial x_\alpha}{\partial q^i} \middle| e_a \right). \tag{2.30}$$

Then, from (2.9), (2.28), (2.29), and (2.30), it follows that

$$\omega = \sum_{a=1}^{3} \omega^a R(e_a), \quad \omega^a = \Theta^a + \sum_{i=1}^{f} \beta_i^a dq^i. \tag{2.31}$$

In gauge theory, β_i^a is called a Yang–Mills potential and denoted usually by A_i^a [14]. To write out Θ^a of (2.29) in terms of Euler angles $(\phi^a) = (\phi, \theta, \psi)$, we take g as

$$g = \exp(\phi R(e_3)) \exp(\theta R(e_2)) \exp(\psi R(e_3)). \tag{2.32}$$

Then, Eq. (2.29) is written out to give

$$\begin{aligned} \Theta^1 &= -\sin\phi\, d\theta + \sin\theta \cos\phi\, d\psi, \\ \Theta^2 &= \cos\phi\, d\theta + \sin\theta \sin\phi\, d\psi, \\ \Theta^3 &= d\phi + \cos\theta\, d\psi. \end{aligned} \tag{2.33}$$

We notice further that Eqs. (2.25) and (2.31) imply that β_i^a are subject to the transformation

$$\beta_i^a(gx) = \sum_{b=1}^{3} g_{ab} \beta_i^b(x), \quad g = (g_{ab}) \in SO(3). \tag{2.34}$$

The infinitesimal version of (2.34) with $g = \exp(tR(e_c))$ is expressed as

$$J_c(\beta_i^a) = -\sum_{b=1}^{3} \varepsilon_{cab}\beta_i^b, \tag{2.35}$$

where ε_{abc} is the antisymmetric symbol with $\varepsilon_{123} = 1$.

As for the local expression of ξ_i, we obtain, from (2.27) and (2.31),

$$\xi_i = \frac{\partial}{\partial q^i} - \sum_{a=1}^{3} \beta_i^a J_a =: \left(\frac{\partial}{\partial q^i}\right)^*. \tag{2.36}$$

This is a unique vibrational (or horizontal) vector field which is in one-to-one correspondence with $\partial/\partial q^i$ on $U \subset M$. In connection theory, $\xi_i = (\partial/\partial q^i)^*$ is called the horizontal lift of $\partial/\partial q^i$, which we denote by ∂_i^* in short in the below. Moreover, owing to (2.31), the first equation of (2.26) reduces to $\Theta^a(J_b) = \delta_{ab}$, which provides the well-known local expression of J_a as

$$\begin{aligned} J_1 &= -\cos\phi\cot\theta\frac{\partial}{\partial\phi} - \sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\phi}{\sin\theta}\frac{\partial}{\partial\psi}, \\ J_2 &= -\sin\phi\cot\theta\frac{\partial}{\partial\phi} + \cos\phi\frac{\partial}{\partial\theta} + \frac{\sin\phi}{\sin\theta}\frac{\partial}{\partial\psi}, \\ J_3 &= \frac{\partial}{\partial\phi}. \end{aligned} \tag{2.37}$$

In addition, we have to touch upon the transformation property of the components of the inertia tensor;

$$A_{ab}(x) := \big(e_a | A_x(e_b)\big). \tag{2.38}$$

Indeed, Eq. (2.15) gives rise to the transformation of $A(x) = (A_{ab}(x))$:

$$A_{ab}(gx) = \sum_{c,d} g_{ac}A_{cd}(x)g_{bd}, \quad g = (g_{ab}) \in SO(3). \tag{2.39}$$

The infinitesimal transformation of (2.39) for $g = \exp(tR(e_c))$ proves to be given by

$$J_c(A_{ab}) = \big[R(e_c), A\big]_{ab} = \sum_d \varepsilon_{cda}A_{db} + \sum_d \varepsilon_{cdb}A_{ad}. \tag{2.40}$$

In conclusion, we remark that the connection form vanishes in the direction of dilatation. In fact, the infinitesimal generator of the dilatation $x \mapsto e^t x$, $t \in \mathbb{R}$, is given by

$$\lambda = \sum_{\alpha=1}^{N} \left(x_\alpha \middle| \frac{\partial}{\partial x_\alpha} \right), \tag{2.41}$$

for which ω vanishes;

$$\omega(\lambda) = R\left(A_x^{-1} \sum_\alpha m_\alpha x_\alpha \times x_\alpha \right) = 0. \tag{2.42}$$

This means that λ is a vibrational vector field by definition.

2.3. Curvature

On using (2.24), (2.35), and (2.36), the rotational vector fields J_a and the vibrational vector fields ∂_i^* are shown to satisfy the following commutation relations

$$\begin{aligned} [J_a, J_b] &= -\sum_{c=1}^{3} \varepsilon_{abc} J_c, \\ [\partial_i^*, \partial_j^*] &= -\sum_{c=1}^{3} F_{ij}^c J_c, \\ [\partial_i^*, J_a] &= 0, \end{aligned} \tag{2.43}$$

where F_{ij}^c is defined to be

$$F_{ij}^c := \frac{\partial \beta_j^c}{\partial q^i} - \frac{\partial \beta_i^c}{\partial q^j} - \sum_{a,b=1}^{3} \varepsilon_{abc} \beta_i^a \beta_j^b. \tag{2.44}$$

The middle equation of (2.43) means that two independent vibrational vector fields, ∂_i^* and ∂_j^*, are coupled to give rise to an infinitesimal rotation. This fact implies that molecular vibrations cannot be separated from rotations. Another implication is that the distribution spanned by $\{\partial_i^*\}$ is not completely integrable in the sense of Frobenius [17], so that there are no submanifolds to which ∂_i^*'s are tangent. If there were such a submanifold, only vibrational motions would take place on it, and it would be able to be identified with (an open submanifold of) the internal space M.

We turn to the curvature form, which is defined to be

$$\Omega := d\omega - \omega \wedge \omega. \tag{2.45}$$

In the ordinary connection theory, in which the structure group is assumed to act on a principal bundle to the right [12], the minus sign in the right-hand side of (2.45) should be replaced by the plus sign. Let the components of Ω be denoted by Ω^a;

$$\Omega = \sum_{a=1}^{3} R(e_a)\Omega^a. \tag{2.46}$$

Then a calculation provides

$$\Omega^c = d\omega^c - \sum_{a<b} \varepsilon_{abc}\omega^a \wedge \omega^b. \tag{2.47}$$

On the other hand, the theory of connection gives the formula [12]

$$\Omega(\partial_i^*, \partial_j^*) = -\omega([\partial_i^*, \partial_j^*]), \quad \Omega(J_a, \cdot) = 0. \tag{2.48}$$

Then Eqs. (2.43) and (2.48) are put together to provide

$$\Omega^c = \sum_{i<j} F_{ij}^c \, dq^i \wedge dq^j. \tag{2.49}$$

In view of (2.49) and (2.43), we understand that the presence of non-vanishing curvature makes it impossible to separate rotation from vibration.

In addition, we give the transformation property of the curvature form. From (2.22) and (2.45) it follows that

$$\Omega_{gx} = \mathrm{Ad}_g \Omega_x. \tag{2.50}$$

Then the components of Ω are subject to the transformation

$$\Omega_{gx}^a = \sum_{b=1}^{3} g_{ab}\Omega_x^b, \quad g = (g_{ab}) \in SO(3). \tag{2.51}$$

Alternatively, one finds that

$$F^c_{ij}(gx) = \sum_{a=1}^{3} g_{ca} F^a_{ij}(x), \quad g = (g_{ca}) \in SO(3). \tag{2.52}$$

In conclusion, we wish to show that the Ω vanishes for the vector λ given by (2.41). From (2.9) and (2.11), we observe that the connection form ω is invariant under the dilatation $x \mapsto e^t x$. Hence, the Lie derivative of ω with respect to λ vanishes; $\mathcal{L}_\lambda \omega = 0$. From this and from (2.42) and (2.45), one verifies that

$$0 = \mathcal{L}_\lambda \omega = \iota(\lambda)\Omega, \tag{2.53}$$

where $\iota(\cdot)$ stands for the interior derivative [17]. On setting $\lambda = \sum \lambda^i \partial_i^*$, Eq. (2.53) reads

$$\sum_i \lambda^i F^c_{ij} = 0, \quad c = 1, 2, 3, \tag{2.54}$$

implying that the curvature form is degenerate in the direction of λ.

3. RIEMANNIAN GEOMETRY

3.1. Canonical affine connection

We are to study the infinitesimal displacement, $dx = (dx_1, \ldots, dx_N)$, of $x \in X$. Since ω^a and dq^i form a local basis of the space of one-forms, dx is put in the form

$$dx = \sum_{a=1}^{3} B_a \omega^a + \sum_{i=1}^{f} B_i \, dq^i, \tag{3.1}$$

or

$$dx_\alpha = \sum_{a=1}^{3} B^\alpha_a \omega^a + \sum_{i=1}^{f} B^\alpha_i \, dq^i, \quad \alpha = 1, \ldots, N, \tag{3.2}$$

where $B_a = (B^1_a, B^2_a, \ldots, B^N_a)$ and $B_i = (B^1_i, B^2_i, \ldots, B^N_i)$ are determined to be

$$\begin{aligned} B_a &= J_a x, \quad \text{i.e., } B^\alpha_a = J_a x_\alpha = e_a \times x_\alpha, \\ B_i &= \partial_i^* x, \quad \text{i.e., } B^\alpha_i = \partial_i^* x_\alpha, \end{aligned} \tag{3.3}$$

respectively. The system $\{B_a, B_i\}$ is called a moving frame in the center-of-mass system X (for an elementary treatment of moving frames, see [18]), which gives conversely rise to J_a and ∂_i^* through

$$J_a = \sum_{\alpha=1}^{N} \left(B_a^\alpha \middle| \frac{\partial}{\partial x_\alpha} \right), \qquad \partial_i^* = \sum_{\alpha=1}^{N} \left(B_i^\alpha \middle| \frac{\partial}{\partial x_\alpha} \right). \tag{3.4}$$

The differentials of the moving frame are put in the form

$$\begin{aligned} dB_a &= \sum_b \gamma_a^b B_b + \sum_i \gamma_a^i B_i, \\ dB_i &= \sum_a \gamma_i^a B_a + \sum_j \gamma_i^j B_j, \end{aligned} \tag{3.5}$$

where $\gamma_a^b, \gamma_a^i, \gamma_i^a, \gamma_i^j$ are one-forms, which are called the connection forms of the canonical affine connection of X [12,18]. These connection forms are expressed as

$$\begin{aligned} \gamma_a^b &= \sum_c \Gamma_{ac}^b \omega^c + \sum_j \Gamma_{aj}^b \, dq^j, \\ \gamma_a^i &= \sum_c \Gamma_{ac}^i \omega^c + \sum_j \Gamma_{aj}^i \, dq^j, \\ \gamma_i^a &= \sum_c \Gamma_{ic}^a \omega^c + \sum_j \Gamma_{ij}^a \, dq^j, \\ \gamma_i^j &= \sum_c \Gamma_{ic}^j \omega^c + \sum_k \Gamma_{ik}^j \, dq^k, \end{aligned} \tag{3.6}$$

where $\Gamma_{ac}^b, \ldots, \Gamma_{ik}^j$ are called the coefficients of the canonical affine connection. We have here to distinguish $\gamma_b^a, \ldots, \gamma_j^i$ from ω^a. The former forms are concerned with the canonical affine connection on the tangent bundle TX, and the latter with the principal $SO(3)$ bundle $X \to M$.

3.2. Levi–Civita connection

In what follows, we study what results from the fact that the canonical affine connection stated above is a flat Levi–Civita connection of the Euclidean space X. The metric defined on X was already given by (2.8), which is clearly a flat metric. Eqs. (2.8) and (3.2) are put together to give

$$ds^2 = \sum_\alpha \sum_{a,b} m_\alpha (B_a^\alpha | B_b^\alpha) \omega^a \omega^b + 2 \sum_\alpha \sum_{a,i} m_\alpha (B_a^\alpha | B_i^\alpha) \omega^a \, dq^i$$
$$+ \sum_\alpha \sum_{i,j} m_\alpha (B_i^\alpha | B_j^\alpha) \, dq^i \, dq^j. \tag{3.7}$$

On the other hand, from the definition (3.3) of B_a^α and B_i^α, we can verify that

$$\sum_{\alpha=1}^{N} m_\alpha (B_a^\alpha | B_b^\alpha) = A_{ab}, \qquad \sum_{\alpha=1}^{N} m_\alpha (B_a^\alpha | B_i^\alpha) = 0, \tag{3.8}$$

where A_{ab} are the components of the inertia tensor given by (2.38). On looking at the last term of the right-hand side of (3.7) along with (3.4), we see that the B_i^α's define a metric tensor a_{ij} on the internal space M,

$$a_{ij} := \sum_{\alpha=1}^{N} m_\alpha (B_i^\alpha | B_j^\alpha) = ds^2 (\partial_i^*, \partial_j^*). \tag{3.9}$$

In fact, since ds^2 is invariant under the $SO(3)$ action and since ∂_i^* and $\partial / \partial q^i$ are in one-to-one correspondence, a_{ij}'s are independent of $SO(3)$, and therefore well defined on M. Thus the metric ds^2 expressed as (3.7) becomes

$$ds^2 = \sum_{a,b=1}^{3} A_{ab} \omega^a \omega^b + \sum_{i,j=1}^{f} a_{ij} \, dq^i \, dq^j. \tag{3.10}$$

We choose to describe Eqs. (3.8) and (3.9) as

$$B_a \cdot B_b = A_{ab}, \quad B_a \cdot B_i = 0, \quad B_i \cdot B_j = a_{ij}, \tag{3.11}$$

where the center dot indicates the inner product with respect to the metric ds^2.

We have to note here that the map $\pi : X \to M$ becomes a Riemannian submersion [19] since π has maximal rank and since π_* preserves lengths of horizontal (i.e., vibrational in our case) vectors.

We proceeds to the structure equations of Cartan [18]. Since X is a Euclidean space, one has

$$d(dx) = 0, \tag{3.12}$$

$$d(dB_a) = 0, \qquad d(dB_i) = 0, \tag{3.13}$$

which mean that the affine connection has no torsion and vanishing curvature, respectively. From (3.12) it follows that the coefficients

appearing in the right-hand sides of (3.6) satisfy

$$\begin{aligned} &\Gamma^c_{ab} - \Gamma^c_{ba} = \varepsilon_{abc}, && \Gamma^i_{ab} = \Gamma^i_{ba}, \\ &\Gamma^c_{ia} - \Gamma^c_{ai} = 0, && \Gamma^j_{ia} = \Gamma^j_{ai}, \\ &\Gamma^a_{ji} - \Gamma^a_{ij} = F^a_{ji}, && \Gamma^k_{ij} = \Gamma^k_{ji}. \end{aligned} \tag{3.14}$$

In fact, the left-hand side of (3.12) are written out as

$$\begin{aligned} d(dx) &= \sum_b \Big(\sum_a \gamma^b_a \wedge \omega^a + \sum_i \gamma^b_i \wedge dq^i + d\omega^b \Big) B_b \\ &\quad + \sum_j \Big(\sum_a \gamma^j_a \wedge \omega^a + \sum_i \gamma^j_i \wedge dq^i \Big) B_j \\ &= \sum_b \Big[\sum_{a<c} (\varepsilon_{acb} - \Gamma^b_{ac} + \Gamma^b_{ca}) \omega^a \wedge \omega^c \\ &\qquad + \sum_a \sum_i (\Gamma^b_{ai} - \Gamma^b_{ia}) dq^i \wedge \omega^a \\ &\qquad + \sum_{i<j} (F^b_{ij} - \Gamma^b_{ij} - \Gamma^b_{ji})\, dq^i \wedge dq^j \Big] B_b \\ &\quad + \sum_j \Big[\sum_{b<a} (\Gamma^j_{ab} - \Gamma^j_{ba}) \omega^b \wedge \omega^a + \sum_a \sum_i (\Gamma^j_{ai} - \Gamma^j_{ia})\, dq^i \wedge \omega^a \\ &\qquad + \sum_{k<i} (\Gamma^j_{ik} - \Gamma^j_{ki})\, dq^k \wedge dq^i \Big] B_j. \end{aligned} \tag{3.15}$$

Hence, the condition (3.12) along with (3.15) brings about (3.14), as is wanted. It is to be noted that the Eqs. (3.14) are also obtained by operating x with the vector fields (2.43).

Before studying what results from (3.13), we are to differentiate (3.11) to obtain the condition that the canonical affine connection on X be a metric connection [18]. Differentiation of the last equation of (3.11) gives

$$da_{ij} = dB_i \cdot B_j + B_i \cdot dB_j. \tag{3.16}$$

Then, it follows that

$$\begin{aligned}\frac{\partial a_{ij}}{\partial q^\ell} &= \sum_k \Gamma^k_{i\ell} a_{kj} + \sum_k \Gamma^k_{j\ell} a_{ik},\\ 0 &= \sum_k \Gamma^k_{ia} a_{kj} + \sum_k \Gamma^k_{ja} a_{ik}.\end{aligned} \tag{3.17}$$

The first equation of (3.17) and the relation $\Gamma^k_{ij} = \Gamma^k_{ji}$ from (3.14) imply that Γ^k_{ij} are equal to the Christoffel symbols formed from the metric tensor a_{ij},

$$\Gamma^i_{jk} = \left\{ \begin{matrix} i \\ j\ k \end{matrix} \right\} := \tfrac{1}{2} \sum_{\ell=1}^{f} a^{i\ell} \left(\frac{\partial a_{\ell k}}{\partial q^j} + \frac{\partial a_{j\ell}}{\partial q^k} - \frac{\partial a_{jk}}{\partial q^\ell} \right), \tag{3.18}$$

where $(a^{ij}) = (a_{ij})^{-1}$. Put another way, the Levi–Civita connection on the center-of-mass system X endowed with the metric ds^2 induces the Levi–Civita connection on the internal space M endowed with the metric $\sum a_{ij}\, dq^i\, dq^j$. This fact is already pointed out in [3].

The differentiation of the first and the second equations of (3.11) yields

$$\begin{aligned} J_d(A_{ab}) &= \sum_c \Gamma^c_{ad} A_{cb} + \sum_c \Gamma^c_{bd} A_{ac},\\ \partial^*_i(A_{ab}) &= \sum_c \Gamma^c_{ai} A_{cb} + \sum_c \Gamma^c_{bi} A_{ac},\end{aligned} \tag{3.19}$$

and

$$\begin{aligned} 0 &= \sum_j \Gamma^j_{ac} a_{ji} + \sum_b \Gamma^b_{ic} A_{ab},\\ 0 &= \sum_j \Gamma^j_{ak} a_{ji} + \sum_b \Gamma^b_{ik} A_{ab},\end{aligned} \tag{3.20}$$

respectively. Eqs. (3.19), (3.20), and the second of (3.17) along with (3.14) are put together to provide

$$\begin{aligned}\Gamma^c_{ad} = &-\tfrac{1}{2}\varepsilon_{adc} + \tfrac{1}{2} \sum_b A^{cb} \big(J_d(A_{ab}) + J_a(A_{db}) - J_b(A_{da}) \big)\\ &+ \tfrac{1}{2} \sum_{b,e} \big(\varepsilon_{bed} A_{ae} A^{cb} + \varepsilon_{bea} A_{de} A^{cb} \big)\end{aligned} \tag{3.21}$$

with $(A^{ab}) := (A_{ab})^{-1}$, and

$$\Gamma^c_{ai} = \tfrac{1}{2} \sum_b A^{bc} \partial^*_i(A_{ab}) = \Gamma^c_{ia}, \tag{3.22}$$

$$\Gamma^b_{ik} = \tfrac{1}{2} F^b_{ik} = -\Gamma^b_{ki}, \tag{3.23}$$

$$\Gamma^i_{ja} = \tfrac{1}{2} \sum_k \sum_b a^{ik} F^b_{jk} A_{ab} = \Gamma^i_{aj}, \tag{3.24}$$

$$\Gamma^j_{ba} = -\tfrac{1}{2} \sum_i a^{ji} \partial^*_i (A_{ab}) = \Gamma^j_{ab}. \tag{3.25}$$

Inserting (2.40) into (3.21), we find that

$$\Gamma^c_{ad} = -\tfrac{1}{2} \left(\varepsilon_{adc} + \sum_{b,e} \varepsilon_{bea} A_{ed} A^{bc} + \sum_{b,e} \varepsilon_{bed} A_{ea} A^{cb} \right), \tag{3.26}$$

which may be written in a symmetric form, if $\Gamma_{ad,c} := \sum_e \Gamma^e_{ad} A_{ec}$ is introduced;

$$\Gamma_{ad,c} = -\tfrac{1}{2} \left(\sum_e \varepsilon_{ade} A_{ec} + \sum_e \varepsilon_{dce} A_{ea} - \sum_e \varepsilon_{cae} A_{ed} \right). \tag{3.27}$$

3.3. Riemann curvature

We proceed to study what results from (3.13), the vanishing curvature condition. From $d(dB_a) = 0$, one obtains

$$\begin{aligned} d\gamma^c_a - \sum_b \gamma^b_a \wedge \gamma^c_b - \sum_i \gamma^i_a \wedge \gamma^c_i &= 0, \\ d\gamma^i_a - \sum_b \gamma^b_a \wedge \gamma^i_b - \sum_j \gamma^j_a \wedge \gamma^i_j &= 0, \end{aligned} \tag{3.28}$$

and from $d(dB_i) = 0$,

$$\begin{aligned} d\gamma^a_i - \sum_b \gamma^b_i \wedge \gamma^a_b - \sum_j \gamma^j_i \wedge \gamma^a_j &= 0, \\ d\gamma^j_i - \sum_b \gamma^b_i \wedge \gamma^j_b - \sum_k \gamma^k_i \wedge \gamma^j_k &= 0. \end{aligned} \tag{3.29}$$

If F^a_{ij} vanished identically, the internal space M would be able to be identified with a submanifold of X. Then Eqs. (3.28) and (3.29) would provide the Ricci, Codazzi, and Gauss equations for the submanifold M of X. However, there are no submanifolds to which B_i's are tangent, so that the above equations are viewed as generalizations of the Ricci, Codazzi, and Gauss ones [19].

One of the consequences of geometric interest from the second equation of (3.29) is that

$$R^j_{im\ell} + \sum_a \Gamma^j_{ia} F^a_{\ell m} + \sum_a \Gamma^a_{im} \Gamma^j_{a\ell} - \sum_a \Gamma^a_{i\ell} \Gamma^j_{am} = 0, \tag{3.30}$$

where $R^j_{im\ell}$ are the components of the Riemann curvature tensor formed from a_{ij},

$$R^j_{i\ell m} := \frac{\partial \Gamma^j_{im}}{\partial q^\ell} - \frac{\partial \Gamma^j_{i\ell}}{\partial q^m} + \sum_k \Gamma^k_{im} \Gamma^j_{k\ell} - \sum_k \Gamma^k_{i\ell} \Gamma^j_{km}. \tag{3.31}$$

Inserting (3.23) and (3.24) into (3.30) results in

$$R^j_{i\ell m} + \tfrac{1}{4} \sum_k \sum_{a,b} a^{jk} A_{ab} \left(F^a_{im} F^b_{\ell k} - 2F^a_{m\ell} F^b_{ik} + F^a_{\ell i} F^b_{mk} \right) = 0. \tag{3.32}$$

Note here that the second term of the left-hand side of (3.32) is independent of $g \in SO(3)$, since $\sum_{a,b} A_{ab} F^a_{\cdot\cdot} F^b_{\cdot\cdot}$ are independent of g because of (2.52) and (2.39). Eq. (3.32) is a specialized form of O'Neill's formula [19], which links the Riemann curvatures of the total space and that of the base space of a Riemannian submersion. On account of (3.32), the Ricci tensor and the scalar curvature defined as $R_{ij} := \sum_k R^k_{ikj}$ and as $R := \sum_{ij} a^{ij} R_{ij}$, respectively, satisfy

$$R_{im} - \tfrac{3}{4} \sum_{j,k} \sum_{a,b} a^{jk} A_{ab} F^a_{ij} F^b_{mk} = 0, \tag{3.33}$$

$$R - \tfrac{3}{4} \sum_{i,m,j,k} \sum_{a,b} a^{im} a^{jk} A_{ab} F^a_{ij} F^b_{mk} = 0. \tag{3.34}$$

These formula are also found in [6].

In conclusion, we mention of sectional curvature. Let $\sum_i u^i \partial/\partial q^i$ and $\sum_i v^i \partial/\partial q^i$ be mutually orthogonal unit tangent vector fields on M. Then the sectional curvature for the plane κ spanned by (u^i) and (v^i) at a point $q \in M$ is defined to be

$$K_\kappa := \sum_{j,i,\ell,m,k} R^j_{i\ell m} u^\ell v^m v^i u^k a_{kj}, \tag{3.35}$$

which takes, from (3.32), the form

$$K_\kappa = \tfrac{3}{4} \sum_{a,b} \sum_{i,j,k,\ell} A_{ab} F^a_{ij} u^i v^j F^b_{k\ell} u^k v^\ell. \tag{3.36}$$

We note here that the right-hand sides of (3.36) is independent of $g \in SO(3)$. Since the right-hand side of (3.36) is a quadratic form in the quantity $\sum F^a_{ij} u^i v^j$, we observe that K_κ is non-negative. However, it is unlikely that K_κ is strictly positive, since M is not a compact space. In fact, for a class of planes, the K_κ vanishes. To show this, we take the vector λ given by (2.41). Since λ is a vibrational vector field by definition, the projected vector $\pi_*\lambda$ is a non-vanishing tangent vector field on M. If κ is a plane including $\pi_*\lambda$, then the sectional curvature K_κ vanishes on account of (2.54) and (3.36). Furthermore, the Ricci tensor is non-negative as well,

$$\sum_{i,j} R_{ij} u^i u^j \geqslant 0, \tag{3.37}$$

which is known from (3.33). We see also that the Ricci tensor vanishes for $u = \pi_*\lambda$ on account of (2.54). This means that the Ricci tensor (R_{ij}) is not strictly positive. We will give an example of (R_{ij}) in Section 6.

4. EQUATIONS OF MOTION

4.1. Setting up equations of motion

In this section, we are to obtain the equations of motion for multi-particle systems in the Lagrangian formalism adapted for the bundle structure of the center-of-mass system X. To this end, the Lagrangian formalism described in terms of "quasi-coordinates" is of great use [20–23], a brief review of which is as follows: For local expression of the equations of motion, it is sufficient for us to work in an open subset W of $\mathbb{R}^{3N-3}$. Let ξ^λ, $\lambda = 1, 2, \ldots, 3N-3$, be a local coordinate system in W. Let X_λ and θ^λ be a local basis of vector fields and its dual on W, respectively, which are denoted by

$$X_\lambda = \sum_\mu B^\mu_\lambda \frac{\partial}{\partial \xi^\mu}, \qquad \theta^\lambda = \sum_\mu A^\lambda_\mu \, d\xi^\mu, \tag{4.1}$$

respectively, with $\sum_\lambda A^\mu_\lambda B^\lambda_\nu = \delta^\mu_\nu$. Then, one has, after differentiation,

$$d\theta^\lambda = \sum_{\sigma<\kappa} \gamma^\lambda_{\sigma\kappa} \theta^\kappa \wedge \theta^\sigma, \quad \gamma^\lambda_{\sigma\kappa} := \sum_{\mu,\nu} \left(\frac{\partial A^\lambda_\mu}{\partial \xi^\nu} - \frac{\partial A^\lambda_\nu}{\partial \xi^\mu} \right) B^\mu_\sigma B^\nu_\kappa. \tag{4.2}$$

It is clear that $\gamma^\lambda_{\sigma\kappa}$ is anti-symmetric in σ and κ.

Let

$$\dot{\pi}^{\lambda} = \sum_{\mu} A^{\lambda}_{\mu}(\xi)\dot{\xi}^{\mu} \tag{4.3}$$

be "quasi-velocities", the time derivatives of "quasi-coordinates". The equations of motion can be described in terms of quasi-velocities $\dot{\pi}^{\lambda}$ and coordinates ξ^{λ}. We express the Lagrangian $L(\xi, \dot{\xi})$ as

$$L^*(\xi, \dot{\pi}) = L(\xi, \dot{\xi}). \tag{4.4}$$

Then the Lagrangian equations of motion for L^* takes the form

$$\frac{d}{dt}\left(\frac{\partial L^*}{\partial \dot{\pi}^{\sigma}}\right) - X_{\sigma} L^* + \sum_{\mu,\kappa} \gamma^{\mu}_{\sigma\kappa} \frac{\partial L^*}{\partial \dot{\pi}^{\mu}} \dot{\pi}^{\kappa} = 0, \quad \sigma = 1, \ldots, 3N-3, \tag{4.5}$$

where X_{σ} and $\gamma^{\mu}_{\sigma\kappa}$ are the vector fields and the coefficients given in (4.1) and (4.2), respectively. Occasionally, the symbols $\partial/\partial\pi_{\sigma}$ are used for X_{σ}.

We are to apply these equations to our multi-particle system in the open subset $\pi^{-1}(U) \cong U \times SO(3)$ referred to in (2.5). From (2.26) and (2.27), the system of one-forms is given by

$$\theta^a = \omega^a, \qquad \theta^{3+i} = dq^i, \quad a = 1, 2, 3, \ i = 1, \ldots, f = \dim M, \tag{4.6}$$

and the dual system of vector fields is written as

$$X_a = J_a, \qquad X_{3+i} = \partial^*_i, \quad a = 1, 2, 3, \ i = 1, \ldots, f = \dim M. \tag{4.7}$$

Then, Eqs. (2.47), (2.49), and $d(dq^i) = 0$ provide, when compared with (4.2),

$$\gamma^a_{bc} = -\varepsilon_{bca}, \qquad \gamma^a_{3+i,3+j} = -F^a_{ij} \tag{4.8}$$

with the other $\gamma^{\lambda}_{\mu\nu}$'s all vanishing. To express the Lagrangian L^*, we introduce quasi-velocities according to (4.3) by

$$\dot{\pi}^a = \omega^a_t, \qquad \dot{\pi}^{3+i} = \dot{q}^i, \tag{4.9}$$

where ω^a_t are defined through (2.31) as

$$\omega^a_t := \omega^a\left(\frac{d}{dt}\right) = \Theta^a_t + \sum_i \beta^a_i \dot{q}^i, \qquad \Theta^a_t = \sum_b \Theta^a_b \dot{\phi}^b. \tag{4.10}$$

Then, from (3.10) together with the potential function V, one has the Lagrangian

$$L^* = \tfrac{1}{2}\sum_{a,b} A_{ab}\omega_t^a\omega_t^b + \tfrac{1}{2}\sum_{i,j} a_{ij}\dot{q}^i\dot{q}^j - V. \tag{4.11}$$

The application of (4.5) to (4.11) then provides

$$\frac{d}{dt}\left(\frac{\partial L^*}{\partial \omega_t^a}\right) - J_a L^* - \sum_{b,c} \varepsilon_{acb}\frac{\partial L^*}{\partial \omega_t^b}\omega_t^c = 0, \tag{4.12}$$

$$\frac{d}{dt}\left(\frac{\partial L^*}{\partial \dot{q}^i}\right) - \partial_i^* L^* - \sum_a\sum_j F_{ij}^a \frac{\partial L^*}{\partial \omega_t^a}\dot{q}^j = 0. \tag{4.13}$$

PROPOSITION 4.1. – *The Lagrangian equations of motion of a molecule are given by* (4.12) *and* (4.13) *in terms of internal coordinates* q^i *and quasi-velocities* ω_t^a. *A point to make is that they contain the the structure constants* ε_{acb} *of the structure group* $SO(3)$ *and the curvature* F_{ij}^a *on the bundle* $X \to M$.

We are going to look into (4.12). In the vector notation with $A = (A_{ab})$ and $\omega_t = (\omega_t^a)$, one has, by using (2.40),

$$J_a L^* = e_a \cdot (A\omega_t \times \omega_t), \qquad \sum_{b,c} \varepsilon_{acb}\frac{\partial L^*}{\partial \omega_t^b}\omega_t^c = (\omega_t \times A\omega_t)_a, \tag{4.14}$$

so that Eq. (4.12) comes to be expressed as

$$\frac{d}{dt}(A\omega_t) + JV = 0, \qquad JV = \sum_a e_a J_a V. \tag{4.15}$$

Since the total angular momentum is expressed as

$$L = \sum_\alpha m_\alpha x_\alpha \times \dot{x}_\alpha = A\omega_t, \tag{4.16}$$

as is easily seen from (2.9), Eq. (4.15) is put in the form

$$\frac{d}{dt}L = -JV. \tag{4.17}$$

If the potential is rotational invariant, this equation implies the conservation of the total angular momentum.

On the other hand, Eq. (4.13) becomes

$$\frac{d}{dt}\left(\sum_j a_{ij}\dot{q}^j\right) - \tfrac{1}{2}\sum_{k,j}\frac{\partial a_{kj}}{\partial q^i}\dot{q}^k\dot{q}^j - \tfrac{1}{2}\sum_{a,b}\partial_i^*(A_{ab})\omega_t^a\omega_t^b$$
$$-\sum_j\sum_{a,b}F_{ij}^a A_{ab}\omega_t^b\dot{q}^j + \partial_i^* V = 0, \tag{4.18}$$

which proves to be equivalent to

$$\frac{d^2q^i}{dt^2} + \sum_{j,k}\left\{\begin{matrix} i \\ j\,k\end{matrix}\right\}\frac{dq^j}{dt}\frac{dq^k}{dt} = \tfrac{1}{2}\sum_k\sum_{a,b}\partial_k^*(A_{ab})a^{ik}\omega_t^a\omega_t^b$$
$$-\sum_{j,k}\sum_c A_{ab}F_{jk}^b a^{ik}\frac{dq^j}{dt}\omega_t^a - \sum_j a^{ij}\partial_j^* V. \tag{4.19}$$

If the molecule is allowed to be regarded as a rigid molecule, the variables (q^i) are fixed, so that A_{ab}, V, and x_α are constant in (q^i), and hence $\beta_i^a = 0$ from (2.30). Thus, one has $\partial_i^*(A_{ab}) = 0$ and $\partial_j^* V = 0$, so that Eq. (4.19) is satisfied identically. On the other hand, Eq. (4.15) can be shown to be equivalent to the Euler equation for a rigid body with the torque $-J(V)$. To this end, we first calculate the time derivative of A in the vector notation,

$$\frac{dA}{dt} = \sum_i \frac{dq^i}{dt}\partial_i^*(A) + [R(\omega_t), A], \tag{4.20}$$

where we have used (2.40). Put together, Eqs. (4.15) and (4.20) provide the equation for the rigid body,

$$A\frac{d\omega_t}{dt} + \omega_t \times A\omega_t = -J(V). \tag{4.21}$$

Further, from Eq. (2.31), one has $\omega_t = \Theta_t = (\Theta_t^a)$ on account of $\beta_i^a = 0$, so that Eq. (4.21) becomes

$$A\frac{d\Theta_t}{dt} + \Theta_t \times A\Theta_t = -J(V). \tag{4.22}$$

What to do for us is to rewrite this equation in terms of constant inertia tensor. To this end, we are to evaluate $A = A(x)$ at a specific point x_0 given by (2.6) along with (q^i) fixed. We denote by A_0 the matrix A evaluated at x_0. Then Eq. (2.39) implies that $A = gA_0g^{-1}$. On using this

relation, Eq. (4.22) turns into

$$A_0 g^{-1}\frac{d\Theta_t}{dt} + g^{-1}\Theta_t \times A_0 g^{-1}\Theta_t = -g^{-1}J(V). \tag{4.23}$$

Incidentally, from (2.29) one verifies that $\dot{g}g^{-1} = R(\Theta_t)$, so that $d(g^{-1}\Theta_t)/dt = g^{-1}(d\Theta_t/dt)$. Therefore, Eq. (4.23) turns over into a preferable form

$$A_0 \frac{d}{dt}\Pi_t + \Pi_t \times A_0\Pi_t = -g^{-1}J(V), \qquad \Pi_t := g^{-1}\Theta_t, \tag{4.24}$$

which is the Euler equation for a rigid body with Π_t and $-g^{-1}J(V)$ the angular velocity in the body and the torque, respectively, [24]. We note in addition that $g^{-1}\dot{g} = R(\Pi_t)$.

In the case of molecular dynamics, the potential function V is assumed to be rotationally invariant, so that one has

$$J_a(V) = 0, \qquad \partial_j^*(V) = \frac{\partial V}{\partial q^j}. \tag{4.25}$$

Thus we have the following.

PROPOSITION 4.2. – *If the potential is rotationally invariant, then Eq.* (4.12), *a part of the equations of motion, implies the conservation of the total angular momentum. Moreover, if the molecule is assumed to be rigid, Eq.* (4.12) *becomes equivalent to the Euler equation for a rigid body.*

4.2. Reduction of the equations of motion

In what follows, under the assumption that the potential function is rotationally invariant, we treat the total angular momentum L as a constant vector, and thereby reduce the equations of motion. Eq. (4.19) along with (4.16) and (4.25) can be put in the form

$$\begin{aligned}\frac{d^2q^i}{dt^2} + \sum_{j,k}\left\{ {i \atop j\,k} \right\}\frac{dq^j}{dt}\frac{dq^k}{dt} &= -\tfrac{1}{2}\sum_k\sum_{a,b} a^{ik}\partial_k^*(A^{ab})L_aL_b \\ &\quad - \sum_{j,k}\sum_c a^{ik}L_cF^c_{jk}\frac{dq^j}{dt} - \sum_j a^{ij}\frac{\partial V}{\partial q^j},\end{aligned} \tag{4.26}$$

where use has been made of $\sum_b A^{ab}A_{bc} = \delta_{ac}$. This equation was also found in [6].

What to note about (4.26) is that this equation is not in a closed form, if L is fixed during the motion. In fact, the right-hand side contains angular variables, i.e., depends on $SO(3)$ through A^{ab} and F^c_{jk}, but the left-hand side is independent of $SO(3)$. This implies that we need another equation for angular variables in order to obtain equations of motion in the closed form. However, we can observe that, if L is constant, the right-hand side of (4.26) is invariant under the rotation about L, i.e., under the action of $h \in SO(3)$ satisfying $hL = L$. In fact, $\partial^*_k(A^{ab})$ is subject to the transformation

$$\left(\partial^*_k A^{-1}\right)_{gx} = \mathrm{Ad}_g\left(\partial^*_k A^{-1}\right)_x, \tag{4.27}$$

the same transformation as A^{-1}, and (F^c_{jk}) subject to (2.52). We have to notice here that Eq. (4.27) is a consequence of the fact that ∂^*_k is invariant under the $SO(3)$ action; $\Phi_{g*}\partial^*_k = \partial^*_k$, the infinitesimal version of which is $[\partial^*_k, J_a] = 0$, the last equation of (2.43). Thus we need in reality equations for angular variables which do not keep L invariant. Since the set of $h \in SO(3)$ satisfying $hL = L$, $L \neq 0$, forms a subgroup $SO(2)$, the angular variables we need lie on the sphere $S^2 \simeq SO(3)/SO(2)$. To find equations on S^2, we consider the vector defined by

$$\Lambda := g^{-1}L, \tag{4.28}$$

where $g \in SO(3)$ is the angular variable introduced in (2.7). The magnitude of Λ, of course, conserved; $\|\Lambda\| = \|L\| = \text{const}$, and hence Λ varies in the sphere S^2. A calculation along with $\dot{g}g^{-1} = R(\Theta_t)$ shows that Λ is subject to the equation

$$\frac{d\Lambda}{dt} = -g^{-1}\Theta_t \times \Lambda. \tag{4.29}$$

To look into (4.29), we use the relation resulting from (4.10), (4.16), and (4.28),

$$\Lambda = A_0 g^{-1}\omega_t = A_0\left(g^{-1}\Theta_t + \sum_i \beta^0_i \frac{dq^i}{dt}\right), \tag{4.30}$$

where A_0 is the inertia tensor evaluated at $x_0 = \sigma(q)$, and $\beta^0_i := g^{-1}\beta_i$ is a vector $\beta_i = (\beta^a_i)$ evaluated also at x_0 (see the transformation property (2.34) and (2.39)). Then, Eq. (4.29) is rewritten as

$$\frac{d\Lambda}{dt} = -(A_0^{-1}\Lambda) \times \Lambda + \sum_i \frac{dq^i}{dt}(\beta^0_i \times \Lambda). \tag{4.31}$$

This is the equation for Λ, depending on internal coordinates.

Returning to Eq. (4.26), we have to rewrite it by replacing $g\Lambda$ for L. To this end, we use the formulae (2.52) and (4.27). Then Eq. (4.26) becomes expressible as

$$\frac{d^2q^i}{dt^2}+\sum_{j,k}\left\{\begin{matrix} i \\ j\,k\end{matrix}\right\}\frac{dq^j}{dt}\frac{dq^k}{dt}=-\tfrac{1}{2}\sum_k\sum_{a,b}a^{ik}(\partial_k^*A^{ab})_0\Lambda_a\Lambda_b$$
$$-\sum_{j,k}\sum_c a^{ik}\Lambda_c(F^c_{jk})_0\frac{dq^j}{dt}-\sum_j a^{ij}\frac{\partial V}{\partial q^j}, \tag{4.32}$$

where the subscript 0 indicates that those quantities are evaluated at $x_0=\sigma(q)$. The second term of the right-hand side of (4.32) is a generalization of the Lorenz force in electrodynamics. The quantity $(\partial_k^*A^{-1})_0$ $(A^{-1}=(A^{ab}))$ in the first term of the right-hand side of (4.32) turns out to be put in the form

$$(\partial_k^*A^{-1})_0=\frac{\partial A_0^{-1}}{\partial q^k}-[R(\beta_k^0),A_0^{-1}], \tag{4.33}$$

which can be verified by using (2.36) and $J_a(A^{-1})=[R(e_a),A^{-1}]$, a consequence of (2.40). From (4.33), the first and the third terms of the right-hand side of (4.32) are put together to be written as

$$-\sum_k a^{ik}\frac{\partial}{\partial q^k}\left(\tfrac{1}{2}\sum_{a,b}A_0^{ab}\Lambda_a\Lambda_b+V\right)+\sum_k a^{ik}((A_0^{-1}\Lambda)\times\Lambda|\beta_k^0), \tag{4.34}$$

the first term of which stands for minus the gradient of an effective potential. Thus we have found that Eq. (4.32) is written as

$$\frac{d^2q^i}{dt^2}+\sum_{j,k}\left\{\begin{matrix} i \\ j\,k\end{matrix}\right\}\frac{dq^j}{dt}\frac{dq^k}{dt}=-\sum_k a^{ik}\frac{\partial}{\partial q^k}\left(\tfrac{1}{2}\sum_{a,b}A_0^{ab}\Lambda_a\Lambda_b+V\right)$$
$$+\sum_k a^{ik}((A_0^{-1}\Lambda)\times\Lambda|\beta_k^0)]-\sum_{j,k}\sum_c a^{ik}\Lambda_c(F^c_{jk})_0\frac{dq^j}{dt}. \tag{4.35}$$

PROPOSITION 4.3. – *Along with the conservation of the total angular momentum, the equations of motion are reduced to* (4.35) *and* (4.31). *The set of these equations is reminiscent of Wong's equation* [25], *if the terms appearing in* (4.34) *are dropped from the right-hand side of* (4.35). *In the case of* $L=\Lambda=0$, *Eq.* (4.35) *reduces to the usual Newton's equations of motion on the internal space, and Eq.* (4.31) *vanishes.*

4.3. Equilibrium states

We are to consider the equilibrium state of the molecule with non-vanishing total angular momentum. From (4.31) and (4.35), it follows that the equilibrium state determined by $(\dot{q}, \dot{\Lambda}) = 0$ occurs under the conditions

$$(A_0^{-1}\Lambda) \times \Lambda = 0, \qquad \frac{\partial}{\partial q^i}\left(\tfrac{1}{2}\sum_{a,b} A_0^{ab}\Lambda_a\dot{\Lambda}_b + V\right) = 0. \tag{4.36}$$

The first condition of (4.36) means that Λ has to be an eigenvector of A_0^{-1}; $A_0^{-1}\Lambda = \mu^{-1}\Lambda$, where μ is an eigenvalue of A_0, which depends on q, of course. Then the second equation of (4.36) becomes

$$\frac{\partial}{\partial q^i}\left(\frac{\|L\|^2}{2\mu(q)} + V\right) = 0, \tag{4.37}$$

where use has been made of the relation $\|L\| = \|\Lambda\|$. The condition (4.37) was suggested in [6] in the name of the condition for relative equilibria.

PROPOSITION 4.4. – *The shape of the molecule in the relative equilibrium* $(\dot{q}, \dot{\Lambda}) = 0$ *is determined by* (4.37).

Now suppose that an equilibrium state with $L = 0$, described as q_0, undergoes a small amount of change in L. We denote $\|L\|^2/2$ by ε, an infinitesimal parameter. Then Eq. (4.37) has a one-parameter solution $q(\varepsilon)$ satisfying

$$\frac{\partial V}{\partial q^i}(q(\varepsilon)) - \varepsilon\frac{1}{\mu(\varepsilon)^2}\frac{\partial \mu}{\partial q^i}(\varepsilon) = 0, \qquad \frac{\partial V}{\partial q^i}(q_0) = 0, \tag{4.38}$$

where $q_0 = q(0)$. Differentiation of Eq. (4.38) with respect to ε at $\varepsilon = 0$ provides

$$\sum_j \frac{\partial^2 V}{\partial q^j \partial q^i}(q_0)\frac{dq^j}{d\varepsilon}(0) - \frac{1}{\mu(q_0)^2}\frac{\partial \mu}{\partial q^i}(q_0) = 0. \tag{4.39}$$

Assume that q_0 is a non-degenerate equilibrium position, that is, the Hessian matrix for V at q_0 is non-degenerate. We may then set

$$(K^{ij}(q_0)) = \left(\frac{\partial^2 V}{\partial q^i \partial q^j}(q_0)\right)^{-1}. \tag{4.40}$$

Eqs. (4.39) and (4.40) hence imply that

$$\frac{dq^i}{d\varepsilon}(0) = \frac{1}{\mu(q_0)^2} \sum_j K^{ij}(q_0) \frac{\partial \mu}{\partial q^j}(q_0). \tag{4.41}$$

This provides an infinitesimal change in the equilibrium states as the angular momentum vector is turned on.

For $\|L\| \neq 0$ of finite magnitude, a solution to (4.37) can be found by the use of the gradient method. In fact, along with an initial value, the gradient flow defined through

$$\frac{dq^i}{dt} = -\sum_j a^{ij} \frac{\partial}{\partial q^j} \left(\frac{\|L\|^2}{2\mu(q)} + V \right) \tag{4.42}$$

will approach a solution to (4.37).

5. VARIATIONAL EQUATIONS

In this section, we consider first the equation of motion with vanishing total angular momentum. Then Eq. (4.26) reduces to the equations on the internal space,

$$\frac{d^2 q^i}{dt^2} + \sum_{j,k} \left\{ \begin{matrix} i \\ j\,k \end{matrix} \right\} \frac{dq^j}{dt} \frac{dq^k}{dt} = -\sum_j a^{ij} \frac{\partial V}{\partial q^j}. \tag{5.1}$$

Let $c(t, s)$, $-\varepsilon_0 < s < \varepsilon_0$, be a one-parameter family of solutions to Eq. (5.1). That is, for each s fixed, $t \mapsto c(t, s)$ is a solution to Eq. (5.1). In particular, we set $c(t) := c(t, 0)$. Further, a variation vector field $\eta = (\eta^i)$ is defined, along $c(t)$, to be

$$\eta = \left. \frac{\partial c}{\partial s} \right|_{s=0}. \tag{5.2}$$

Let us denote by D/dt the covariant differentiation along the curve $c(t)$. Then, in the same method as that for obtaining the equation for geodesic deviations or the Jacobi equation [24], we find the equation for the variation vector field η in the form

$$\frac{D^2 \eta^i}{dt^2} - \sum_{j,\ell,m} R^i_{j\ell m} \frac{dq^j}{dt} \frac{dq^\ell}{dt} \eta^m = -\sum_{k,j} a^{ik} H_{jk} \eta^j, \tag{5.3}$$

where $H_{jk} := \nabla_j \nabla_k V$ is the Hessian for V with ∇_i the covariant differentiation.

We now use (3.32) to put (5.3) in the form

$$\frac{D^2\eta^i}{dt^2} + \frac{3}{4} \sum_{k,j,\ell,m} \sum_{a,b} a^{ik} A_{ab} F^a_{jm} \frac{dq^j}{dt} \eta^m F^b_{\ell k} \frac{dq^\ell}{dt} = -\sum_{k,j} a^{ik} H_{jk} \eta^j. \quad (5.4)$$

To have a compact expression, we use the notation $\Omega^a = (F^a_{ij})$ (see (2.49)). Then Eq. (5.4) turns into

$$\frac{D^2\eta}{dt^2} = -\frac{3}{4} \sum_{a,b} A_{ab} \Omega^a(\dot{c}^*, \eta^*) \Omega^b(\dot{c}^*, \cdot)^\# - H(\eta, \cdot)^\#, \quad (5.5)$$

where $\dot{c}^* = \sum \dot{q}^i \partial_i^*$, $\eta^* = \sum \eta^i \partial_i^*$, and $\Omega^b(\dot{c}^*, \cdot)^\#$ and $H(\eta, \cdot)^\#$ stand for the vector fields associated with the 1-forms $\Omega^b(\dot{c}^*, \cdot)$ and $H(\eta, \cdot)$ with $H = (H_{ij})$, respectively. The right-hand side of this equation is viewed as a force acting on the variation vector field η. This force can be derived from the potential function in η,

$$\frac{3}{8} \sum_{a,b} A_{ab} \Omega^a(\dot{c}^*, \eta^*) \Omega^b(\dot{c}^*, \eta^*) + \frac{1}{2} H(\eta, \eta). \quad (5.6)$$

Incidentally, the term $(3/8) \sum A_{ab} \Omega^a(\dot{c}^*, \eta^*) \Omega^b(\dot{c}^*, \eta^*)$ is positive semi-definite in η and is a function multiple of the sectional curvature for the plane formed by $\dot{c}$ and η (see (3.36), and remember that $\dot{c}$ and η are not assumed here to be unit vectors). Therefore, we observe that the curvature Ω^a does not make the trajectory $c(t)$ unstable, rather keeps it semi-stable. However, we note that if η is parallel to $\dot{c}$, the term $(3/8) \sum A_{ab} \Omega^a(\dot{c}^*, \eta^*) \Omega^b(\dot{c}^*, \eta^*)$ vanishes, so that the force $-(3/4) \sum A_{ab} \Omega^a(\dot{c}^*, \eta^*) \Omega^b(\dot{c}^*, \cdot^*)^\#$ has no effect in the direction of $\dot{c}$. Moreover, if η is parallel to λ given by (2.41), the potential $(3/8) \sum A_{ab}$ $\Omega^a(\dot{c}^*, \eta^*) \Omega^b(\dot{c}^*, \eta^*)$ vanishes because of (2.53), which implies that the dilatation does not contribute to keeping the trajectory $c(t)$ stable. This is a reasonable consequence.

If the potential V has a critical point at q_0, the point is a particular solution, $q(t) = q_0$, to Eq. (5.1). If we take this point as the solution $c(t) = q_0$, then the variation vector (5.2) is viewed as a small vibration at the equilibrium state, in the traditional sense. We note here that $\eta \in T_{q_0}(M)$ in this case. Since $\dot{c} = 0$, the variational equation (5.3) is put in

the form

$$\frac{d^2\eta^i}{dt^2} = -\sum_{k,j} a^{ik} H_{jk}\eta^j, \tag{5.7}$$

where a^{ik} and $H_{ij} = \partial^2 V/\partial q^i \partial q^j$ are both evaluated at q_0. Eq. (5.7) is just the equation of small vibrations with (a^{ik}) the **G** matrix and (H_{jk}) the force constant matrix [1].

PROPOSITION 5.1. – *The variational equations of the equations of motion for the multi-particle system with the vanishing total angular momentum are given by Eq.* (5.5), *which shows that the curvature Ω arising from the rotation of the system does not make the trajectory unstable. Further, at a critical point of the potential, the variational equations reduce to the traditional equations for small vibrations.*

We turn to the variational equations at an equilibrium state determine by (4.37). On denoting by ζ the variation vector for Λ, we obtain, from (4.35) and (4.31),

$$\begin{aligned}\frac{d^2\eta^i}{dt^2} = &-\sum_{j,k}\sum_{c} a^{ik}\Lambda_c (F^c_{jk})_0 \frac{d\eta^j}{dt} - \sum_{j,k} a^{ik}\frac{\partial^2 V_{\text{eff}}}{\partial q^j \partial q^k}\eta^j \\ &- \sum_{k}\sum_{a,b} a^{ik}\frac{\partial A_0^{ab}}{\partial q^k}\zeta_a\Lambda_b + \sum_{k,j} a^{ik}\left(\left(\frac{\partial A_0^{-1}}{\partial q^i}\Lambda\right)\times\Lambda|\beta_k^0\right)\eta^j \\ &+ \sum_k a^{ik}((A_0^{-1}\zeta)\times\Lambda + (A_0^{-1}\Lambda)\times\zeta|\beta_k^0)\end{aligned} \tag{5.8}$$

with $V_{\text{eff}} = (1/2)(\Lambda|A_0^{-1}\Lambda) + V$, and

$$\begin{aligned}\frac{d\zeta}{dt} = &-\sum_i \eta^i\left(\frac{\partial A_0^{-1}}{\partial q^i}\Lambda\right)\times\Lambda - A_0^{-1}\zeta\times\Lambda - A_0^{-1}\Lambda\times\zeta \\ &+ \sum_i \frac{d\eta^i}{dt}(\beta_i^0\times\Lambda),\end{aligned} \tag{5.9}$$

respectively, where the functions appearing in the coefficients are evaluated at (q, Λ) satisfying (4.37) with $A_0(q)\Lambda = \mu(q)\Lambda$, and further ζ is subject to $\sum_a \zeta_a\Lambda_a = 0$. Eq. (5.8) reduces to Eq. (5.7), if $\Lambda = 0$.

6. AN EXAMPLE

In conclusion, we give an example of the geometry for a tri-atomic molecule. Let us denote by c_0 a position vector of the center-of-mass of two particles at x_2 and at x_3. Let r and ρ be the length of the vector $x_2 - x_3$ and of $x_1 - c_0$, respectively, and φ the angle made by two vectors $x_2 - c_0$ and $x_1 - c_0$. We choose to lay the tri-atomic molecule in the plane so that the position vectors x_1 and x_2 may lie, respectively, in the positive half of the e_1-axis and in the upper half plane spanned by e_1 and e_2. The third position vector x_3 takes a due position so that the system may be the center-of-mass system. Then the position vectors are expressed as

$$\begin{aligned} x_1^0 &= \frac{(m_2+m_3)\rho}{m_1+m_2+m_3} e_1, \\ x_2^0 &= -\frac{m_1\rho}{m_1+m_2+m_3} e_1 + \frac{m_3 r}{m_2+m_3}(\cos\varphi\, e_1 + \sin\varphi\, e_2), \\ x_3^0 &= -\frac{m_1}{m_3} x_1^0 - \frac{m_2}{m_3} x_2^0. \end{aligned} \tag{6.1}$$

This expression is a specialization of (2.6) for the tri-atomic molecule and defines a local section, $x_0 = \sigma(q)$ along with $q^1 = \rho$, $q^2 = r$, $q^3 = \varphi$, in the center-of-mass system X. Generic position vectors are then given by $x_\alpha = g x_\alpha^0$, $\alpha = 1, 2, 3$, with $g \in SO(3)$.

From the definition (2.11), the inertia tensor A turns out to have the components, at x_0,

$$A_0 = \begin{pmatrix} A_{11}^0 & A_{12}^0 & 0 \\ A_{21}^0 & A_{22}^0 & 0 \\ 0 & 0 & A_{33}^0 \end{pmatrix}$$

with

$$\begin{aligned} A_{11}^0 &= \frac{m_2 m_3}{m_2+m_3} r^2 \sin^2\varphi, \\ A_{12}^0 = A_{21}^0 &= -\frac{m_2 m_3}{m_2+m_3} r^2 \sin\varphi\cos\varphi, \\ A_{22}^0 &= \frac{m_1(m_2+m_3)}{m_1+m_2+m_3}\rho^2 + \frac{m_2 m_3}{m_2+m_3} r^2 \cos^2\varphi, \\ A_{33}^0 &= \frac{m_1(m_2+m_3)}{m_1+m_2+m_3}\rho^2 + \frac{m_2 m_3}{m_2+m_3} r^2. \end{aligned} \tag{6.2}$$

The value of A at a generic point $x = gx_0$ is given by $A = gA_0g^{-1}$ on account of (2.39).

Now we are in a position to calculate the connection form. A straightforward calculation of (2.30) along with (6.1) provides, at x_0,

$$\sum_a \sum_i \beta_i^a(x_0)\, dq^i\, e_a = \frac{m_2 m_3}{m_2 + m_3} \frac{r^2}{C}\, d\varphi\, e_3, \quad \text{with } C = A_{33}^0. \tag{6.3}$$

This shows that the only non-vanishing component is $\beta_3^3(x_0)$. The value of β_i^a at a generic point $x = gx_0$ is calculated by using (2.34). The components of the connection form at x are then given through (2.31). The components of the curvature form evaluated at x_0 then turns out to take the form

$$\Omega_0^1 = \Omega_0^2 = 0, \quad \Omega_0^3 = \frac{m_1 m_2 m_3}{m_1 + m_2 + m_3} \frac{2r\rho}{C^2} (\rho\, dr \wedge d\varphi - r\, d\rho \wedge d\varphi), \tag{6.4}$$

giving the values $F_{13}^3(x_0)$ and $F_{23}^3(x_0)$ with the others vanishing. The value of Ω^a at a generic point $x = gx_0$ is obtained by using (2.51).

We now turn to the moving frame associated with J_a and ∂_i^*. From the definition (3.3), the B_a^α are easy to obtain; $B_a^\alpha = e_a \times gx_\alpha^0$ with x_α^0 given by (6.1). However, the B_i^α needs calculation. By operating x with

$$\partial_1^* = \frac{\partial}{\partial \rho}, \qquad \partial_2^* = \frac{\partial}{\partial r}, \qquad \partial_3^* = \frac{\partial}{\partial \varphi} - \sum_a \beta_3^a J_a,$$

and by using (3.3), we obtain, at x_0,

$$\begin{aligned}
B_1^1(x_0) &= \frac{m_2 + m_3}{m_1 + m_2 + m_3} e_1, \\
B_1^2(x_0) &= -\frac{m_1}{m_1 + m_2 + m_3} e_1, \\
B_1^3(x_0) &= -\frac{m_1}{m_1 + m_2 + m_3} e_1, \\
B_2^1(x_0) &= 0, \\
B_2^2(x_0) &= \frac{m_3}{m_2 + m_3} (\cos\varphi\, e_1 + \sin\varphi\, e_2), \\
B_2^3(x_0) &= -\frac{m_2}{m_2 + m_3} (\cos\varphi\, e_1 + \sin\varphi\, e_2),
\end{aligned} \tag{6.5}$$

$$B_3^1(x_0) = -\beta_3^3(x_0)Q^1 e_2,$$
$$B_3^2(x_0) = \frac{m_3}{m_2+m_3} r(-\sin\varphi\, e_1 + \cos\varphi\, e_2) - \beta_3^3(x_0)(-Q^3 e_1 + Q^2 e_2),$$
$$B_3^3(x_0) = \frac{m_2}{m_2+m_3} r(\sin\varphi\, e_1 - \cos\varphi\, e_2) - \beta_3^3(x_0)$$
$$\times \left(\frac{m_2}{m_3} Q^3 e_1 - \frac{m_1 Q^1 + m_2 Q^2}{m_3} e_2\right),$$

where Q^1, Q^2, Q^3 are functions given by

$$Q^1 = \frac{m_2+m_3}{m_1+m_2+m_3}\rho,$$
$$Q^2 = \frac{m_3}{m_2+m_3} r\cos\varphi - \frac{m_1}{m_1+m_2+m_3}\rho,$$
$$Q^3 = \frac{m_3}{m_2+m_3} r\sin\varphi.$$

At a generic point $x = gx_0$, the above vectors take the form $B_i^\alpha(x) = gB_i^\alpha(x_0)$. This is because the transformation property of B_i^α results from the definition (3.3) along with $\Phi_{g*}\partial_i^* = \partial_i^*$.

Using (3.9) and (6.5), we can find the expression of the the metric tensor on the internal space in the form

$$a_{11} = \frac{m_1(m_2+m_3)}{m_1+m_2+m_3},$$
$$a_{22} = \frac{m_2 m_3}{m_2+m_3}, \qquad a_{ij} = 0 \quad (i \neq j), \tag{6.6}$$
$$a_{33} = \frac{m_1 m_2 m_3}{m_1+m_2+m_3}\frac{r^2\rho^2}{C}.$$

To obtain the Riemann curvature tensor is now a matter of calculation, which can be done through (3.32). It is to be noted that we do not use the Christoffel symbols, but use a^{ij}, A_{ab}, and F_{ij}^a to calculate the Riemann curvature. However, we do not give here the Riemann curvature tensor but give the Ricci curvature tensor only for simplicity, which can be obtained through (3.33). A calculation results in

$$(R_{ij}) = \begin{pmatrix} R_{11} & R_{12} & 0 \\ R_{21} & R_{22} & 0 \\ 0 & 0 & R_{33} \end{pmatrix} \tag{6.7}$$

with

$$R_{11} = \frac{3}{4}\frac{m_2 + m_3}{m_2 m_3 r^2} C(F_1)^2,$$

$$R_{12} = R_{21} = \frac{3}{4}\frac{m_2 + m_3}{m_2 m_3 r^2} C F_1 F_2,$$

$$R_{22} = \frac{3}{4}\frac{m_2 + m_3}{m_2 m_3 r^2} C(F_2)^2,$$

$$R_{33} = \frac{3}{4}\frac{m_1 + m_2 + m_3}{m_1(m_2 + m_3)} C(F_1)^2 + \frac{3}{4}\frac{m_2 + m_3}{m_2 m_3} C(F_2)^2,$$

where $F_1 = F^3_{12}(x_0)$, $F_2 = F^3_{23}(x_0)$, the expression of which are known from (6.4). It is easy to see that the tensor (6.7) is positive semi-definite (see (3.37)). There exists a zero eigenvalue, for which the associated eigenvector is a function multiple of the dilatation vector $\rho\partial/\partial\rho + r\partial/\partial r$, as is expected.

In conclusion, we remark that some of numerical calculations for equilibrium state of a tri-atomic molecule are found in [26].

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