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Stratified reduction of many-body kinetic energy operators

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The center-of-mass system of many bodies 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 is stratified into three types of strata. The principal stratum consists of nonsingular configurations for which the isotropy subgroup is trivial, and the other two types of strata consist of singular configurations for which the isotropy subgroup is isomorphic with either SO(2) or SO(3). Depending on whether the isotropy subgroup is isomorphic with SO(2) or SO(3), the stratum in question consists of collinear configurations or of a single configuration of the multiple collision. It is shown that the kinetic energy operator is expressed as the sum of rotational and vibrational energy operators on each stratum except for the stratum of multiple collision. The energy operator for nonsingular configurations has singularity at singular configurations. However, the singularity is not essential in the sense that both of the rotational and vibrational energy integrals have a finite value. This can be proved by using the boundary conditions of wave functions at singular configurations for three-body systems, for simplicity. It is shown, in addition, that the energy operator for collinear configurations has also singularity at the multiple collision, but the singularity is not essential either in the sense that the kinetic energy integral is not divergent at the multiple collision. Reduction procedure is applied to the respective energy operators for the nonsingular and the collinear configurations to obtain respective reduced operators, both of which are expressed in terms of internal coordinates.
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I. INTRODUCTION

This article has an aim to study n-body Hamiltonians by means of a transformation group. A key idea is as follows: Consider a quantum system on a manifold on which a compact Lie group acts. The manifold is then stratified into the disjoint union of strata according to the orbit types of the group action. If a Hamiltonian operator defined on the manifold is invariant under the group action, it will be stratified in such a manner that the Hamiltonian operator has a description on each stratum. The restricted Hamiltonian operator on each stratum will be reduced, by using a unitary irreducible representation of the group, to an operator on the orbit space formed from the stratum in question.

The center-of-mass system for n bodies admits the action of the rotation group SO(3) in a natural manner. According to the orbit types for the SO(3) action, the center-of-mass system is stratified into strata. The principal (or maximal) stratum consists of nonsingular configurations for which the isotropy subgroup is trivial, so that it is made into an SO(3) principal fiber bundle.[1] The strata of lower dimension consist of singular configurations for which the isotropy subgroup is not trivial. Practically, singular configurations are collinear ones and simultaneous multiple collision, and nonsingular configurations are planar or spatial ones.

To study quantum systems for nonsingular configurations, one can apply connection theory on the SO(3) bundle, through which the kinetic energy operator is determined to be the sum of

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rotational and vibrational energy operators.[2–5] However, these operators fail to be defined at singular configurations. In contrast with the case of nonsingular configurations, the stratum of collinear configurations is not made into a principal fiber bundle, but it remains to have a bundle structure. The present article shows that one can set up quantum systems on each stratum on the basis of the bundle structure of each stratum. The quantum systems defined on respective strata will be reduced to quantum systems defined on respective orbit spaces formed from the respective strata.

On each stratum except for the multiple collision stratum, the kinetic energy operator is decomposed into the sum of rotational and vibrational energy operators. The energy operator for nonsingular configurations has singularity at singular configuration, but it is shown that the singularity is not essential in the sense that both of the rotational and vibrational energy integrals have a finite value. This can be proved by using the boundary conditions of wave functions at singular configurations, while the proof is given only for three-body systems for simplicity. Furthermore, the energy operator for collinear configurations, which is also expressed as the sum of rotational and vibrational energy operators, has also singularity at the multiple collision, but the singularity is not essential either in the sense that the kinetic energy integral is not divergent at the multiple collision. The description of the kinetic energy operator as the sum of rotational and vibrational energy operators is effectively used to provide reduced kinetic energy operators in terms of internal (or shape) coordinates.

The organization of this article is as follows: In Sec. II, a brief review is made of the center-of-mass system along with the stratification by means of the SO(3) action. Section III is a review of the Fourier analysis of wave functions,[6,7] which is an application of the Peter–Weyl theorem on unitary irreducible representations of compact Lie groups. Section IV is concerned with a geometric setting for nonsingular configurations. A connection form and a metric are defined and expressed in terms of local coordinates. Transformation law for locally defined connection forms is discussed also. In Sec. V, the kinetic energy operator is defined for nonsingular configurations, which is broken up into the sum of rotational and vibrational energy operators. Operating on equivariant functions with these operators, one obtains reduced rotational and vibrational energy operators in terms of local coordinates for the shape of nonsingular configurations. Transformation law for locally defined reduced operators is studied as well. Section VI is specialized to three-body systems. Though the three-body system was already studied in the same manner,[4] this section deals with it in a different coordinate system to discuss the singularity of the kinetic energy operator. It is shown that the rotational and the vibrational energy operators are not singular in the sense that the rotational and vibrational energy integrals are not divergent at singular configurations. Section VII deals with collinear configurations. A (singular) connection form will be defined on the stratum of collinear configurations. In Sec. VIII, the kinetic energy operator for collinear configurations is studied on the basis of the singular connection treated in Sec. VII. Operating on equivariant wave functions with the kinetic energy operator, one obtains a reduced kinetic energy operator, which is defined on the shape space of collinear configurations.

II. THE CENTER-OF-MASS SYSTEM

Let $\mathbf{x}_i$ and m_i with $i=1,\ldots,N$ be position vectors and masses of point particles in $\mathbf{R}^3$, respectively. Then the configurations of the point particles are denoted by $x=(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N)$. The center-of-mass system M is defined to be

$$M=\left\{ x=(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N) \,\middle|\, \mathbf{x}_i\in\mathbf{R}^3, \sum_{i=1}^{N} m_i\mathbf{x}_i=0 \right\}. \tag{1}$$

The configuration x is characterized by the linear subspace

$$F_x := \mathrm{span}\{\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N\}. \tag{2}$$

According as $\dim F_x = 0,1,2,3$, the configurations of the particles are pointlike, collinear, planar, and spatial, respectively. Thus M is broken up into four subsets:

$$M = \bigcup_{k=0}^{3} M_k, \quad M_k := \{x \in M \mid \dim F_x = k\}, \quad k = 0,1,2,3. \tag{3}$$

The center-of-mass system admits a natural SO(3) action:

$$\Phi_g(x) = gx = (g\mathbf{x}_1, g\mathbf{x}_2, \ldots, g\mathbf{x}_N), \quad g \in \mathrm{SO}(3), \quad x \in M. \tag{4}$$

The isotropy subgroup G_x of $G = \mathrm{SO}(3)$ at $x \in M$ is defined, as usual, to be $G_x = \{g \in G \mid gx = x\}$. Now one can show that the isotropy subgroups are trivial, $G_x = \{e\}$, on $M_2 \cup M_3$, that is, SO(3) acts on $M_2 \cup M_3$ freely. However, on M_1 and on M_0, the isotropy subgroups are nontrivial; at $x \in M_1$ and at $x \in M_0$, they are isomorphic with SO(2) and with SO(3), respectively. Configurations in $M_0 \cup M_1$ are called singular, which are pointlike or collinear. Depending on the dimensionality of the isotropy subgroups G_x, orbits $\mathcal{O}_x$ of G through $x \in M$ are classified into three cases:

$$\mathcal{O}_x \cong \begin{cases} \mathrm{SO}(3) & \text{for} \quad x \in M_2 \cup M_3, \\ S^2 \cong \mathrm{SO}(3)/\mathrm{SO}(2) & \text{for} \quad x \in M_1, \\ \{0\} & \text{for} \quad x \in M_0. \end{cases} \tag{5}$$

According to the orbit types, M is stratified into strata:

$$M = \dot{M} \cup M_1 \cup M_0, \quad \dot{M} := M_2 \cup M_3. \tag{6}$$

On restricting M to $\dot{M} = M_2 \cup M_3$, we can make $\dot{M}$ into a principal fiber bundle $\dot{M} \rightarrow \dot{Q} := \dot{M}/\mathrm{SO}(3)$,[1] since SO(3) is compact and since SO(3) acts on $\dot{M}$ freely. However, the total space M cannot be made into a principal fiber bundle. The orbit space $Q := M/\mathrm{SO}(3)$ is not a manifold in general. In fact, in the case of the three-body system, the orbit space is homeomorphic with the closed half space of $\mathbf{R}^3$.[4] In the case of the four-body system, the orbit space is shown to be homeomorphic with $\mathbf{R}^6$.[8] Though M itself is not a principal fiber bundle, we may make M into a stratified fiber bundle with respective projections

$$\dot{M} \rightarrow \dot{M}/\mathrm{SO}(3), \quad M_1 \rightarrow M_1/S^2, \quad M_0 \rightarrow M_0/M_0. \tag{7}$$

It is to be noted that $\dot{M}$ and M_1 are viewed as the configuration spaces for "nonlinear molecules" and for "linear molecules," respectively. Equation (7) implies that we can discuss nonlinear and linear molecules separately, but on an equal footing from the viewpoint of transformation group theory.

It is of great use to employ Jacobi vectors in working with the center-of-mass system. The Jacobi vectors $\mathbf{r}_j$, $j = 1,\ldots,N-1$, are defined to be

$$\mathbf{r}_j := \left(\frac{1}{\mu_j} + \frac{1}{m_{j+1}}\right)^{-1/2} \left(\mathbf{x}_{j+1} - \frac{1}{\mu_j}\sum_{i=1}^{j} m_i \mathbf{x}_i\right), \quad \mu_j := \sum_{i=1}^{j} m_i. \tag{8}$$

Since the position vectors $\mathbf{x}_i$ in the center-of-mass system are uniquely described in terms of Jacobi vectors, we can identify the center-of-mass system with the set of collections of Jacobi vectors:

$$M \cong \{x = (\mathbf{r}_1, \ldots, \mathbf{r}_{N-1}) \mid \mathbf{r}_j \in \mathbf{R}^3, \quad j = 1,\ldots,N-1\}. \tag{9}$$

Thus, M is viewed as the linear space formed by $x=(\mathbf{r}_1,\ldots,\mathbf{r}_{N-1})$, or as the space of $3\times(N-1)$ matrices. Since $\operatorname{rank} x=\dim F_x$, we can regard $\dot{M}:=M_2\cup M_3$ as the space of $3\times(N-1)$ matrices of rank greater than or equal to two. M_1 and M_0 are the spaces of $3\times(N-1)$ matrices of rank 1 and of rank 0, respectively. The space of singular configurations, M_1 and M_0, forms the boundary of the space of nonsingular configurations, $M_2\cup M_3$. Note that $\dim\dot{M}=3N-3$, $\dim M_1=N+1$, and $\dim M_0=0$. We note, in conclusion, that the SO(3) action is expressed as

$$(\mathbf{r}_1,\ldots,\mathbf{r}_{N-1})\mapsto(g\mathbf{r}_1,\ldots,g\mathbf{r}_{N-1}). \tag{10}$$

III. FOURIER ANALYSIS OF WAVE FUNCTIONS

To treat wave functions irrespectively of the orbit type of the SO(3) action on the center-of-mass system, it is of great use to apply Fourier analysis on the basis of the Peter–Weyl theorem on unitary irreducible representations of compact Lie groups. To describe this method,[6,7] we put the problem in a general setting. Let M be a manifold on which a compact Lie group G acts. Let μ_M be a G-invariant measure on M. We take the space $L^2(M)$ of square integrable functions on M as the Hilbert space of wave functions, in which the G is represented unitarily through $(U(g)f)(x)=f(g^{-1}x)$, $g\in G$, $x\in M$.

Let μ_G and $L^2(G)$ denote the normalized invariant measure on G and the space of square integrable functions on G with respect to μ_G, respectively. Let $(\mathcal{H}^\chi,\rho^\chi)$ be irreducible unitary representations of G, where χ ranges over all the inequivalent representations. We denote by ρ^χ_{ij} the matrix elements of the representation ρ^χ with respect to some orthonormal basis e^χ_i of $\mathcal{H}^\chi$, where $i,j=1,\ldots,d_\chi$, with $d_\chi=\dim\mathcal{H}^\chi$. The Peter–Weyl theorem states that the set of all the matrix elements $\{\sqrt{d_\chi}\rho^\chi_{ij}\}_{\chi,i,j}$ forms a complete orthonormal system in $L^2(G)$. By this theorem, any function φ of $L^2(G)$ is expanded into

$$\varphi(h)=\sum_{\chi,i,j} d_\chi\rho^\chi_{ij}(h)\int_G\overline{\rho^\chi_{ij}(g)}\varphi(g)d\mu_G(g). \tag{11}$$

We turn to wave functions on M. For a function $f\in L^2(M)$, we may view $f(hx)$ as a function on G with x fixed arbitrarily, $f_x(h):=f(hx)$, and apply the above expansion to f_x to obtain

$$f(hx)=\sum_{\chi,i,j} d_\chi\rho^\chi_{ij}(h)\int_G\overline{\rho^\chi_{ij}(g)}f(gx)d\mu_G(g). \tag{12}$$

We here introduce the operators P^χ_{ij} and P^χ_i on $L^2(M)$ by

$$P^\chi_{ij}:=d_\chi\int_G\rho^\chi_{ij}(g)U(g)d\mu_G(g), \tag{13}$$

$$P^\chi_i:=P^\chi_{ii}, \tag{14}$$

respectively. These operators satisfy that

$$(P^\chi_{ij})^\dagger=P^\chi_{ji}, \quad P^\chi_{ij}P^{\chi'}_{k\ell}=\delta^{\chi\chi'}\delta_{jk}P^\chi_{i\ell}, \tag{15}$$

and

$$(P^\chi_i)^\dagger=P^\chi_i, \quad P^\chi_iP^{\chi'}_j=\delta^{\chi\chi'}\delta_{ij}P^\chi_i, \tag{16}$$

respectively. Moreover, one verifies that

$$(P^\chi_{ij})^\dagger P^\chi_{ij}=P^\chi_j, \quad P^\chi_{ij}(P^\chi_{ij})^\dagger=P^\chi_i. \tag{17}$$

It then follows that when restricted to $\mathrm{Im}\, P_j^\chi$, the P_{ij}^χ provides the unitary isomorphism

$$P_{ij}^\chi : \mathrm{Im}\, P_j^\chi \xrightarrow{\sim} \mathrm{Im}\, P_i^\chi . \tag{18}$$

Furthermore, we can show that P_{ij}^χ and $U(g)$ are put together to give

$$P_{ij}^\chi U(g) = \sum_k \rho_{kj}^\chi (g^{-1}) P_{ik}^\chi , \tag{19}$$

$$U(g) P_{ij}^\chi = \sum_k \rho_{ik}^\chi (g^{-1}) P_{kj}^\chi . \tag{20}$$

From (20), it turns out that the map $E_j^\chi : L^2(M) \to \mathcal{H}^\chi \otimes L^2(M)$ defined by

$$E_j^\chi := \frac{1}{\sqrt{d_\chi}} \sum_{i=1}^{d_\chi} e_i^\chi \otimes P_{ij}^\chi \tag{21}$$

satisfies $U(g^{-1}) E_j^\chi = \rho^\chi(g) E_j^\chi$, or equivalently

$$(E_j^\chi f)(gx) = \rho^\chi(g)(E_j^\chi f)(x), \quad f \in L^2(M), \tag{22}$$

which implies that the $\mathcal{H}^\chi$-valued function $E_j^\chi f$ is a ρ^χ-equivariant function.

We here introduce the space, $L^2(M;\mathcal{H}^\chi)^G$, of square integrable equivariant $\mathcal{H}^\chi$-valued functions by

$$L^2(M;\mathcal{H}^\chi)^G := \left\{ \psi : M \to \mathcal{H}^\chi \,\middle|\, \int_M \|\psi(x)\|^2 d\mu_M(x) < \infty,\ \psi(gx) = \rho^\chi(g)\psi(g) \right\}, \tag{23}$$

where $g \in G$, $x \in M$, and $\|\cdot\|$ denotes the norm in $\mathcal{H}^\chi$. Then we can view the operator E_j^χ as a map $L^2(M) \to L^2(M;\mathcal{H}^\chi)^G$. The adjoint operator $(E_j^\chi)^\dagger : L^2(M;\mathcal{H}^\chi)^G \to L^2(M)$ is defined, of course, through

$$\langle \psi, E_j^\chi f \rangle_{\mathcal{H}^\chi \otimes L^2(M)} = \langle (E_j^\chi)^\dagger \psi, f \rangle_{L^2(M)}, \quad \psi \in L^2(M;\mathcal{H}^\chi)^G, \quad f \in L^2(M), \tag{24}$$

where the subscripts $\mathcal{H}^\chi \otimes L^2(M)$ and $L^2(M)$ attached to $\langle \, , \rangle$ indicate the spaces on which the respective inner products are defined. Then one can observe that

$$(E_j^\chi)^\dagger E_j^\chi = P_j^\chi , \quad E_j^\chi (E_j^\chi)^\dagger = \mathrm{id}_{L^2(M;\mathcal{H}^\chi)^G} . \tag{25}$$

These relations imply that when restricted to $\mathrm{Im}\, P_j^\chi$, the E_j^χ provides a unitary isomorphism

$$E_j^\chi : \ \mathrm{Im}\, P_j^\chi \xrightarrow{\sim} L^2(M;\mathcal{H}^\chi)^G, \quad j = 1,\ldots,d_\chi . \tag{26}$$

We now apply the above-mentioned Fourier analysis to N-body systems. The manifold M we take is the center-of-mass system for N bodies. We introduce the Euler angles (ϕ, θ, ψ) through

$$g = e^{\phi R(\mathbf{e}_3)} e^{\theta R(\mathbf{e}_2)} e^{\psi R(\mathbf{e}_3)}, \quad g \in \mathrm{SO}(3), \tag{27}$$

where $\mathbf{e}_k$, $k = 1,2,3$, are the standard basis of $\mathbf{R}^3$ and $R(\mathbf{e}_k)$ denote the 3×3 antisymmetric matrices defined through $R(\mathbf{e}_k)\mathbf{a} = \mathbf{e}_k \times \mathbf{a}$ for $\mathbf{a} \in \mathbf{R}^3$. Let $D_{nm}^\ell(g)$ denote the matrix elements of unitary irreducible representations of SO(3) with $\ell = 0,1,2,\ldots$, and $|m|,|n| \leq \ell$.[9] They are expressed as

$$D^{\ell}_{nm}(g)=e^{-in\phi}d^{\ell}_{nm}(\theta)e^{-im\psi}, \tag{28}$$

where $d^{\ell}_{nm}(\theta)$ are given by

$$\begin{aligned} d^{\ell}_{nm}(\theta) &= (-1)^{n-m}\sqrt{(\ell+n)(\ell-n)(\ell+m)(\ell-m)} \\ &\times \sum_{k=0}^{\ell-m} \frac{(-1)^k}{k!(\ell-n-k)!(\ell+m-k)!(n-m+k)!}\left(\sin\frac{\theta}{2}\right)^{2k+n-m}\left(\cos\frac{\theta}{2}\right)^{2\ell-2k-(n-m)}. \end{aligned} \tag{29}$$

Let $d\mu(g)$ denote the invariant volume element on SO(3), which is expressed, in terms of the Euler angles, as

$$d\mu(g)=\sin\theta\, d\theta d\phi d\psi \quad \text{with} \quad \int_{\mathrm{SO}(3)} d\mu(g)=8\pi^2. \tag{30}$$

According to (12) with $\rho^{\chi}_{ij}=D^{\ell}_{mn}$, $d_{\chi}=2\ell+1$, and $d\mu_G(g)=d\mu(g)/(8\pi^2)$, a wave function $f(hx)$ on M is expanded into a Fourier series

$$f(hx)=\sum_{\ell=0}^{\infty}\sum_{|m|,|n|\le\ell}\frac{2\ell+1}{8\pi^2}D^{\ell}_{mn}(h)\int_{\mathrm{SO}(3)}\overline{D}^{\ell}_{mn}(g)f(gx)d\mu(g), \quad x\in M. \tag{31}$$

The map $E^{\ell}_m : L^2(M)\to\mathcal{H}^{\ell}\otimes L^2(M)$ is defined as in (21):

$$E^{\ell}_m f=\frac{1}{\sqrt{2\ell+1}}\sum_{|m'|\le\ell} e^{\ell}_{m'}\otimes P^{\ell}_{m'm}f, \tag{32}$$

where $e^{\ell}_{m'}$, denoted usually by $|\ell\, m'\rangle$, is the basis of the representation space $\mathcal{H}^{\ell}$. The ρ^{χ}-equivariance condition (22) now takes the form

$$(E^{\ell}_m f)(hx)=D^{\ell}(h)(E^{\ell}_m f)(x). \tag{33}$$

IV. NONSINGULAR CONFIGURATIONS

In this section, we make a brief review of the geometric setting-up for the nonsingular configurations.[4] We note first that the center-of-mass system is now identified with the set of collections of the Jacobi vectors [see (9)]. As is already mentioned, SO(3) acts on $\dot{M}$ freely, so that $\dot{M}$ is made into an SO(3) bundle,

$$\pi: \quad \dot{M}\to\dot{Q}:=\dot{M}/\mathrm{SO}(3). \tag{34}$$

The inertia tensor, $A_x: \ \mathbf{R}^3\to\mathbf{R}^3$, is defined for $x\in M$ through

$$A_x(\mathbf{v})=\sum_{j=1}^{N-1}\mathbf{r}_j\times(\mathbf{v}\times\mathbf{r}_j), \quad \mathbf{v}\in\mathbf{R}^3, \tag{35}$$

and the connection form ω is defined for $x\in\dot{M}$ to be

$$\omega_x=R\left(A_x^{-1}\left(\sum_{j=1}^{N-1}\mathbf{r}_j\times d\mathbf{r}_j\right)\right), \tag{36}$$

where $R:\mathbf{R}^3\rightarrow \mathrm{so}(3)$ is the isomorphism already mentioned in Sec. III. Note that A_x^{-1} exists only for $x\in\dot{M}$. The connection form ω gives rise to a direct sum decomposition of the tangent space to $\dot{M}$ at $x\in\dot{M}$,

$$T_x(\dot{M})=V_x\oplus H_x, \tag{37}$$

where $V_x:=T_x(\mathcal{O}_x)$ is the tangent space to the SO(3)-orbit $\mathcal{O}_x$ through $x\in\dot{M}$ and $H_x:=\ker\omega_x$ with $\omega_x:T_x(\dot{M})\rightarrow \mathrm{so}(3)$. Tangent vectors in V_x and in H_x are called rotational (or vertical) and vibrational (or horizontal), respectively. By definition, rotational vectors are put in the form $R(\mathbf{a})x$ with $\mathbf{a}\in\mathbf{R}^3$. In fact, for a one-parameter group of rotations $e^{tR(\mathbf{a})}$ acting on M, its infinitesimal generator is given by

$$\frac{d}{dt}e^{tR(\mathbf{a})}x\bigg|_{t=0}=R(\mathbf{a})x=(R(\mathbf{a})\mathbf{r}_1,\ldots,R(\mathbf{a})\mathbf{r}_{N-1}). \tag{38}$$

In contrast with this, the definition of H_x implies that

$$u=(\mathbf{u}_1,\ldots,\mathbf{u}_{N-1})\in H_x\Leftrightarrow \sum_{j=1}^{N-1}\mathbf{r}_j\times\mathbf{u}_j=0. \tag{39}$$

Further, it is easy to see that V_x and H_x are orthogonal to each other with respect to the metric

$$ds^2=\sum_{j=1}^{N-1}d\mathbf{r}_j\cdot d\mathbf{r}_j. \tag{40}$$

In fact, for $R(\mathbf{a})x\in V_x$ and $u\in H_x$, one has

$$\sum_j R(\mathbf{a})\mathbf{r}_j\cdot\mathbf{u}_j=\mathbf{a}\cdot\sum_j \mathbf{r}_j\times\mathbf{u}_j=0. \tag{41}$$

For a tangent vector $v=(\mathbf{v}_1,\ldots,\mathbf{v}_{N-1})\in T_x(\dot{M})$, its vertical components $P_x(v)=(P_x(v)_1,\ldots,P_x(v)_{N-1})\in V_x$ are given by

$$P_x(v)_j=\left(A_x^{-1}\left(\sum_{k=1}^{N-1}\mathbf{r}_k\times\mathbf{v}_k\right)\right)\times\mathbf{r}_j. \tag{42}$$

In what follows, we describe the connection form ω and the metric ds^2 in terms of local coordinates. Let σ be a local section defined on an open subset U of $\dot{Q}$, σ: $U\rightarrow\dot{M}$. Then any point $x\in\pi^{-1}(U)$ is expressed as

$$x=g\sigma(q)=(g\boldsymbol{\sigma}_1(q),\ldots,g\boldsymbol{\sigma}_{N-1}(q)),\quad q\in U. \tag{43}$$

Let $g\in\mathrm{SO}(3)$ and $q\in U$ be assigned by the Euler angles $(\theta,\ \phi,\ \psi)$ and by local coordinates q^α, $\alpha=1,\ldots,3N-6$, respectively. Then a straightforward calculation along with (36) and (43) provides

$$\omega_{g\sigma(q)}=dgg^{-1}+g\omega_{\sigma(q)}g^{-1}=g(g^{-1}dg+\omega_{\sigma(q)})g^{-1}, \tag{44}$$

where

$$\omega_{\sigma(q)}:=R\left(A_{\sigma(q)}^{-1}\left(\sum_{j=1}^{N-1}\boldsymbol{\sigma}_j(q)\times d\boldsymbol{\sigma}_j(q)\right)\right). \tag{45}$$

We here express $\omega_{\sigma(q)}$ as

$$\omega_{\sigma(q)}=\sum_{a=1}^{3}\sum_{\alpha=1}^{3N-6}\Lambda_{\alpha}^{a}(q)dq^{\alpha}R(\mathbf{e}_a), \tag{46}$$

and introduce a moving frame $\mathbf{u}_a$, $a=1,2,3$, and the left-invariant one-forms Ψ^a, $a=1,2,3$, on SO(3) by

$$\mathbf{u}_a=g\mathbf{e}_a, \tag{47}$$

$$g^{-1}dg=\sum_{a=1}^{3}\Psi^a R(\mathbf{e}_a), \tag{48}$$

respectively. Then the connection form ω given by (44) is put in the form

$$\omega_{g\sigma(q)}=\sum_a \Theta^a R(\mathbf{u}_a), \quad \Theta^a := \Psi^a+\sum_\alpha \Lambda_\alpha^a(q)dq^\alpha, \tag{49}$$

where we have used the formula $R(g\mathbf{e}_a)=gR(\mathbf{e}_a)g^{-1}$.

The horizontal lift, $(\partial/\partial q^\alpha)^*$, of a local vector field $\partial/\partial q^\alpha$ on U is defined through

$$\omega_{g\sigma(q)}\left(\left(\frac{\partial}{\partial q^\alpha}\right)^*\right)=0, \quad \pi_*\left(\left(\frac{\partial}{\partial q^\alpha}\right)^*\right)=\frac{\partial}{\partial q^\alpha}, \tag{50}$$

and proves to be given by

$$\left(\frac{\partial}{\partial q^\alpha}\right)^*=\frac{\partial}{\partial q^\alpha}-\sum_a \Lambda_\alpha^a(q)K_a, \quad \alpha=1,2,\ldots,3N-6, \tag{51}$$

where K_a are the left-invariant vector fields on SO(3), which are dual to Ψ^a:

$$\Psi^a(K_b)=\delta_b^a, \quad a,b=1,2,3. \tag{52}$$

The dq^α,Θ^a and the $(\partial/\partial q^\alpha)^*,K_a$ form local bases of one-forms and of vector fields on $\pi^{-1}(U)\cong U\times \mathrm{SO}(3)$, respectively, in accordance with the decomposition (37). They are dual to each other:

$$dq^\alpha\left(\left(\frac{\partial}{\partial q^\beta}\right)^*\right)=\delta_\beta^\alpha, \quad dq^\alpha(K_a)=0, \tag{53}$$

$$\Theta^a\left(\left(\frac{\partial}{\partial q^\alpha}\right)^*\right)=0, \quad \Theta^a(K_b)=\delta_b^a. \tag{54}$$

In contrast with left-invariant one-forms and vector fields, right-invariant one-forms Φ^a and vector fields J_a are defined through

$$dgg^{-1}=\sum_{a=1}^{3}\Phi^a R(\mathbf{e}_a), \tag{55}$$

$$\Phi^a(J_b)=\delta_b^a, \quad a,b=1,2,3, \tag{56}$$

respectively. Since $g(g^{-1}dg)g^{-1}=dgg^{-1}$, the right- and left-invariant one-forms are related to each other, and so are the right- and left-invariant vector fields,

$$\Phi^a = \sum_{b=1}^{3} g_{ab}\Psi^b, \quad J_a = \sum_{b=1}^{3} g_{ab} K_b, \tag{57}$$

where g_{ab} denote the matrix elements of g.

We here associate the vector fields K_a and J_a with the angular momentum operator. The infinitesimal rotation (38) is put in the form of operator,

$$\sum_{k=1}^{N-1} R(\mathbf{a})\mathbf{r}_k \cdot \frac{\partial}{\partial \mathbf{r}_k} = \mathbf{a} \cdot \left(\sum_{k=1}^{N-1} \mathbf{r}_k \times \frac{\partial}{\partial \mathbf{r}_k} \right) = \mathbf{a}\cdot\mathbf{J}, \tag{58}$$

where we have set

$$\mathbf{J} = \sum_{k=1}^{N-1} \mathbf{r}_k \times \frac{\partial}{\partial \mathbf{r}_k}. \tag{59}$$

Since one has, from (58) with $\mathbf{a} = \mathbf{e}_a$,

$$\mathbf{e}_a \cdot \mathbf{J} = \frac{d}{dt} e^{tR(\mathbf{e}_a)} x \Big|_{t=0} = \frac{d}{dt} e^{tR(\mathbf{e}_a)} g\sigma(q) \Big|_{t=0}, \tag{60}$$

$\mathbf{e}_a \cdot \mathbf{J}$ can be identified with the right-invariant vector fields J_a on SO(3), $J_a = \mathbf{e}_a \cdot \mathbf{J}$. Further, on account of (47) and (57), we obtain

$$\mathbf{J} = \sum_{a=1}^{3} \mathbf{e}_a J_a = \sum_{a=1}^{3} \mathbf{u}_a K_a. \tag{61}$$

The last equality of the above equation also means that

$$K_a = \mathbf{u}_a \cdot \mathbf{J} = \frac{d}{dt} e^{tR(\mathbf{u}_a)} x \Big|_{t=0} = \frac{d}{dt} g e^{tR(\mathbf{e}_a)} \sigma(q) \Big|_{t=0}. \tag{62}$$

This implies that K_a can be identified with an infinitesimal rotation with respect to the so-called body frame.

In terms of the Euler angles given by $g = e^{\phi R(\mathbf{e}_3)} e^{\theta R(\mathbf{e}_2)} e^{\psi R(\mathbf{e}_3)}$, the K_a and J_a and the Ψ^a and Φ^a are expressed, respectively, as

$$\begin{aligned} K_1 &= -\frac{\cos\psi}{\sin\theta}\frac{\partial}{\partial\phi} + \sin\psi\frac{\partial}{\partial\theta} + \cot\theta\cos\psi\frac{\partial}{\partial\psi}, \\ K_2 &= \frac{\sin\psi}{\sin\theta}\frac{\partial}{\partial\phi} + \cos\psi\frac{\partial}{\partial\theta} - \cot\theta\sin\psi\frac{\partial}{\partial\psi}, \\ K_3 &= \frac{\partial}{\partial\psi}, \end{aligned} \tag{63}$$

$$\begin{aligned} \Psi^1 &= \sin\psi\, d\theta - \sin\theta\cos\psi\, d\phi, \\ \Psi^2 &= \cos\psi\, d\theta + \sin\theta\sin\psi\, d\phi, \\ \Psi^3 &= d\psi + \cos\theta\, d\phi, \end{aligned} \tag{64}$$

$$J_1 = -\cos\phi \cot\theta \frac{\partial}{\partial\phi} - \sin\phi \frac{\partial}{\partial\theta} + \frac{\cos\phi}{\sin\theta}\frac{\partial}{\partial\psi},$$

$$J_2 = -\sin\phi \cot\theta \frac{\partial}{\partial\phi} + \cos\phi \frac{\partial}{\partial\theta} + \frac{\sin\phi}{\sin\theta}\frac{\partial}{\partial\psi}, \tag{65}$$

$$J_3 = \frac{\partial}{\partial\phi},$$

$$\Phi^1 = -\sin\phi\, d\theta + \sin\theta\cos\phi\, d\psi,$$

$$\Phi^2 = \cos\phi\, d\theta + \sin\theta\sin\phi\, d\psi, \tag{66}$$

$$\Phi^3 = d\phi + \cos\theta\, d\psi.$$

We now wish to express the metric (40) in terms of dq^α, Θ^a. We first note that the basis vector fields $(\partial/\partial q^\alpha)^*$, K_a are expressed also as

$$\left(\frac{\partial}{\partial q^\alpha}\right)^* = \sum_j \left(\frac{\partial}{\partial q^\alpha}\right)^* \mathbf{r}_j \cdot \frac{\partial}{\partial \mathbf{r}_j}, \quad K_a = \sum_j K_a \mathbf{r}_j \cdot \frac{\partial}{\partial \mathbf{r}_j}, \tag{67}$$

respectively. Since vibrational and rotational vectors are orthogonal to each other, one has

$$ds^2\left(\left(\frac{\partial}{\partial q^\alpha}\right)^*, K_a\right) = \sum_j \left(\frac{\partial}{\partial q^\alpha}\right)^* \mathbf{r}_j \cdot K_a \mathbf{r}_j = 0. \tag{68}$$

We further introduce the quantities $a_{\alpha\beta}$ and A_{ab} by

$$a_{\alpha\beta} := ds^2\left(\left(\frac{\partial}{\partial q^\alpha}\right)^*, \left(\frac{\partial}{\partial q^\beta}\right)^*\right) = \sum_j \left(\frac{\partial}{\partial q^\alpha}\right)^* \mathbf{r}_j \cdot \left(\frac{\partial}{\partial q^\beta}\right)^* \mathbf{r}_j, \tag{69}$$

$$A_{ab} := ds^2(K_a, K_b) = \sum_j K_a \mathbf{r}_j \cdot K_b \mathbf{r}_j. \tag{70}$$

Then the metric ds^2 is put in the form

$$ds^2 = \sum_{\alpha,\beta} a_{\alpha\beta} dq^\alpha dq^\beta + \sum_{a,b} A_{ab} \Theta^a \Theta^b. \tag{71}$$

Since $K_a \mathbf{r}_j = \mathbf{u}_a \times \mathbf{r}_j = g(\mathbf{e}_a \times \boldsymbol{\sigma}_j(q))$, one obtains, from (51),

$$\left(\frac{\partial}{\partial q^\alpha}\right)^* \mathbf{r}_j = g\left(\frac{\partial \boldsymbol{\sigma}_j(q)}{\partial q^\alpha} - \sum_a \Lambda^a_\alpha(q)(\mathbf{e}_a \times \boldsymbol{\sigma}_j(q))\right), \tag{72}$$

and then the quantities $a_{\alpha\beta}$ and A_{ab} are put, respectively, in the form

$$a_{\alpha\beta} = \sum_j \left(\frac{\partial \boldsymbol{\sigma}_j}{\partial q^\alpha} - \sum_a \Lambda^a_\alpha(q)(\mathbf{e}_a \times \boldsymbol{\sigma}_j)\right) \cdot \left(\frac{\partial \boldsymbol{\sigma}_j}{\partial q^\beta} - \sum_b \Lambda^b_\beta(q)(\mathbf{e}_b \times \boldsymbol{\sigma}_j)\right), \tag{73}$$

$$A_{ab} = \sum_j (\mathbf{u}_a \times \mathbf{r}_j) \cdot (\mathbf{u}_b \times \mathbf{r}_j) = \mathbf{u}_a \cdot A_x(\mathbf{u}_b) = \mathbf{e}_a \cdot A_{\sigma(q)}(\mathbf{e}_b). \tag{74}$$

In the remainder of this section, we consider the transformation law for local expressions of the connection form. Let $\tau: V \to \dot{M}$ be another local section defined on an open subset V with $V \cap U \neq \emptyset$. Then the local sections τ and σ are related by $\tau(q) = k(q)\sigma(q), q \in V \cap U$ with $k(q) \in \mathrm{SO}(3)$. From (44), it follows that

$$\omega_{\tau(q)} = dkk^{-1} + k\omega_{\sigma(q)}k^{-1}. \tag{75}$$

Like (46), we describe the connection form $\omega_{\tau(q)}$ as

$$\omega_{\tau(q)} = \sum_a \sum_\alpha \tilde{\Lambda}^a_\alpha(q) dq^\alpha R(\mathbf{e}_a). \tag{76}$$

Then the transformation law (75) brings about

$$\sum_\alpha \tilde{\Lambda}^a_\alpha dq^\alpha = \Phi^a(k) + \sum_b k_{ab} \sum_\alpha \Lambda^b_\alpha dq^\alpha, \tag{77}$$

where $\Phi^a(k)$ are defined through $dkk^{-1} = \Sigma_a \Phi^a(k) R(\mathbf{e}_a)$ and k_{ab} denote the components of $k \in \mathrm{SO}(3)$. Furthermore, we note that the inertia tensor is subject to the transformation $A_{hx} = hA_x h^{-1}$ for any $h \in \mathrm{SO}(3)$, so that the components (A_{ab}) transform according to

$$\tilde{A}_{ab} = \sum_{c,d} k_{ad} A_{dc} k_{bc}, \quad k = (k_{ab}), \tag{78}$$

where

$$\tilde{A}_{ab} = \mathbf{e}_a \cdot A_{\tau(q)}(\mathbf{e}_b). \tag{79}$$

We note also that since the metric ds^2 is SO(3)-invariant, $a_{\alpha\beta}$ are defined independently of the choice of sections, so that the $(a_{\alpha\beta})$ defines a metric tensor on $U \subset \dot{Q}$.

V. KINETIC ENERGY OPERATOR FOR NONSINGULAR CONFIGURATIONS

In this section, we study the kinetic energy operator for nonsingular configurations by using the setup stated in Secs. III and IV, and obtain a reduced kinetic energy operator which is defined on $\dot{Q}$. We begin by considering the gradient vector

$$\nabla = \left(\frac{\partial}{\partial \mathbf{r}_1}, \ldots, \frac{\partial}{\partial \mathbf{r}_{N-1}} \right). \tag{80}$$

For a smooth wave function f, we regard ∇f as a tangent vector to $\dot{M}$, and decompose ∇f according to (37):

$$\nabla f = (\nabla f)_{\mathrm{rot}} + (\nabla f)_{\mathrm{vib}}. \tag{81}$$

The rotational vector $(\nabla f)_{\mathrm{rot}}$ is given by $(\nabla f)_{\mathrm{rot}} := P_x(\nabla f)$, so that its components are expressed, on using (42) with $\mathbf{v}_k = \partial f / \partial \mathbf{r}_k$, as

$$\begin{aligned} P_x(\nabla f)_j &= \left(A_x^{-1} \left(\sum_k \mathbf{r}_k \times \frac{\partial f}{\partial \mathbf{r}_k} \right) \right) \times \mathbf{r}_j \\ &= (A_x^{-1}(\mathbf{J} f)) \times \mathbf{r}_j \\ &= \left(A_x^{-1} \left(\sum_a \mathbf{u}_a K_a f \right) \right) \times \mathbf{r}_j \\ &= \sum_a ((A_x^{-1}(\mathbf{u}_a)) \times \mathbf{r}_j) K_a f. \end{aligned} \tag{82}$$

Then $(\nabla f)_{\mathrm{rot}}$ turns out to have the components

$$\left(\frac{\partial f}{\partial \mathbf{r}_j}\right)_{\mathrm{rot}}=\sum_{a=1}^{3}\mathbf{t}_j^a K_a f,\quad \mathbf{t}_j^a:=A_x^{-1}(\mathbf{u}_a)\times\mathbf{r}_j,\quad j=1,\ldots,N-1. \tag{83}$$

In contrast with this, the components of $(\nabla f)_{\mathrm{vib}}$ can be put in the form

$$\left(\frac{\partial f}{\partial \mathbf{r}_j}\right)_{\mathrm{vib}}=\sum_{\alpha=1}^{3N-6}\mathbf{v}_j^\alpha\left(\frac{\partial}{\partial q^\alpha}\right)^* f,\quad j=1,\ldots,N-1, \tag{84}$$

where the vectors $\mathbf{v}_j^\alpha$ will be determined as follows: From (67) along with the decomposition $\partial/\partial\mathbf{r}_j=(\partial/\partial\mathbf{r}_j)_{\mathrm{rot}}+(\partial/\partial\mathbf{r}_j)_{\mathrm{vib}}$, the basis tangent vectors can be expressed as

$$K_a=\sum_j K_a\mathbf{r}_j\cdot\left(\sum_b \mathbf{t}_j^b K_b+\sum_\alpha \mathbf{v}_j^\alpha\left(\frac{\partial}{\partial q^\alpha}\right)^*\right), \tag{85}$$

$$\left(\frac{\partial}{\partial q^\beta}\right)^*=\sum_j \left(\frac{\partial}{\partial q^\beta}\right)^*\mathbf{r}_j\cdot\left(\sum_b \mathbf{t}_j^b K_b+\sum_\alpha \mathbf{v}_j^\alpha\left(\frac{\partial}{\partial q^\alpha}\right)^*\right). \tag{86}$$

These equations provide

$$\sum_j K_a\mathbf{r}_j\cdot\mathbf{t}_j^b=\delta_a^b,\quad \sum_j \left(\frac{\partial}{\partial q^\alpha}\right)^*\mathbf{r}_j\cdot\mathbf{t}_j^b=0, \tag{87}$$

$$\sum_j K_a\mathbf{r}_j\cdot\mathbf{v}_j^\alpha=0,\quad \sum_j \left(\frac{\partial}{\partial q^\beta}\right)^*\mathbf{r}_j\cdot\mathbf{v}_j^\alpha=\delta_\beta^\alpha. \tag{88}$$

Equations (88) are used to determine $\mathbf{v}_j^\alpha$ or the vectors $v^\alpha:=\Sigma_j\mathbf{v}_j^\alpha\cdot(\partial/\partial\mathbf{r}_j)$. It then turns out that v^α are expressed as

$$v^\alpha=\sum_\beta a^{\alpha\beta}\left(\frac{\partial}{\partial q^\beta}\right)^*, \tag{89}$$

or

$$\mathbf{v}_j^\alpha=v^\alpha\mathbf{r}_j=\sum_\beta a^{\alpha\beta}\left(\frac{\partial}{\partial q^\beta}\right)^*\mathbf{r}_j, \tag{90}$$

where

$$(a^{\alpha\beta}):=(a_{\alpha\beta})^{-1}. \tag{91}$$

In addition, it is easy to show that

$$\sum_j \mathbf{t}_j^a\cdot\mathbf{t}_j^b=A^{ab}, \tag{92}$$

$$\sum_j \mathbf{t}_j^a\cdot\mathbf{v}_j^\alpha=0, \tag{93}$$

$$\sum_j \mathbf{v}_j^\alpha\cdot\mathbf{v}_j^\beta=a^{\alpha\beta}, \tag{94}$$

where

$$A^{ab} := \mathbf{u}_a \cdot A_x^{-1}(\mathbf{u}_b) = \mathbf{e}_a \cdot A_{\sigma(q)}^{-1}(\mathbf{e}_b). \tag{95}$$

It is to be noted that A_x^{-1} is defined only for $x \in \dot{M}$.

We are now in a position to study the kinetic energy operator. The kinetic energy integral of our N-body system is given by

$$T = \frac{1}{2} \int_M \sum_j \overline{\frac{\partial f}{\partial \mathbf{r}_j}} \cdot \frac{\partial f}{\partial \mathbf{r}_j} dV, \tag{96}$$

where dV is the standard volume element of M. The energy operator, which is equal to $-\frac{1}{2}$ times the Laplacian Δ, is defined through integration by part as follows:

$$T = \int_M \bar{f} \left(-\frac{1}{2} \sum_j \left(\frac{\partial}{\partial \mathbf{r}_j} \right)^2 f \right) dV = \int_M \bar{f} \left(-\frac{1}{2} \Delta f \right) dV, \tag{97}$$

where f is assumed to be a smooth function with compact support. According to the orthogonal decomposition, $\nabla = \nabla_{\mathrm{rot}} + \nabla_{\mathrm{vib}}$, of the gradient operator, the kinetic energy is also broken up into rotational and vibrational energies,

$$T = T_{\mathrm{rot}} + T_{\mathrm{vib}}, \tag{98}$$

where

$$T_{\mathrm{rot}} = \frac{1}{2} \int_M \sum_j \left(\overline{\frac{\partial f}{\partial \mathbf{r}_j}} \right)_{\mathrm{rot}} \cdot \left(\frac{\partial f}{\partial \mathbf{r}_j} \right)_{\mathrm{rot}} dV, \tag{99}$$

$$T_{\mathrm{vib}} = \frac{1}{2} \int_M \sum_j \left(\overline{\frac{\partial f}{\partial \mathbf{r}_j}} \right)_{\mathrm{vib}} \cdot \left(\frac{\partial f}{\partial \mathbf{r}_j} \right)_{\mathrm{vib}} dV. \tag{100}$$

The rotational and vibrational energy operators will be defined by carrying out the integration by part for the energy integrals T_{rot} and T_{vib}, respectively. Accordingly, the Laplacian Δ is broken up into two,

$$\Delta = \Delta_{\mathrm{rot}} + \Delta_{\mathrm{vib}}. \tag{101}$$

We wish to express Δ_{rot} and Δ_{vib} in terms of local coordinates. From (71) together with (49), the volume element dV proves to be expressed as

$$dV = dQ \wedge d\mu(g), \tag{102}$$

where

$$dQ = \rho(q) dq^1 \wedge \cdots \wedge dq^{3N-6}, \tag{103}$$

$$\rho(q) = \sqrt{\det(A_{ab}) \det(a_{\alpha\beta})}, \tag{104}$$

$$d\mu(g) = \Psi^1 \wedge \Psi^2 \wedge \Psi^3 = \sin\theta d\theta \wedge d\phi \wedge d\psi. \tag{105}$$

By using (83) and (92) and performing integration by part, we obtain

$$T_{\mathrm{rot}} = \frac{1}{2} \int_M \sum_j \sum_a \mathbf{t}_j^a \overline{K_a f} \cdot \sum_b \mathbf{t}_j^b K_b f \, dV = -\frac{1}{2} \int_M \bar{f} \sum_{a,b} K_a (A^{ab} K_b f) \, dV, \tag{106}$$

where we have used the fact that K_a are volume-preserving operators on SO(3). In the same manner, it follows from (84) and (94) that

$$T_{\mathrm{vib}}=\frac{1}{2}\int_M \sum_j \sum_\alpha \overline{\mathbf{v}_j^\alpha \left(\frac{\partial}{\partial q^\alpha}\right)^* f}\cdot \sum_\beta \mathbf{v}_j^\beta \left(\frac{\partial}{\partial q^\beta}\right)^* f\, dV$$

$$=-\frac{1}{2}\int_M \overline{f}\frac{1}{\rho(q)}\sum_{\alpha,\beta}\left(\frac{\partial}{\partial q^\alpha}\right)^*\left(a^{\alpha\beta}\rho(q)\left(\frac{\partial}{\partial q^\beta}\right)^* f\right) dV. \tag{107}$$

Thus we have found the respective expressions of Δ_{rot} and Δ_{vib}:

$$\Delta_{\mathrm{rot}}=\sum_{a,b} K_a(A^{ab}K_b), \tag{108}$$

$$\Delta_{\mathrm{vib}}=\frac{1}{\rho(q)}\sum_{\alpha,\beta}\left(\frac{\partial}{\partial q^\alpha}\right)^*\left(a^{\alpha\beta}\rho(q)\left(\frac{\partial}{\partial q^\beta}\right)^*\right). \tag{109}$$

Note that these operators fail to be defined at singular configurations. In fact, for singular configurations, one has $\det(A_{ab})=0$, so that A^{ab} is not defined, and further $\rho(q)=0$.

In the remainder of this section, we show that the rotational and vibrational energy operators, $-\frac{1}{2}\Delta_{\mathrm{rot}}$ and $-\frac{1}{2}\Delta_{\mathrm{vib}}$, will reduce to operators acting on wave functions of internal variables (q^α). To this end, we restrict ourselves to the subspace $\mathrm{Im}\, P_m^\ell$ of $L^2(M)$. Then we obtain, from (26),

$$\langle P_m^\ell f_1, P_m^\ell f_2\rangle_{L^2(M)}=\int_M \langle E_m^\ell f_1, E_m^\ell f_2\rangle_{\mathcal{H}^\ell} dV, \quad f_1, f_2\in L^2(M), \tag{110}$$

where we have used the fact that $E_m^\ell P_m^\ell f=E_m^\ell f$, and $\langle\, ,\, \rangle_{\mathcal{H}^\ell}$ denotes the inner product on the representation space $\mathcal{H}^\ell$ assigned by ℓ. From (33) together with (43), one finds that the $\mathcal{H}^\ell$-valued function $E_m^\ell f$ is locally expressed as

$$(E_m^\ell f)(g\sigma(q))=D^\ell(g)(E_m^\ell f)(\sigma(q)). \tag{111}$$

If f has a compact support in $\pi^{-1}(U)$, Eq. (110) becomes

$$\langle P_m^\ell f_1, P_m^\ell f_2\rangle_{L^2(M)}=8\pi^2\int_{\dot{Q}}\langle (E_m^\ell f_1)(\sigma(q)),(E_m^\ell f_2)(\sigma(q))\rangle_{\mathcal{H}^\ell} dQ, \tag{112}$$

where we have used the fact that $D^\ell(g)$ is a unitary matrix. This equation means that we may view $(E_m^\ell f)(\sigma(q))$ as a (locally defined) $\mathcal{H}^\ell$-valued wave function on the internal space $\dot{Q}$. If f is smooth enough, the projection operator $P_{m'm}^\ell$ and a differential operator such as $(\partial/\partial q^\alpha)^*$ commute, so that we obtain

$$E_m^\ell\left(\frac{\partial}{\partial q^\alpha}\right)^* f=\left(\mathrm{id}_{\mathcal{H}^\ell}\otimes\left(\frac{\partial}{\partial q^\alpha}\right)^*\right)E_m^\ell f, \tag{113}$$

where $\mathrm{id}_{\mathcal{H}^\ell}$ denotes the identity of $\mathcal{H}^\ell$. The right-hand side of this equation means that we may differentiate $E_m^\ell f$ componentwise. We recall here that the operator K_a acts on the D-functions[10] as

$$K_a D^\ell(g)=-iD^\ell(g)[\hat{J}_a^{(\ell)}], \tag{114}$$

where $\hat{J}_a$ are the angular momentum operators defined to be $\hat{J}_a=-iJ_a$, and $[\hat{J}_a^{(\ell)}]$ denote their representation matrices which are, as usual, given by

$$[\hat{J}_1^{(\ell)}]_{m-1\,m}=\frac{1}{2}\sqrt{(\ell+m)(\ell-m+1)},\quad [\hat{J}_1^{(\ell)}]_{m+1\,m}=\frac{1}{2}\sqrt{(\ell-m)(\ell+m+1)},$$

$$[\hat{J}_2^{(\ell)}]_{m-1\,m}=-\frac{1}{2i}\sqrt{(\ell+m)(\ell-m+1)},\quad [\hat{J}_2^{(\ell)}]_{m+1\,m}=\frac{1}{2i}\sqrt{(\ell-m)(\ell+m+1)},\tag{115}$$

$$[\hat{J}_3^{(\ell)}]_{mm}=m,\qquad \text{the others vanishing.}$$

Operating on $D^\ell(g)(E_m^\ell f)(\sigma(q))$ with $\mathrm{id}_{\mathcal{H}^\ell}\otimes(\partial/\partial q^\alpha)^*$ and using (114), we obtain

$$\left(\mathrm{id}_{\mathcal{H}^\ell}\otimes\left(\frac{\partial}{\partial q^\alpha}\right)^*\right)D^\ell(g)(E_m^\ell f)(\sigma(q))=D^\ell(g)\nabla_\alpha(E_m^\ell f)(\sigma(q)),\tag{116}$$

where

$$\nabla_\alpha=I_{2\ell+1}\otimes\frac{\partial}{\partial q^\alpha}+i\sum_a \Lambda_\alpha^a(q)[\hat{J}_a^{(\ell)}],\tag{117}$$

and $I_{2\ell+1}$ denotes the $(2\ell+1)\times(2\ell+1)$ identity matrix.

We have to point out that the operators ∇_α may be defined independently of the choice of local sections. We recall here that the $\dot{M}$ is made into the fiber bundle (34). Take a representation space $\mathcal{H}^\ell\cong\mathbf{C}^{2\ell+1}$ of SO(3). Then the associated complex vector bundle is defined to be $\dot{M}\times_\ell\mathcal{H}^\ell:=(\dot{M}\times\mathcal{H}^\ell)/\mathrm{SO}(3)$, where the SO(3) action on the product space $\dot{M}\times\mathcal{H}^\ell$ is defined by $(gx,D^\ell(g)v)$ for $(x,v)\in\dot{M}\times\mathcal{H}^\ell$. The space of equivariant functions on $\dot{M}$ is in one-to-one correspondence with the space of sections in $\dot{M}\times_\ell\mathcal{H}^\ell$; $s(\pi(x))=[(x,F(x))]$, where s and F are a section and an equivariant function, respectively, and $[\,\cdot\,]$ denotes the equivalence class. We denote this correspondence by $s=\gamma F$. For a local section σ in $\dot{M}$ and the equivariant function $E_m^\ell f$, one has $[(x,(E_m^\ell f)(x))]=[(\sigma(q),(E_m^\ell f)(\sigma(q)))]$, which means that $(E_m^\ell f)(\sigma(q))$ serves as a local expression of the section $s(\pi(x))=[(x,(E_m^\ell f)(x))]$. For a section s in $\dot{M}\times_\ell\mathcal{H}^\ell$, the covariant derivative of s with respect to a vector field X on $\dot{Q}=\dot{M}/\mathrm{SO}(3)$ is defined by

$$\nabla_X s=\gamma X^*(\gamma^{-1}s),\tag{118}$$

where X^* denotes the horizontal lift of X. Equation (117) is a local expression of the covariant differential operator with respect to $\partial/\partial q^\alpha$.

For confirmation, we show that locally defined operators (117) can be pieced together to define an operator independently of the choice of sections. For another local section τ in $\dot{M}$, we have another local expression $(E_m^\ell f)(\tau(q))$ of the section $s(\pi(x))=[(x,(E_m^\ell f)(x))]$. The locally defined $\mathcal{H}^\ell$-valued functions $(E_m^\ell f)(\tau(q))$ and $(E_m^\ell f)(\sigma(q))$ are related by the gauge transformation

$$(E_m^\ell f)(\tau(q))=D^\ell(k(q))(E_m^\ell f)(\sigma(q)),\quad q\in V\cap U.\tag{119}$$

For $(E_m^\ell f)(\tau(q))$, we have the covariant differential operator, instead of (117),

$$\tilde{\nabla}_\alpha=I_{2\ell+1}\otimes\frac{\partial}{\partial q^\alpha}+i\sum_a \tilde{\Lambda}_\alpha^a(q)[\hat{J}_a^{(\ell)}].\tag{120}$$

We show that the locally defined covariant differential operators, ∇_α and $\tilde{\nabla}_\alpha$, are subject to the transformation law

$$\tilde{\nabla}_\alpha(E_m^\ell f)(\tau(q))=D^\ell(k(q))\nabla_\alpha(E_m^\ell f)(\sigma(q)),\tag{121}$$

or, equivalently,

$$\sum_{\alpha} \tilde{\nabla}_{\alpha}(E_m^{\ell} f)(\tau(q))dq^{\alpha} = D^{\ell}(k(q)) \sum_{\alpha} \nabla_{\alpha}(E_m^{\ell} f)(\sigma(q))dq^{\alpha}. \tag{122}$$

The transformation law (121) shows that locally defined covariant differential operators are pieced together to define a covariant differential operator acting on sections in $\dot{M} \times_{\ell} \mathcal{H}^{\ell}$;

$$[(\sigma(q), \nabla_{\alpha}(E_m^{\ell} f)(\sigma(q)))] = [(\tau(q), \tilde{\nabla}_{\alpha}(E_m^{\ell} f)(\tau(q)))]. \tag{123}$$

To prove (122), we need some formulas on D-functions. In contrast with (114), we have the formula[10]

$$J_a D^{\ell}(g) = -i[\hat{J}_a^{(\ell)}] D^{\ell}(g). \tag{124}$$

From (114) and (124) together with (57), we obtain the formula

$$[\hat{J}_a^{(\ell)}] D^{\ell}(g) = \sum_{b} g_{ab} D^{\ell}(g)[\hat{J}_b^{(\ell)}]. \tag{125}$$

Using the transformation law (77) along with the above formulas and the equation

$$dD^{\ell}(k) = \sum_{a} K_a D^{\ell}(k) \Psi^a(k), \tag{126}$$

we can verify (122) in a straightforward manner.

We proceed to the operators Δ_{rot} and Δ_{vib}. Operating on $D^{\ell}(g)(E_m^{\ell} f)(\sigma(q))$ with $\mathrm{id}_{\mathcal{H}^{\ell}} \otimes \Delta_{\mathrm{rot}}$ and $\mathrm{id}_{\mathcal{H}^{\ell}} \otimes \Delta_{\mathrm{vib}}$, we obtain

$$(\mathrm{id}_{\mathcal{H}^{\ell}} \otimes \Delta_{\mathrm{rot}}) D^{\ell}(g)(E_m^{\ell} f)(\sigma(q)) = -D^{\ell}(g) \sum_{a,b} A^{ab}[\hat{J}_a^{(\ell)}][\hat{J}_b^{(\ell)}](E_m^{\ell} f)(\sigma(q)), \tag{127}$$

$$(\mathrm{id}_{\mathcal{H}^{\ell}} \otimes \Delta_{\mathrm{vib}}) D^{\ell}(g)(E_m^{\ell} f)(\sigma(q)) = D^{\ell}(g) \frac{1}{\rho(q)} \sum_{\alpha,\beta} \nabla_{\alpha}(a^{\alpha\beta} \rho(q) \nabla_{\beta}(E_m^{\ell} f)(\sigma(q))), \tag{128}$$

respectively. From these equations, it turns out that the Laplacian $\Delta = \Delta_{\mathrm{vib}} + \Delta_{\mathrm{rot}}$ reduces to the operator acting on vector-valued wave functions $(E_m^{\ell} f)(\sigma(q))$,

$$\Delta^{\mathrm{red}} := \frac{1}{\rho(q)} \sum_{\alpha,\beta} \nabla_{\alpha}(a^{\alpha\beta} \rho(q) \nabla_{\beta}) - \sum_{a,b} A^{ab}[\hat{J}_a^{(\ell)}][\hat{J}_b^{(\ell)}]. \tag{129}$$

We here have to mention the transformation law for the locally defined reduced Laplacians. For $(E_m^{\ell} f)(\tau(q))$, we have the reduced Laplacian expressed as

$$\tilde{\Delta}^{\mathrm{red}} := \frac{1}{\rho(q)} \sum_{\alpha,\beta} \tilde{\nabla}_{\alpha}(a^{\alpha\beta} \rho(q) \tilde{\nabla}_{\beta}) - \sum_{a,b} \tilde{A}^{ab}[\hat{J}_a^{(\ell)}][\hat{J}_b^{(\ell)}]. \tag{130}$$

Using the transformation law (78) and the formula (125) in addition to (121), we can also show that $\tilde{\Delta}^{\mathrm{red}}$ and Δ^{red} are related by

$$\tilde{\Delta}^{\mathrm{red}}(E_m^{\ell} f)(\tau(q)) = D^{\ell}(k(q)) \Delta^{\mathrm{red}}(E_m^{\ell} f)(\sigma(q)). \tag{131}$$

Thus we obtain the following.

Theorem 1: For nonsingular configurations, the Laplacian reduces to an operator acting on the sections in the associated vector bundle $\dot{M}\times_{\ell}\mathcal{H}^{\ell}$, which is expressed locally as Δ^{red} given by (129) or $\tilde{\Delta}^{\mathrm{red}}$ given by (130) according to the choice of local sections in $\dot{M}\to\dot{Q}$. The reduced local operators Δ^{red} and $\tilde{\Delta}^{\mathrm{red}}$ are subject to the transformation law (131).

VI. THREE-BODY SYSTEMS

Our aim in this section is to show that in spite of the singularity of Δ_{rot} and Δ_{vib} at singular configurations, the rotational and vibrational energy integrals are not divergent at singular configurations. To this end, we need to understand the detailed behavior of wave functions at singular configurations. For this reason, we specialize in three-body systems for simplicity. Let us introduce internal coordinates $(\zeta_1,\zeta_2,\zeta_3)$ by

$$\zeta_1=r_1,\quad \zeta_2=r_2\cos\varphi,\quad \zeta_3=r_2\sin\varphi, \tag{132}$$

where

$$r_1=\|\mathbf{r}_1\|,\quad r_2=\|\mathbf{r}_2\|,\quad \mathbf{r}_1\cdot\mathbf{r}_2=r_1r_2\cos\varphi. \tag{133}$$

Using ζ_α, $\alpha=1,2,3$, we define a local section σ by

$$\boldsymbol{\sigma}_1(q)=\zeta_1\mathbf{e}_3,\quad \boldsymbol{\sigma}_2(q)=\zeta_2\mathbf{e}_3+\zeta_3\mathbf{e}_1. \tag{134}$$

We note here that the local section σ is defined originally on an open subset U of $\dot{Q}=\dot{M}/\mathrm{SO}(3)$. If we are strict in using the term "local section," we must pose the restriction that $\zeta_1>0$ and $\zeta_3>0$ to identify the open subset U. However, $(\zeta_1,\zeta_2,\zeta_3)$ can serve as local coordinates beyond U,

$$\{(\zeta_1,\zeta_2,\zeta_3)|\ \zeta_1\geqslant 0,\zeta_3\geqslant 0\}. \tag{135}$$

The coordinates $(\zeta_1,\zeta_2,\zeta_3)$ work well in the orbit space $M/\mathrm{SO}(3)$ for describing singular configurations. In fact, we have collinear configurations if $\zeta_3=0$, and the configurations that two of three particles collide but the remainder is separate, if $\zeta_1=0$. If $\zeta_1=\zeta_2=\zeta_3=0$, we have a triple collision. With this interpretation, we are allowed to make ζ_3 tend to zero, for example.

From the definition (74) along with (134), the inertia tensor and its inverse at $\sigma(q)$ are put, respectively, in the form

$$(A_{ab})=\begin{pmatrix}\zeta_1^2+\zeta_2^2 & 0 & -\zeta_2\zeta_3\\ 0 & \zeta_1^2+\zeta_2^2+\zeta_3^2 & 0\\ -\zeta_2\zeta_3 & 0 & \zeta_3^2\end{pmatrix}, \tag{136}$$

$$(A^{ab})=\begin{pmatrix}\dfrac{1}{\zeta_1^2} & 0 & \dfrac{\zeta_2}{\zeta_1^2\zeta_3}\\ 0 & \dfrac{1}{\zeta_1^2+\zeta_2^2+\zeta_3^2} & 0\\ \dfrac{\zeta_2}{\zeta_1^2\zeta_3} & 0 & \dfrac{\zeta_1^2+\zeta_2^2}{\zeta_1^2\zeta_3^2}\end{pmatrix}. \tag{137}$$

From (45), (134), and (137), the connection form proves to be expressed as

$$\omega_{\sigma(q)}=\frac{\zeta_2d\zeta_3-\zeta_3d\zeta_2}{\zeta_1^2+\zeta_2^2+\zeta_3^2}R(\mathbf{e}_2). \tag{138}$$

From (51) together with (138), the horizontal lifts of $\partial/\partial\zeta_\alpha$ are given by

$$\left(\frac{\partial}{\partial\zeta_1}\right)^* = \frac{\partial}{\partial\zeta_1},$$
$$\left(\frac{\partial}{\partial\zeta_2}\right)^* = \frac{\partial}{\partial\zeta_2} + \frac{\zeta_3}{\zeta_1^2+\zeta_2^2+\zeta_3^2}K_2, \tag{139}$$
$$\left(\frac{\partial}{\partial\zeta_3}\right)^* = \frac{\partial}{\partial\zeta_3} - \frac{\zeta_2}{\zeta_1^2+\zeta_2^2+\zeta_3^2}K_2.$$

From (73) and (139), the metric tensor and its inverse are calculated, respectively, as

$$(a_{\alpha\beta}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \dfrac{\zeta_1^2+\zeta_2^2}{\zeta_1^2+\zeta_2^2+\zeta_3^2} & \dfrac{\zeta_2\zeta_3}{\zeta_1^2+\zeta_2^2+\zeta_3^2} \\ 0 & \dfrac{\zeta_2\zeta_3}{\zeta_1^2+\zeta_2^2+\zeta_3^2} & \dfrac{\zeta_1^2+\zeta_3^2}{\zeta_1^2+\zeta_2^2+\zeta_3^2} \end{pmatrix}, \tag{140}$$

$$(a^{\alpha\beta}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \dfrac{\zeta_1^2+\zeta_3^2}{\zeta_1^2} & -\dfrac{\zeta_2\zeta_3}{\zeta_1^2} \\ 0 & -\dfrac{\zeta_2\zeta_3}{\zeta_1^2} & \dfrac{\zeta_1^2+\zeta_2^2}{\zeta_1^2} \end{pmatrix}. \tag{141}$$

Further, the volume density $\rho(q)$ given in (104) is expressed as

$$\rho(q) = \zeta_1^2\zeta_3. \tag{142}$$

Thus we have obtained all the quantities needed for expressing the rotational and the vibrational energy operators given by (108) and (109), respectively. The resultant expression looks singular at the singular configurations, i.e., at the triple collision, $\zeta_1=\zeta_2=\zeta_3=0$, and at the collinear configuration, $\zeta_1=0$ or $\zeta_3=0$.

To investigate how singular the operators are at singular configurations, we treat the rotational and the vibrational energy integrals in detail. The vibrational energy integral for the three-body system is expressed as

$$T_{\mathrm{vib}} = \frac{1}{2}\int_M \Bigg(\left(\left|\frac{\partial f}{\partial\zeta_1}\right|^2 + \frac{\zeta_1^2+\zeta_3^2}{\zeta_1^2}\left|\left(\frac{\partial}{\partial\zeta_2}\right)^* f\right|^2 + \frac{\zeta_1^2+\zeta_2^2}{\zeta_1^2}\left|\left(\frac{\partial}{\partial\zeta_3}\right)^* f\right|^2 - \frac{\zeta_2\zeta_3}{\zeta_1^2}\left(\overline{\left(\frac{\partial}{\partial\zeta_2}\right)^* f}\left(\frac{\partial}{\partial\zeta_3}\right)^* f \right.\right.$$
$$\left.\left. + \overline{\left(\frac{\partial}{\partial\zeta_3}\right)^* f}\left(\frac{\partial}{\partial\zeta_2}\right)^* f \right)\right) \zeta_1^2\zeta_3 d\zeta_1 d\zeta_2 d\zeta_3 d\mu(g). \tag{143}$$

From this along with (139), we can observe that the integral T_{vib} is not divergent at singular configurations. In fact, at a glance, we see that no singularity occurs at $\zeta_1=0$. Turning to the singular configuration given by $\zeta_1=\zeta_2=\zeta_3=0$, we pick up one of the terms in the integrand, say,

$$\frac{\zeta_1^2+\zeta_3^2}{\zeta_1^2}\left|\left(\frac{\partial}{\partial\zeta_2}\right)^* f\right|^2 = \frac{\zeta_1^2+\zeta_3^2}{\zeta_1^2}\left(\left|\frac{\partial f}{\partial\zeta_2}\right|^2 + \frac{\zeta_3}{\zeta_1^2+\zeta_2^2+\zeta_3^2}\left(\frac{\overline{\partial f}}{\partial\zeta_2}K_2 f + \frac{\partial f}{\partial\zeta_2}\overline{K_2 f}\right) + \frac{\zeta_3^2|K_2 f|^2}{(\zeta_1^2+\zeta_2^2+\zeta_3^2)^2}\right). \tag{144}$$

If we take the spherical polar coordinates for $(\zeta_1,\zeta_2,\zeta_3)$ with the radial variable $r=\sqrt{\zeta_1^2+\zeta_2^2+\zeta_3^2}$, the volume element $dQ=\zeta_1^2\zeta_3 d\zeta_1 d\zeta_2 d\zeta_3$ is put in the form $dQ=r^5 dr d\nu$, where $d\nu$ denotes the area element induced on the quarter sphere given by $\zeta_1^2+\zeta_2^2+\zeta_3^2=1$, $\zeta_1\geqslant 0$, and $\zeta_3\geqslant 0$. Now it is easy to see that if f is smooth in a neighborhood of $r=0$, no divergence occurs at $r=0$ in the integral of the above term with respect to $r^5 dr d\nu$. For the other terms of the integrand, the same proof of non-divergence also runs well.

The rotational energy integral for the three-body system is expressed as

$$T_{\rm rot}=\frac{1}{2}\int_M\left(\frac{1}{\zeta_1^2}|K_1 f|^2+\frac{1}{\zeta_1^2+\zeta_2^2+\zeta_3^2}|K_2 f|^2+\frac{\zeta_1^2+\zeta_2^2}{\zeta_1^2\zeta_3^2}|K_3 f|^2+\frac{\zeta_2}{\zeta_1^2\zeta_3}(\overline{K_1 f}K_3 f+\overline{K_3 f}K_1 f)\right)\times\zeta_1^2\zeta_3 d\zeta_1 d\zeta_2 d\zeta_3 d\mu(g). \tag{145}$$

It is clear that no divergence occurs at $\zeta_1=0$. We are now interested in the singularity at $\zeta_3=0$. Among the terms of the integrand of the right-hand side of (145), $[(\zeta_1^2+\zeta_2^2)/\zeta_1^2\zeta_3^2]|K_3 f|^2$ might cause the divergence of the integral at $\zeta_3=0$:

$$\int_M\frac{\zeta_1^2+\zeta_2^2}{\zeta_3}|K_3 f|^2 d\zeta_1 d\zeta_2 d\zeta_3 d\mu(g). \tag{146}$$

However, we can show that the integral (146) is not divergent on account of the boundary condition for the wave function f at $\zeta_3=0$. To this end, we may restrict M to $\pi^{-1}(U)$ and use the fact that if f is assumed to be analytic at $\zeta_3=0$, f can be expanded into a Fourier series, with respect to D-functions, of the form

$$f(g\sigma(q))=\sum_{\ell=0}^{\infty}\frac{2\ell+1}{4\pi}\sum_{|n|,|m|\leqslant\ell}D_{mn}^{\ell}(g)\zeta_3^{|n|}\sum_{j=0}^{\infty}\zeta_3^{2j}C_{nmj}(\zeta_1,\zeta_2). \tag{147}$$

We notice here that in Ref. 11 Mitchell and Littlejohn proved that the analyticity assumption for an equivariant function gives rise to a power series in ζ_3 with the exponents of the form $|n|+2j$. By the Fubini theorem, the integral (146) restricted on $\pi^{-1}(U)$ can be written as

$$\int_U d\zeta_1 d\zeta_2 d\zeta_3\frac{\zeta_1^2+\zeta_2^2}{\zeta_3}\int_{\rm SO(3)}|K_3 f|^2 d\mu(g). \tag{148}$$

Carrying out the integration over SO(3) along with (147), we obtain

$$\int_{\rm SO(3)}|K_3 f|^2 d\mu(g)=\frac{1}{2}\sum_{\ell=0}^{\infty}(2\ell+1)\sum_{|m|,|n|\leqslant\ell}n^2\zeta_3^{2|n|}F_{nm}(\zeta_1,\zeta_2,\zeta_3), \tag{149}$$

where

$$F_{nm}(\zeta_1,\zeta_2,\zeta_3):=\sum_{j,j'=0}^{\infty}\zeta_3^{2j+2j'}\overline{C_{nmj}}(\zeta_1,\zeta_2)C_{nmj'}(\zeta_1,\zeta_2), \tag{150}$$

and we have used the orthogonality of D-functions,

$$\int_{\rm SO(3)}\overline{D_{mn}^{\ell}(g)}D_{m'n'}^{\ell'}(g)d\mu(g)=\frac{8\pi^2}{2\ell+1}\delta_{\ell\ell'}\delta_{mm'}\delta_{nn'}, \tag{151}$$

and the fact that $K_3 D_{mn}^{\ell}(g)=-inD_{mn}^{\ell}(g)$. Hence, we obtain

$$\int_U d\zeta_1 d\zeta_2 d\zeta_3 \frac{\zeta_1^2+\zeta_2^2}{\zeta_3}\int_{\mathrm{SO}(3)}|K_3 f|^2 d\mu(g)$$

$$=\frac{1}{2}\sum_{\ell=0}^{\infty}(2\ell+1)\sum_{|m|,|n|\leq\ell}\int_U \frac{\zeta_1^2+\zeta_2^2}{\zeta_3}n^2\zeta_3^{2|n|}F_{nm}(\zeta_1,\zeta_2,\zeta_3)d\zeta_1 d\zeta_2 d\zeta_3. \tag{152}$$

From this, we observe that the integral (146) is not divergent at $\zeta_3=0$. We may weaken the analyticity assumption on wave functions at $\zeta_3=0$ to smoothness assumption to some extent.

We turn to the singularity at $\zeta_1=\zeta_2=\zeta_3=0$. In this case, we have to consider whether the integral

$$\int_{\pi^{-1}(U)}\left(\frac{\zeta_1^2\zeta_3}{\zeta_1^2+\zeta_2^2+\zeta_3^2}|K_2 f|^2+\frac{\zeta_1^2+\zeta_2^2}{\zeta_3}|K_3 f|^2\right)d\zeta_1 d\zeta_2 d\zeta_3 d\mu(g) \tag{153}$$

is divergent at $\zeta_1=\zeta_2=\zeta_3=0$ or not. In the spherical polar coordinates for $(\zeta_1,\zeta_2,\zeta_3)$, the three-form $d\zeta_1 d\zeta_2 d\zeta_3$ is expressed as $r^2 dr d\nu$. Hence the integral (153) is not divergent at $\zeta_1=\zeta_2=\zeta_3=0$, if f is smooth in the neighborhood of $r=0$. Thus we conclude that

Theorem 2: While the rotational and the vibrational energy operators look singular at singular configurations, the singularity is not essential in the sense that the rotational and the vibrational energy integrals are not divergent at singular configurations on account of the boundary behavior of wave functions there. The reduced kinetic energy operator looks singular as well, but the singularity is not essential in the same sense.

VII. COLLINEAR CONFIGURATIONS

In this section, we consider the space M_1 of collinear configurations. Though M_1 is a part of the boundary of $\dot{M}$, and the rotational and the vibrational energy operators defined on $\dot{M}$ have singularity at M_1, we will be able to define restricted rotational and vibrational energy operators for collinear configurations, if we restrict ourselves to M_1. The rotation group SO(3) does not act freely on M_1, but it has the isotropy subgroup which is isomorphic with SO(2), so that the orbit of SO(3) through $x\in M_1$ is identified with S^2; $\mathcal{O}_x\cong \mathrm{SO}(3)/\mathrm{SO}(2)\cong S^2$. We can decompose the tangent space to M_1 at $x\in M_1$ into a direct sum of vertical and horizontal subspaces; the vertical subspace $V_x^{(1)}$ is defined to be the tangent space to the orbit $\mathcal{O}_x$ through $x\in M_1$, and the horizontal subspace $H_x^{(1)}$ to be the orthogonal complement of $V_x^{(1)}$:

$$T_x(M_1)=V_x^{(1)}\oplus H_x^{(1)},\quad V_x^{(1)}:=T_x(\mathcal{O}_x),\quad H_x^{(1)}:=(V_x^{(1)})^{\perp}, \tag{154}$$

where the metric with respect to which the orthogonality is referred is induced on M_1 from that on the center-of-mass system M.

We are to express basis vectors in $V_x^{(1)}$ in terms of local coordinates. To this end, we recall here the formula (62) which holds for singular configurations as well. However, in the present case, we must take the $\sigma(q)$ as a local section in M_1: $\sigma_0: U^{(1)}\subset M_1/S^2\to M_1$. The formula (62) restricted to $x\in M_1$ implies that K_a are tangent vectors in $V_x^{(1)}$. To find an explicit local expression of K_a, we take the section σ_0 to be

$$\sigma_0(q)=(\xi_1\mathbf{e}_3,\dots,\xi_{N-1}\mathbf{e}_3),\qquad q\in U^{(1)}, \tag{155}$$

where ξ_j are local coordinates in $U^{(1)}$. Then a generic point $x\in\pi^{-1}(U^{(1)})$ is expressed as

$$x=g\sigma_0(q)=(\xi_1 g\mathbf{e}_3,\dots,\xi_{N-1}g\mathbf{e}_3),\qquad g\in \mathrm{SO}(3). \tag{156}$$

We put g in the form $g=e^{\phi R(\mathbf{e}_3)}e^{\theta R(\mathbf{e}_2)}e^{\psi R(\mathbf{e}_3)}$. Then the point x is assigned by the local coordinates $(\theta,\phi,\xi_1,\dots,\xi_{N-1})$, ψ being eliminated on account of $e^{\psi R(\mathbf{e}_3)}\mathbf{e}_3=\mathbf{e}_3$. Hence we may take the matrix g as $e^{\phi R(\mathbf{e}_3)}e^{\theta R(\mathbf{e}_2)}$.

We first deal with K_1. Using the formula (62) restricted to M_1, one has

$$K_1 = \frac{d}{dt} g e^{tR(\mathbf{e}_1)} \sigma_0(q) \bigg|_{t=0} = -(\xi_j g \mathbf{e}_2) = -(\xi_j(-\sin\phi\, \mathbf{e}_1 + \cos\phi\, \mathbf{e}_2)). \tag{157}$$

On the other hand, the curve $x(t) = g e^{tR(\mathbf{e}_1)} \sigma_0(q)$ is put, in terms of (θ, ϕ, ξ_j), in the form

$$x(t) = (\xi_j(\sin\theta\cos\phi\, \mathbf{e}_1 + \sin\theta\sin\phi\, \mathbf{e}_2 + \cos\theta\, \mathbf{e}_3)), \tag{158}$$

where θ and ϕ are viewed as functions of t. Differentiating this with respect to t at $t=0$, and setting the resultant tangent vector equal to K_1 given by (157), we find that

$$K_1^{(1)} = \frac{-1}{\sin\theta} \frac{\partial}{\partial\phi}, \tag{159}$$

where the superscript $^{(1)}$ indicates that the vector field $K_1^{(1)}$ is defined on M_1. In the same manner as above, we have

$$K_2^{(1)} = \frac{\partial}{\partial\theta}. \tag{160}$$

For K_3, we can easily find that

$$K_3^{(1)} = \frac{d}{dt} g e^{tR(\mathbf{e}_3)} \sigma_0(q) \bigg|_{t=0} = 0. \tag{161}$$

The vector fields $K_1^{(1)}$ and $K_2^{(1)}$ form a local basis of vertical vector fields on M_1. We have observed, in the course of the above calculation, that $K_1^{(1)}$ and $K_2^{(2)}$ can also be expressed as

$$K_1^{(1)} = -\sum_{j=1}^{N-1} \xi_j \mathbf{u}_2 \cdot \frac{\partial}{\partial \mathbf{r}_j}, \quad K_2^{(1)} = \sum_{j=1}^{N-1} \xi_j \mathbf{u}_1 \cdot \frac{\partial}{\partial \mathbf{r}_j}, \tag{162}$$

respectively.

We proceed to find a local basis in $H_x^{(1)}$. The local vector fields $\partial/\partial\xi_j$ can be put in the form

$$\frac{\partial}{\partial\xi_j} = \sum_{i=1}^{N-1} \frac{\partial \mathbf{r}_i}{\partial\xi_j} \cdot \frac{\partial}{\partial \mathbf{r}_i} = \mathbf{u}_3 \cdot \frac{\partial}{\partial \mathbf{r}_j}. \tag{163}$$

From (162) and (163), it follows that $\partial/\partial\xi_j$ are orthogonal to $K_1^{(1)}, K_2^{(1)}$;

$$ds^2(K_a^{(1)}, \partial/\partial\xi_j) = 0, \quad a = 1,2, \quad j = 1,\ldots,N-1. \tag{164}$$

This implies that $\partial/\partial\xi_j$, $j = 1,\ldots,N-1$, form a local basis of horizontal vector fields. The inner product among these basis vector fields are given by

$$ds^2(K_a^{(1)}, K_b^{(1)}) = \sum_{j=1}^{N-1} \xi_j^2 \delta_{ab}, \quad a,b = 1,2, \tag{165}$$

$$ds^2(\partial/\partial\xi_i, \partial/\partial\xi_j) = \delta_{ij}, \quad i,j = 1,\ldots,N-1. \tag{166}$$

It is easy to see that the basis of one-forms dual to $K_a^{(1)}$ and $\partial/\partial\xi_j$ are given by

$$-\sin\theta\, d\phi, \quad d\theta, \quad d\xi_1, \ldots, d\xi_{N-1}, \tag{167}$$

of which the first two are vertical and the remainder horizontal. From (165)–(167), the induced metric on M_1 proves to be expressed as

$$ds^{2(1)}=\sum_{j=1}^{N-1}\xi_j^2(d\theta^2+\sin^2\theta\, d\phi^2)+\sum_{j=1}^{N-1}d\xi_j^2. \tag{168}$$

The volume element on M_1 is then given by

$$dV^{(1)}=dQ^{(1)}\wedge dS, \tag{169}$$

where

$$dQ^{(1)}=\rho_1(\xi)d\xi_1\wedge\cdots\wedge d\xi_{N-1},\quad \rho_1(\xi):=\sum_{j=1}^{N-1}\xi_j^2, \tag{170}$$

$$dS=\sin\theta\, d\theta\wedge d\phi. \tag{171}$$

As was already mentioned in Sec. IV, the inertia tensor A_x is singular at $x\in M_1$. However, to study collinear configurations, we have to know to what extent the A_x is singular at $x\in M_1$. For $x=(\mathbf{r}_1,\ldots,\mathbf{r}_{N-1})\in M_1$, one has rank $x=1$. Hence we can express Jacobi vectors as $\mathbf{r}_j=\lambda_j\mathbf{a}$, where $\lambda_j\in\mathbf{R}$ and $\mathbf{a}\neq 0$. Then for $\mathbf{v}$, the inertia tensor takes the value

$$A_x(\mathbf{v})=\sum_{j=1}^{N-1}\lambda_j^2(|\mathbf{a}|^2\mathbf{v}-(\mathbf{a}\cdot\mathbf{v})\mathbf{a}). \tag{172}$$

Suppose now that $\mathbf{v}\in\ker A_x$. Then one has $\mathbf{v}=(\mathbf{a}\cdot\mathbf{v})\mathbf{a}/|\mathbf{a}|^2$, which means that

$$\ker A_x=\mathrm{span}\{\mathbf{a}\},\quad x\in M_1. \tag{173}$$

In contrast with this, for any vector $\mathbf{u}\in\mathrm{span}\{\mathbf{a}\}^\perp$, one has

$$A_x(\mathbf{u})=\sum_{j-1}^{N-1}\lambda_j^2|\mathbf{a}|^2\mathbf{u}, \tag{174}$$

which implies that $\mathrm{span}\{\mathbf{a}\}^\perp$ is the eigenspace associated with the multiple eigenvalue $\Sigma_{j=1}^{N-1}\lambda_j^2|\mathbf{a}|^2=\Sigma_{j=1}^{N-1}|\mathbf{r}_j|^2$.

If we take $\mathbf{a}=g\mathbf{e}_3=\mathbf{u}_3$ and set $\lambda_j=\xi_j$, and if we restrict the domain of A_x to the subspace $\mathrm{span}\{\mathbf{u}_1,\mathbf{u}_2\}=\mathrm{span}\{\mathbf{u}_3\}^\perp$, the restricted A_x becomes invertible:

$$(A_x^{(1)})^{-1}(\mathbf{u}_a)=\left(\sum_{j=1}^{N-1}\xi_j^2\right)^{-1}\mathbf{u}_a,\quad x\in M_1,\quad a=1,2. \tag{175}$$

The connection form (36) fails to be defined for $x\in M_1$, as is easily seen. However, taking (175) into account, we may define a restricted connection form. We recall here that we have obtained the decomposition (154), which allows the interpretation that M_1 admits a "singular" connection, since (154) may be viewed as an analog to the decomposition (37). We now look into the connection form associated with the decomposition (154). By using the local coordinates given in (156), we obtain

$$\mathbf{r}_j\times d\mathbf{r}_j=\xi_j^2(\Psi^{1(1)}\mathbf{u}_1+\Psi^{2(1)}\mathbf{u}_2), \tag{176}$$

where $\Psi^{a(1)}$ are given by

$$\Psi^{1(1)}=-\sin\theta\, d\phi,\quad \Psi^{2(1)}=d\theta. \tag{177}$$

Note that $\Psi^{a(1)}$ are the reduced form of Ψ^a given in (64). Thus the total angular momentum is put in the form

$$\sum_{j=1}^{N-1} \mathbf{r}_j \times d\mathbf{r}_j = \sum_{j=1}^{N-1} \xi_j^2 (\Psi^{1(1)}\mathbf{u}_1 + \Psi^{2(1)}\mathbf{u}_2). \tag{178}$$

Since this vector is in the space span$\{\mathbf{u}_1, \mathbf{u}_2\}$, we can apply the restricted inverse operator $(A_x^{(1)})^{-1}$ to (178) to obtain a one-form,

$$\omega^{(1)} := R\left((A_x^{(1)})^{-1} \left(\sum_{j=1}^{N-1} \mathbf{r}_j \times d\mathbf{r}_j \right) \right) = \Psi^{1(1)} R(\mathbf{u}_1) + \Psi^{2(1)} R(\mathbf{u}_2). \tag{179}$$

For horizontal and vertical vectors on M_1, the form $\omega^{(1)}$ takes values as follows:

$$\omega^{(1)}(\partial/\partial \xi_j) = 0, \quad j = 1, \ldots, N-1, \tag{180}$$

$$\omega^{(1)}(K_a^{(1)}) = R(\mathbf{u}_a), \quad a = 1,2. \tag{181}$$

Since these equations are in keeping with the decomposition (154), we may call the form $\omega^{(1)}$ a (singular) connection form on M_1. Since $\partial/\partial \xi_i$ form a basis of the horizontal subspace $V_x^{(1)}$ and since $[\partial/\partial \xi_j, \partial/\partial \xi_i] = 0$, the curvature of the connection $\omega^{(1)}$ vanishes.

In conclusion of this section, we show that

$$M_1/S^2 \cong \mathbf{R}_+ \times \mathbf{R}P^{N-2}, \tag{182}$$

where $\mathbf{R}_+ = \{r \in \mathbf{R} | \ r > 0\}$ and $\mathbf{R}P^{N-2}$ denotes the real projective space of dimension $N-2$. Since $x \in M_1$ is of rank 1, we can describe x as $x = (\xi_1 \mathbf{u}, \ldots \xi_{N-1}\mathbf{u})$ with $|\mathbf{u}| = 1$ and $(\xi_1, \ldots, \xi_{N-1}) \neq 0$. If $(\xi_1 \mathbf{u}, \ldots, \xi_{N-1}\mathbf{u})$ and $(\eta_1 \mathbf{v}, \ldots, \eta_{N-1}\mathbf{v})$ are equivalent under the SO(3) action, we have $\eta_k \mathbf{v} = \xi_k g \mathbf{u}$, $k = 1, \ldots, N-1$, for some $g \in \mathrm{SO}(3)$. This implies that $|\eta_k| = |\xi_k|$, hence $\eta_k = \pm \xi_k$, and further the choice of sign should be independent of k. Conversely, if $\eta_k = \pm \xi_k$, then there exist $g \in \mathrm{SO}(3)$ such that $(\eta_1 \mathbf{v}, \ldots, \eta_{N-1}\mathbf{v}) = g(\xi_1 \mathbf{u}, \ldots, \xi_{N-1}\mathbf{u})$. This is because one has $-\mathbf{u} = e^{\pi R(\mathbf{w})}\mathbf{u}$ for a vector $\mathbf{w}$ such that $\mathbf{w} \perp \mathbf{u}$. It then follows that the map

$$\dot{\mathbf{R}}^{N-1} := \mathbf{R}^{N-1} - \{0\} \to M_1/S^2; \quad (\xi_1, \ldots, \xi_{N-1}) \mapsto [(\xi_1 \mathbf{u}, \ldots, \xi_{N-1}\mathbf{u})], \tag{183}$$

where $[(\cdots)]$ denotes the equivalence class, is two-to-one, that is, $\pm(\xi_1, \ldots, \xi_{N-1})$ maps to the same point of M_1/S^2. This results in

$$\dot{\mathbf{R}}^{N-1}/\mathbf{Z}_2 \cong M_1/S^2, \tag{184}$$

where $\mathbf{Z}_2$ acts on $\dot{\mathbf{R}}^{N-1}$ by $(\xi_k) \mapsto \pm(\xi_k)$. Since $\dot{\mathbf{R}}^{N-1} \cong \mathbf{R}_+ \times S^{N-2}$, one obtains

$$M_1/S^2 \cong \mathbf{R}_+ \times S^{N-2}/\mathbf{Z}_2 \cong \mathbf{R}_+ \times \mathbf{R}P^{N-2}. \tag{185}$$

In Ref. 12, they showed that the orbit of the shape, $\pi(x)$, of a collinear configuration $x \in M_1$ by the action of the kinetic group $\mathrm{O}(N-1)$ on $M/\mathrm{SO}(3)$ to the right is diffeomorphic with $\mathbf{R}P^{N-2}$.

VIII. KINETIC ENERGY OPERATOR FOR COLLINEAR CONFIGURATIONS

In the same manner as that used to obtain the kinetic energy operator Δ for nonsingular configurations, we can obtain the kinetic energy operator for singular configurations. From (168), it follows that the kinetic energy integral for collinear configurations is given by

$$\frac{1}{2}\int_{M_1}\left(\frac{1}{\rho_1(\xi)}\left(\left|\frac{\partial f}{\partial\theta}\right|^2+\frac{1}{\sin^2\theta}\left|\frac{\partial f}{\partial\phi}\right|^2\right)+\sum_{j=1}^{N-1}\left|\frac{\partial f}{\partial\xi_j}\right|^2\right)dV^{(1)}, \tag{186}$$

where $dV^{(1)}$ is the volume element given in (169). Integrated by part, this integral is expressed as

$$-\frac{1}{2}\int_{M_1}\overline{f}\left(\frac{1}{\rho_1(\xi)}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 f}{\partial\phi^2}\right)+\frac{1}{\rho_1(\xi)}\sum_{j=1}^{N-1}\frac{\partial}{\partial\xi_j}\left(\rho_1(\xi)\frac{\partial f}{\partial\xi_j}\right)\right)dV^{(1)}. \tag{187}$$

Thus we obtain the kinetic energy operator $-\frac{1}{2}\Delta^{(1)}$ with the Laplacian $\Delta^{(1)}$ on M_1,

$$\Delta^{(1)}=\frac{1}{\rho_1(\xi)}\Lambda+\frac{1}{\rho_1(\xi)}\sum_{j=1}^{N-1}\frac{\partial}{\partial\xi_j}\left(\rho_1(\xi)\frac{\partial}{\partial\xi_j}\right), \tag{188}$$

where Λ is the spherical Laplacian on S^2,

$$\Lambda=\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}. \tag{189}$$

The first and second terms on the right-hand side of (188) are a rotational and a vibrational operator, respectively.

The operator $\Delta^{(1)}$ has singularity at multiple collision for which $\rho_1(\xi)=0$. However, it is clear that the energy integral (186) is not divergent at the multiple collision $\xi_j=0$. Note also that the spherical Laplacian Λ has no singularity at $\theta=0,\pi$, as is well known.

We proceed to show that the Laplacian $\Delta^{(1)}$ will reduce to an operator acting on the wave functions of variables (ξ_j). For $x=\sigma_0(q)$ and $h=e^{tR(\mathbf{e}_3)}$, the equivariance condition (33) specializes to

$$(E_m^\ell f)(\sigma_0(q))=(E_m^\ell f)(e^{tR(\mathbf{e}_3)}\sigma_0(q))=D^\ell(e^{tR(\mathbf{e}_3)})(E_m^\ell f)(\sigma_0(q)). \tag{190}$$

Since

$$D^\ell(e^{tR(\mathbf{e}_3)})=\mathrm{diag}(e^{-i\ell t},\dots,e^{-it},0,e^{it},\dots,e^{i\ell t}), \tag{191}$$

the above condition implies that the $\mathcal{H}^\ell$-valued function $(E_m^\ell f)(\sigma_0(q))$ has only one non-zero component $(P_{0m}^\ell f)(\sigma(q))/\sqrt{2\ell+1}$, and hence the $\mathcal{H}^\ell$-valued function $(E_m^\ell f)(g\sigma_0(q))=D^\ell(g)(E_m^\ell f)(\sigma_0(q))$ has the nth $(|n|\leqslant\ell)$ component expressed as

$$\frac{1}{\sqrt{2\ell+1}}D_{n0}^\ell(g)(P_{0m}^\ell f)(\sigma_0(q))=\sqrt{4\pi}\;\overline{Y_{\ell n}(g\mathbf{e}_3)}(P_{0m}^\ell f)(\sigma_0(q)), \tag{192}$$

where $Y_{\ell n}$ are the spherical harmonics and $g\mathbf{e}_3$ denotes a point of the unit sphere S^2, which are designated by the variables $(\theta,\,\phi)$.

Operating on (192) with the Laplacian $\Delta^{(1)}$, we obtain (up to the factor $\sqrt{4\pi}$)

$$\Delta^{(1)}\overline{Y_{\ell n}(g\mathbf{e}_3)}(P_{0m}^\ell f)(\sigma_0(q))=\overline{Y_{\ell n}(g\mathbf{e}_3)}\left(-\frac{\ell(\ell+1)}{\rho_1(\xi)}+\frac{1}{\rho_1(\xi)}\sum_{j=1}^{N-1}\frac{\partial}{\partial\xi_j}\left(\rho_1(\xi)\frac{\partial}{\partial\xi_j}\right)\right)\times(P_{0m}^\ell f)(\sigma_0(q)). \tag{193}$$

Thus we find an operator acting on functions $(P_{0m}^\ell f)(\sigma_0(q))$,

$$\Delta^{(1)\mathrm{red}} := \frac{1}{\rho_1(\xi)} \sum_{j=1}^{N-1} \frac{\partial}{\partial \xi_j}\left(\rho_1(\xi)\frac{\partial}{\partial \xi_j}\right) - \frac{\ell(\ell+1)}{\rho_1(\xi)}. \tag{194}$$

We have to note here that this reduced operator is globally expressed on the orbit space M_1/S^2 on account of (184). In fact, the operator (194) is expressed in terms of $(\xi_1,\ldots,\xi_{N-1}) \in \dot{\mathbf{R}}^{N-1}$ and invariant under the inversion $(\xi_k) \mapsto -(\xi_k)$. Thus we have the following.

Theorem 3: For collinear configurations, the reduced kinetic energy operator $-\frac{1}{2}\Delta^{(1)\mathrm{red}}$ on M_1/S^2 is given by (194). It looks singular at the multiple collision configuration $(\xi_j=0)$, but the singularity is not essential in the sense that the kinetic energy integral is not divergent at the multiple collision.

We note that the Hamiltonian operator for linear molecules was already discussed in an elementary manner.[13] The method taken in this article to derive the kinetic energy operator is quite different from that in Ref. 13. Ours is clear and natural from the viewpoint of differential geometry.

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