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Rotating frames and gauge invariance in three-dimensional many-body quantum systems

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Abstract

We study the quantization of many-body systems in three dimensions in rotating coordinate frames using a gauge invariant formulation of the dynamics. We consider reference frames defined by linear gauge conditions, and discuss their Gribov ambiguities and commutator algebra. We construct the momentum operators, inner product and Hamiltonian in those gauges, for systems with and without translation invariance. The analogy with the quantization of non-Abelian Yang–Mills theories in non-covariant gauges is emphasized. Our results are applied to quasi-rigid systems in the Eckart frame.

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1. Introduction

The problem of quantizing a many-body mechanical system in a rotating reference frame is of interest both by itself and for its possible applications to specific problems in, e.g., molecular and nuclear physics. In this paper, we study the quantization of many-body systems in three dimensions in rotating coordinate frames, using a gauge-invariant formulation. The two-dimensional case was considered in a previous paper [1], in which the method was developed in detail and a close parallel with the quantization of electrodynamics in non-covariant gauges established. The main lines of the method are the same in both cases. Due to the non-Abelianity of the rotation group in three dimensions, however, the technical treatment of the systems considered here is considerably different from the planar case, the differences being already apparent at the Lagrangian level as discussed in the following section.

We consider systems of N spinless particles interacting through central potentials. Since the underlying dynamics are rotationally symmetric, the coordinate transformation from a space-fixed reference frame to a rotating one with the same origin is a time-dependent symmetry transformation, or gauge transformation. If the dynamics are described in terms of a gauge-invariant action, since we know how to quantize a mechanical system in a space-fixed coordinate frame, we can perform a gauge transformation in order to obtain the quantum theory in a rotating frame. Gauge invariance implies that both theories are physically equivalent.

Rotating frames are often defined implicitly, by restrictions on the trajectories of the system in that frame. In the gauge-invariant approach to the quantization in rotating frames, such restrictions are incorporated into the theory as gauge conditions. The action is then given in terms of degrees of freedom that are not independent, but must satisfy certain functional relations. This situation is familiar from the theory of gauge fields [2, 3], where the vector potential $\boldsymbol{A}(t, \boldsymbol{x})$ may be required to satisfy such relations as $\boldsymbol{\nabla} \cdot \boldsymbol{A} = 0$ (Coulomb gauge), or $\boldsymbol{n} \cdot \boldsymbol{A} = 0$ (axial gauge), at all times t. In this paper, we consider only gauge conditions depending linearly on the particles coordinates, which are most useful in practical applications involving perturbative expansions. We do not consider quadratic gauge conditions, in particular, because we expect the formalism in those gauges to be considerably more complicated, in view of the results of [1] in the simpler two-dimensional, Abelian case. Furthermore, the quadratic gauge conditions most common in the literature [4, 5] are those defining the instantaneous principal axes frame, in which the total angular momentum of the system is strongly coupled to the other degrees of freedom through the inertia tensor and the Coriolis terms. Without a strong physical motivation for quadratic gauges, we have no reason to pursue that technically more involved approach here. As discussed in [1], however, there is no problem of principle to deal with those and other kinds of gauge conditions within the formalism espoused in this paper.

We closely follow the approach to non-Abelian Yang–Mills theories in non-covariant gauges of [2, 6], stressing throughout the paper the strict formal similarity between our results for many-body systems and the corresponding ones in [6] for Yang–Mills theories. Our goals are both to illustrate the formalism of gauge theories in the more familiar context of mechanical systems, and to apply the gauge-theoretical techniques to the quantization of three-dimensional N-body systems in rotating frames. Previous treatments of the latter problem within a gauge-invariant approach have been given in [4] and references therein. A gauge theory of rotations and internal motions of deformable bodies, including classical and quantum N-body systems, is developed in [7] (see also [8]) from a point of view different from ours. Non-gauge-invariant treatments can be found, e.g., in [5] in the context of nuclear physics, and in [9, 10] in molecular physics.

The outline of the paper is as follows. In section 2, we describe the class of systems to be considered throughout the paper, and their formulation in terms of a Lagrangian invariant under time-dependent rotations. Their quantization in a space-fixed frame is given, and shown to be equivalent to the non-gauge-invariant formulation. The central results of the paper are given in section 3, where we consider the quantization in rotating frames defined by linear gauge conditions. We discuss in detail the commutator algebra for both linear and angular momentum operators, and give explicit realizations of that algebra in terms of differential operators. Those operators are used to construct the Hamiltonian in terms of position vectors referred to the rotating frame, and their conjugate momenta. The elimination of orientational degrees of freedom from the formalism is subsequently carried out, and the resulting Hamiltonian and its Weyl-ordered form and related quantum potential are obtained. As emphasized throughout, by describing a many-body system from a rotating frame defined by gauge conditions, we are introducing orthogonal curvilinear coordinates in configuration space. The singularities of those coordinates occur at the Gribov horizons where the gauge conditions become ambiguous. Gribov ambiguities [11, 6, 3, 1] are discussed in detail in relation to the construction of the inner product in the reduced state-space of the system.

In section 4, we extend the results of section 3 to translation-invariant systems. We show how the gauge-invariant approach can be used to describe a mechanical system in a reference frame in an arbitrary state of rotation and translation. In particular, we obtain explicit results for the quantization of N-body systems in rotating frames with origin at the centre of mass. Those results are then applied to quasi-rigid systems in the Eckart frame [12, 9, 1] in section 5, where two simple three- and four-body examples are briefly discussed. In section 6, we give our final remarks. Some complementary material is gathered in the appendices.

2. *N*-particle system

We consider a system of N spinless particles with central interactions in three dimensions, described by the Lagrangian

$$\mathcal{L} = \mathcal{L}_N + \mathcal{L}_{\mathrm{rt}} \qquad \mathcal{L}_N = \frac{1}{2}\sum_{\alpha=1}^{N} m_\alpha \dot{\boldsymbol{r}}_\alpha^2 - \mathcal{V}$$
$$\mathcal{V} = \sum_{\alpha<\beta=1}^{N} V_{\alpha\beta}(|\boldsymbol{r}_\alpha - \boldsymbol{r}_\beta|) + \sum_{\alpha=1}^{N} U(r_\alpha) \qquad \mathcal{L}_{\mathrm{rt}} = \frac{\mathcal{I}}{2}(\widehat{\boldsymbol{e}} \wedge \dot{\widehat{\boldsymbol{e}}})^2 = \frac{\mathcal{I}}{2}\dot{\widehat{\boldsymbol{e}}}^2 \quad \widehat{\boldsymbol{e}}\cdot\widehat{\boldsymbol{e}} = 1. \tag{1}$$

The potential energy $\mathcal{V}$ is chosen for concreteness to include only one- and two-body interactions. Our results do not depend on that fact and apply equally well to more general rotationally invariant potentials. If the one-body potential $U = 0$, $\mathcal{L}$ is invariant under the group of Euclidean motions of three-dimensional space. In this and the following sections, we consider $U \neq 0$ and focus on the non-Abelian group of three-dimensional rotations, deferring the discussion of translation invariance until section 4. Besides the kinetic and potential energy for the N-particle system $\mathcal{L}$ also contains the Lagrangian $\mathcal{L}_{\mathrm{rt}}$ for a free rigid rotator, described by a unit vector $\widehat{\boldsymbol{e}}$. This rotator is not coupled to the particle system, so it does not affect its dynamical evolution. $\mathcal{L}_{\mathrm{rt}}$ can be made to vanish by letting the rotator's inertia moment $\mathcal{I} \to \infty$ while keeping constant the magnitude of its angular momentum $\boldsymbol{s} = \mathcal{I}\widehat{\boldsymbol{e}} \wedge \dot{\widehat{\boldsymbol{e}}}$. Whereas $\mathcal{L}_{\mathrm{rt}}$ does not play any role in $\mathcal{L}$ as given in (1), it will serve as a source of angular momentum for the particle system in the gauge-invariant formulation to which we now turn.

$\mathcal{L}$ is invariant under time-independent rotations of the coordinate frame. In order to make $\mathcal{L}$ invariant under changes of arbitrarily rotating coordinate frames we apply the Yang–Mills construction [13] to (1). We introduce a 3×3 real antisymmetric matrix $\boldsymbol{\xi}$, thus adding three new degrees of freedom to the system, and postulate the following transformation laws under rotations of the coordinate frame,

$$\boldsymbol{r}'_\alpha = \boldsymbol{U}\boldsymbol{r}_\alpha \qquad \widehat{\boldsymbol{e}}\,' = \boldsymbol{U}\widehat{\boldsymbol{e}} \qquad \boldsymbol{\xi}' = \boldsymbol{U}\boldsymbol{\xi}\boldsymbol{U}^\dagger + \dot{\boldsymbol{U}}\boldsymbol{U}^\dagger \tag{2}$$

with $\boldsymbol{U}$ a time-dependent real orthogonal matrix and $\boldsymbol{U}^\dagger$ its transpose. These are the gauge transformations of the system. We define the covariant time derivative $D_t\boldsymbol{r}_\alpha \equiv \dot{\boldsymbol{r}}_\alpha - \boldsymbol{\xi}\boldsymbol{r}_\alpha$, which transforms like a vector under gauge transformations, $(D_t\boldsymbol{r}_\alpha)' = \boldsymbol{U}(D_t\boldsymbol{r}_\alpha)$. Analogously, $D_t\widehat{\boldsymbol{e}} = \dot{\widehat{\boldsymbol{e}}} - \boldsymbol{\xi}\widehat{\boldsymbol{e}}$. We can, equivalently, use instead of the matrix $\boldsymbol{\xi}$ the axial vector $\widetilde{\boldsymbol{\xi}}$ dual to $\boldsymbol{\xi}$, $\xi_{ik} = \varepsilon_{ijk}\widetilde{\xi}_j$, whose gauge transformations can be derived from (2). In terms of $\widetilde{\boldsymbol{\xi}}$, covariant derivatives take the form $D_t\boldsymbol{r}_\alpha = \dot{\boldsymbol{r}}_\alpha - \widetilde{\boldsymbol{\xi}} \wedge \boldsymbol{r}_\alpha$. Substituting time derivatives in (1) by covariant derivatives we obtain a Lagrangian invariant under time-dependent rotations of the coordinate frame. Explicitly, we write

$$\mathcal{L} = \mathcal{L}_N + \mathcal{L}_{\mathrm{rt}}$$
$$\mathcal{L}_N = \frac{1}{2}\sum_{\alpha=1}^{N} m_\alpha (D_t \boldsymbol{r}_\alpha)^2 - \mathcal{V} = \frac{1}{2}\sum_{\alpha=1}^{N} m_\alpha \dot{\boldsymbol{r}}_\alpha^2 + \frac{1}{2}\sum_{\alpha=1}^{N} m_\alpha (\widetilde{\boldsymbol{\xi}} \wedge \boldsymbol{r}_\alpha)^2 - \widetilde{\boldsymbol{\xi}} \cdot \sum_{\alpha=1}^{N} m_\alpha (\boldsymbol{r}_\alpha \wedge \dot{\boldsymbol{r}}_\alpha) - \mathcal{V}$$
$$\mathcal{L}_{\mathrm{rt}} = \frac{\mathcal{I}}{2}(\widehat{\boldsymbol{e}} \wedge (D_t\widehat{\boldsymbol{e}}))^2 = \frac{\mathcal{I}}{2}(D_t\widehat{\boldsymbol{e}})^2 = \frac{\mathcal{I}}{2}\dot{\widehat{\boldsymbol{e}}}^2 + \frac{\mathcal{I}}{2}(\widetilde{\boldsymbol{\xi}} \wedge \widehat{\boldsymbol{e}})^2 - \mathcal{I}\widetilde{\boldsymbol{\xi}} \cdot (\widehat{\boldsymbol{e}} \wedge \dot{\widehat{\boldsymbol{e}}}) \qquad (3)$$

where the potential energy $\mathcal{V}$ is defined in (1). $\mathcal{L}$ is exactly invariant under the gauge transformations (2) and, in fact, $\mathcal{L}_N$ and $\mathcal{L}_{\mathrm{rt}}$ are separately invariant under (2).[1]

$\mathcal{L}_N$ in (3) has the form of a Lagrangian for an N-particle system described from a coordinate frame rotating with the angular velocity $-\widetilde{\boldsymbol{\xi}}$ with respect to the laboratory frame [14]. Note, however, that $\widetilde{\boldsymbol{\xi}}$ is a dynamical variable describing the coupling of the particles and the rotator to the inertial forces. The equations of motion for $\boldsymbol{r}_\alpha$, $\widehat{\boldsymbol{e}}$ and $\widetilde{\boldsymbol{\xi}}$ derived from $\mathcal{L}$ are

$$m_\alpha D_t D_t \boldsymbol{r}_\alpha + \nabla_\alpha \mathcal{V} = m_\alpha \ddot{\boldsymbol{r}}_\alpha - 2m_\alpha \widetilde{\boldsymbol{\xi}} \wedge \dot{\boldsymbol{r}}_\alpha - m_\alpha \dot{\widetilde{\boldsymbol{\xi}}} \wedge \boldsymbol{r}_\alpha - m_\alpha \widetilde{\boldsymbol{\xi}} \wedge (\boldsymbol{r}_\alpha \wedge \widetilde{\boldsymbol{\xi}}) + \nabla_\alpha \mathcal{V} = 0 \qquad (4a)$$
$$D_t D_t \widehat{\boldsymbol{e}} + (D_t \widehat{\boldsymbol{e}})^2 \widehat{\boldsymbol{e}} = 0 \qquad \text{with} \quad \widehat{\boldsymbol{e}} \cdot \widehat{\boldsymbol{e}} = 1 \qquad (4b)$$
$$-\frac{\partial \mathcal{L}}{\partial \widetilde{\boldsymbol{\xi}}} = \sum_{\alpha=1}^{N} m_\alpha \boldsymbol{r}_\alpha \wedge (D_t \boldsymbol{r}_\alpha) + \mathcal{I}\widehat{\boldsymbol{e}} \wedge (D_t \widehat{\boldsymbol{e}}) = 0. \qquad (4c)$$

In the equation of motion (4a) for $\boldsymbol{r}_\alpha$ the terms due to the Coriolis, azimuthal and centrifugal forces [15] are apparent. As a consequence of the rotational invariance of $\mathcal{L}$ the total angular momentum of the system is conserved, $\mathrm{d}\boldsymbol{j}/\mathrm{d}t = 0$ with

$$\boldsymbol{j} = \boldsymbol{l} + \boldsymbol{s} \qquad \boldsymbol{l} = \sum_{\alpha=1}^{N} m_\alpha \boldsymbol{r}_\alpha \wedge (D_t \boldsymbol{r}_\alpha) \qquad \boldsymbol{s} = \mathcal{I}\widehat{\boldsymbol{e}} \wedge (D_t \widehat{\boldsymbol{e}}). \qquad (5)$$

Clearly, the vector $\boldsymbol{j}$ can be time independent in every rotating reference frame only if it vanishes. This is expressed by (4c), which can be rewritten as $\boldsymbol{j} = 0$. Since in general $\mathcal{L}$ is not invariant under separate rotations of $\{\boldsymbol{r}_\alpha\}$ and $\widehat{\boldsymbol{e}}$, $\boldsymbol{l}$ and $\boldsymbol{s}$ are not separately conserved. Rather, from (4a) and (4b) they are seen to be covariantly conserved,

$$D_t \boldsymbol{l} = 0 \qquad D_t \boldsymbol{s} = 0 \qquad (6)$$

with $D_t \boldsymbol{l} = \dot{\boldsymbol{l}} - \widetilde{\boldsymbol{\xi}} \wedge \boldsymbol{l}$. From (6), the magnitudes of $\boldsymbol{l}$ and $\boldsymbol{s}$ are conserved and frame independent, but their directions in space are time dependent. Only in the lab frame (in which $\boldsymbol{\xi} = 0$ and $D_t = \mathrm{d}/\mathrm{d}t$, as discussed below) are $\boldsymbol{l}$ and $\boldsymbol{s}$ conserved.

Since the system is gauge invariant we can fix the gauge by imposing a set of conditions of the form[2] $\mathfrak{G}_a(\{\boldsymbol{r}_\alpha\}, \boldsymbol{\xi}, \widehat{\boldsymbol{e}}) = 0, a = 1, 2, 3$, which is equivalent to selecting a rotating frame in which the trajectory of the system $(\{\boldsymbol{r}_\alpha(t)\}, \boldsymbol{\xi}(t), \widehat{\boldsymbol{e}}(t))$ in configuration space is constrained by the relations $\mathfrak{G}_a(\{\boldsymbol{r}_\alpha(t)\}, \boldsymbol{\xi}(t), \widehat{\boldsymbol{e}}(t)) = 0$. The functions[3] $\mathfrak{G}_a$, $a = 1, 2, 3$, can be chosen arbitrarily, as long as any trajectory $(\{\boldsymbol{r}'_\alpha\}, \boldsymbol{\xi}', \widehat{\boldsymbol{e}}\,')$ can be transformed into a new one $(\{\boldsymbol{r}_\alpha\}, \boldsymbol{\xi}, \widehat{\boldsymbol{e}})$ satisfying $\mathfrak{G}_a = 0$. The new trajectory must be unique, in the sense that no other trajectory obtained from $(\{\boldsymbol{r}'_\alpha\}, \boldsymbol{\xi}', \widehat{\boldsymbol{e}}\,')$ by a gauge transformation satisfies the gauge conditions. Otherwise, the gauge is said to be ambiguous [11]. Supplementary conditions must then be imposed to fix the ambiguity.

[1] Note that, unlike the two-dimensional (Abelian) case [1], we cannot add external-source terms to $\mathcal{L}$ without breaking gauge invariance, so we have to incorporate the source into the theory as a dynamical degree of freedom. That is the motivation for including $\mathcal{L}_{\mathrm{rt}}$ in $\mathcal{L}$. We stress here that $\mathcal{L}_{\mathrm{rt}}$ is gauge invariant and therefore it is not a gauge-fixing term.

[2] The letters a, b, c, d are used to index quantities which are not necessarily tensor components, such as $\mathfrak{G}_a$. Summation over these indices and their ranges of variation are always explicitly indicated. We only use the summation convention for tensor indices, which are denoted by latin letters $i, j, k, l, \ldots$ and always run from 1 to 3.

[3] In general, $\mathfrak{G}_a$ are functionals of the trajectory $(\{\boldsymbol{r}_\alpha(t)\}, \boldsymbol{\xi}(t), \widehat{\boldsymbol{e}}(t))$.

2.1. The laboratory frame

Given any trajectory of the system $(\{\boldsymbol{r}_\alpha(t)\}, \boldsymbol{\xi}(t), \widehat{\boldsymbol{e}}(t))$ by means of a gauge transformation we can obtain a physically equivalent trajectory with $\boldsymbol{\xi}' = \boldsymbol{U}\boldsymbol{\xi}\boldsymbol{U}^\dagger + \dot{\boldsymbol{U}}\boldsymbol{U}^\dagger = 0$. Indeed, given the antisymmetric matrix-valued function of time $\boldsymbol{\xi}(t)$, there is always an orthogonal matrix $\boldsymbol{U}(t)$ satisfying $\boldsymbol{U}^\dagger\dot{\boldsymbol{U}} = -\boldsymbol{\xi}$. The condition $\boldsymbol{\xi} = 0$ is then admissible as a choice of gauge for the system, which corresponds to selecting a non-rotating coordinate frame referred to as the 'laboratory frame'.

We denote dynamical quantities in the laboratory frame by lower-case symbols, except for the Lagrangian and Hamiltonian. In this gauge, the Lagrangian (3) reduces to (1). $\mathcal{L}$ is invariant under separate rotations of $\{\boldsymbol{r}_\alpha\}$ and $\widehat{\boldsymbol{e}}$, leading to the separate conservation of the angular momenta $\boldsymbol{l} = \sum_{\alpha=1}^N m_\alpha \boldsymbol{r}_\alpha \wedge \dot{\boldsymbol{r}}_\alpha$ of the system of particles and $\boldsymbol{s} = \mathcal{I}\widehat{\boldsymbol{e}} \wedge \dot{\widehat{\boldsymbol{e}}}$ of the rigid rotator. The equation of motion (4*c*) for $\boldsymbol{\xi}$, which cannot be obtained from (1), must be imposed on the system as a constraint [2], $\boldsymbol{j} \equiv \boldsymbol{l} + \boldsymbol{s} = 0$. In the Hamiltonian formulation in this gauge, this is a primary first-class constraint [16], not leading to further secondary ones.

The quantization in the gauge $\boldsymbol{\xi} = 0$ is canonical. In units such that $\hbar = 1$, we have

$$\begin{aligned} &\mathcal{H} = \mathcal{H}_N + \mathcal{H}_{\mathrm{rt}} \qquad \mathcal{H}_N = \sum_{\alpha=1}^N \frac{1}{2m_\alpha}\boldsymbol{p}_\alpha^2 + \mathcal{V} \qquad \mathcal{H}_{\mathrm{rt}} = \frac{1}{2\mathcal{I}}\boldsymbol{s}^2 \\ &[r_{\alpha i}, p_{\beta j}] = \mathrm{i}\delta_{\alpha\beta}\delta_{ij} \qquad \boldsymbol{p}_\alpha = \frac{1}{\mathrm{i}}\boldsymbol{\nabla}_\alpha \qquad [s_i, s_j] = \mathrm{i}\varepsilon_{ijk}s_k \\ &\langle\phi|\psi\rangle = \int \prod_{\beta=1}^N \mathrm{d}^3 r_\beta\, \mathrm{d}^2\widehat{\boldsymbol{e}}\phi^*(\{\boldsymbol{r}_\alpha\}, \widehat{\boldsymbol{e}})\psi(\{\boldsymbol{r}_\alpha\}, \widehat{\boldsymbol{e}}) \end{aligned} \tag{7}$$

with the commutators among $\boldsymbol{r}_\alpha$ and $\boldsymbol{p}_\alpha$ not shown in (7) all vanishing. The first-class constraint is imposed on the state space [16], $\boldsymbol{j}|\psi\rangle = 0$. Since both $\boldsymbol{l}$ and $\boldsymbol{s}$ are constants of motion, this constraint is clearly consistent with the dynamics. We see that the quantized theory in the $\boldsymbol{\xi} = 0$ gauge is completely analogous to Yang–Mills theories in the temporal gauge [6, 17, 18]. The constraint fixing the value of $\boldsymbol{j}$, in particular, is the equivalent of the non-Abelian Gauss law. In the constraint equation, $\boldsymbol{s}$ plays the same role as the fermion colour current in the Gauss law.

If in (7) we let $\mathcal{I} \to \infty$ with $\boldsymbol{s}^2$ fixed, $\mathcal{H}_{\mathrm{rt}} \to 0$ and the rigid rotator drops from the Hamiltonian, entering the dynamics only through the constant value of $\boldsymbol{s}$ in the constraint. Thus, (7) describes in that limit an *N*-body system with interaction potential $\mathcal{V}$ in the sector of fixed angular momentum $\boldsymbol{l} = -\boldsymbol{s}$ (i.e., the null eigenspace of $(\boldsymbol{l} + \boldsymbol{s})^2$). Due to the gauge invariance, the same must be true in any other gauge.

3. Linear gauge conditions

In order to fix a reference frame we need to impose three gauge conditions. The simplest gauge conditions involving the coordinates of the particles depend linearly on $\{\boldsymbol{r}_\alpha\}$, and do not involve $\boldsymbol{\xi}$ or $\widehat{\boldsymbol{e}}$. As discussed below, linear gauges are relevant in the context of perturbative or semiclassical expansions. The general form of the linear gauge conditions is

$$\mathfrak{S}_a(\{\boldsymbol{r}_\alpha\}) \equiv \sum_{\alpha=1}^N m_\alpha \Gamma_{a\alpha j} r_{\alpha j} = 0 \qquad a = 1, 2, 3 \tag{8}$$

with $\Gamma_{a\alpha j}$ a set of $9N$ constants defining the functions $\mathfrak{S}_a$. We denote dynamical quantities in this gauge by capital letters, in particular the position vectors $\boldsymbol{R}_\alpha$, $\widehat{\boldsymbol{E}}$ and the angular momenta

$\boldsymbol{L}$ and $\boldsymbol{S}$, as opposed to the corresponding quantities in the gauge $\boldsymbol{\xi} = 0$ (the laboratory frame) which are denoted as $\boldsymbol{r}_\alpha, \widehat{\boldsymbol{e}}, \boldsymbol{l}, \boldsymbol{s}$. Thus, $\mathfrak{S}_a(\{\boldsymbol{R}_\alpha\}) = 0$ but, in general, $\mathfrak{S}_a(\{\boldsymbol{r}_\alpha\}) \neq 0$. The gauge conditions (8) select a reference frame rotating so that the linear combinations of coordinates $\mathfrak{S}_a$ vanish for all t. If we choose, for instance, all coefficients in (8) vanishing except for $\Gamma_{11Y} = \Gamma_{21Z} = \Gamma_{32Y} = 1$, the coordinate frame must rotate together with particles 1 and 2 so that 1 is on the X-axis and 2 on the X–Z plane for all t. The formalism in these linear gauges is entirely analogous to that of non-Abelian Yang–Mills theories in linear non-covariant gauges, such as the Coulomb or axial gauges, in which the fields are also constrained by linear relations [6] (see also [3, 17, 18]).

For the functions $\mathfrak{S}_a(\{\boldsymbol{r}_\alpha\})$ to be admissible as gauge conditions they must not be rotationally invariant. The variation of $\mathfrak{S}_a$ under an infinitesimal rotation is $\delta\mathfrak{S}_a = \mathfrak{Q}_{ak}\delta\theta_k$, with

$$\mathfrak{Q}_{ai}(\{\boldsymbol{R}_\gamma\}) = \sum_{\beta=1}^{N} m_\beta \Gamma_{a\beta j}\varepsilon_{jik} R_{\beta k} \qquad a = 1, 2, 3. \tag{9}$$

The requirement that $\mathfrak{S}_a$ must not be invariant under infinitesimal rotations is therefore satisfied if the matrix $\mathfrak{Q}_{ai}$ is not singular on the gauge manifold. Thus, the following equations must be simultaneously satisfied:

$$\mathfrak{S}_a(\{\boldsymbol{R}_\alpha\}) = 0 \quad a = 1, 2, 3 \qquad \det(\mathfrak{Q}_{bj}(\{\boldsymbol{R}_\alpha\})) \neq 0 \tag{10}$$

except possibly at exceptional configurations at which the gauge is singular, $\det\mathfrak{Q} = 0$, such as $\boldsymbol{R}_\alpha = 0$ for all α. Furthermore, without loss of generality, we assume that the gauge coefficients have been orthogonalized so that

$$\sum_{\alpha=1}^{N} m_\alpha \Gamma_{a\alpha j}\Gamma_{b\alpha j} = \mathfrak{N}_a^2 \delta_{ab} \qquad \mathfrak{N}_a^2 \equiv \sum_{\alpha=1}^{N} m_\alpha \Gamma_{a\alpha j}\Gamma_{a\alpha j} > 0 \quad 1 \leqslant a, b \leqslant 3. \tag{11}$$

The gauge transformation from the gauge $\boldsymbol{\xi} = 0$ to the gauge $\mathfrak{S}_a = 0$ is of the form (2),

$$\boldsymbol{R}_\alpha = \boldsymbol{U}\boldsymbol{r}_\alpha \qquad \widehat{\boldsymbol{E}} = \boldsymbol{U}\widehat{\boldsymbol{e}} \qquad \boldsymbol{\xi} = \dot{\boldsymbol{U}}\boldsymbol{U}^\dagger. \tag{12}$$

The orthogonal matrix $\boldsymbol{U}$ is parametrized by three angles $\{\theta_a\}_{a=1}^3$. Although our approach and results do not depend on any specific parametrization of the rotation group, some parametrization-dependent quantities, such as the momenta p_{θ_a} conjugate to θ_a, are physically meaningful and play an important role in some intermediate calculations. All the information we will need about the parametrization of $\boldsymbol{U}$ is encoded in the matrices $\boldsymbol{\Lambda}$ and λ defined by

$$\frac{\partial\boldsymbol{U}}{\partial\theta_a}\boldsymbol{U}^\dagger = \Lambda_{ai}\boldsymbol{T}_i \qquad \boldsymbol{U}^\dagger\frac{\partial\boldsymbol{U}}{\partial\theta_a} = \lambda_{ai}\boldsymbol{T}_i \quad a = 1, 2, 3 \tag{13}$$

where the $\boldsymbol{T}_j$ are the standard generators of the $so(3)$ algebra, $(\boldsymbol{T}_j)_{ik} = \varepsilon_{ijk}$. The three matrices $\partial\boldsymbol{U}/\partial\theta_a\boldsymbol{U}^\dagger, a = 1, 2, 3$, must be a basis of $so(3)$ for all values of $\{\theta_b\}$, if the parametrization is to be well defined. Thus, the matrix Λ_{ai} is invertible and, analogously, so is λ_{ai}. From the unimodularity of $\boldsymbol{U}$ it follows that $\boldsymbol{U}^\dagger\boldsymbol{T}_i\boldsymbol{U} = U_{ij}\boldsymbol{T}_j$ and then, from (13), $\lambda_{aj} = \Lambda_{ai}U_{ij}$. We can express $\boldsymbol{\xi}$ in terms of θ_a and their time derivatives as

$$\xi_{ik} = \sum_{a=1}^{3} \dot{\theta}_a \Lambda_{aj}\varepsilon_{ijk} \qquad \text{or} \qquad \widetilde{\xi}_j = \sum_{a=1}^{3} \dot{\theta}_a \Lambda_{aj}. \tag{14}$$

$\boldsymbol{\xi}$ in this gauge can also be written in terms of $\boldsymbol{R}_\alpha, \widehat{\boldsymbol{E}}$ and their time derivatives from the constraint equation $\boldsymbol{L} + \boldsymbol{S} = 0$. The resulting expression, unlike (14), would be valid only within the constrained subspace.

Through (12), the gauge conditions determine the time dependence of $\{\theta_a\}$ so that, given a trajectory $(\{\boldsymbol{r}_\alpha(t)\}, \widehat{e}(t))$ of the system in the gauge $\boldsymbol{\xi} = 0$, we have $\mathfrak{S}_a(\{\boldsymbol{R}_\alpha(t)\}) = \mathfrak{S}_a(\{\boldsymbol{U}(\{\theta_a(t)\})\boldsymbol{r}_\alpha(t)\}) = 0$ for all t. We view (12) as a coordinate transformation in configuration space, specifying the new coordinates $\{\boldsymbol{R}_\alpha(\{\boldsymbol{r}_\alpha\})\}, \{\theta_a(\{\boldsymbol{r}_\alpha\})\}, \widehat{\boldsymbol{E}}(\{\boldsymbol{r}_\alpha\}, \widehat{e})$ in terms of the original ones $\{\boldsymbol{r}_\alpha\}, \widehat{e}$. The number of independent variables is the same in both sets, since the N position vectors $\{\boldsymbol{R}_\alpha\}$ are restricted by the three linear conditions $\mathfrak{S}_a(\{\boldsymbol{R}_\alpha\}) = 0$. From (12), we then have

$$\frac{\partial R_{\beta i}}{\partial r_{\alpha j}} = \delta_{\alpha\beta} U_{ij} + \frac{\partial U_{ik}}{\partial r_{\alpha j}} U_{lk} R_{\beta l}. \tag{15}$$

Substituting (15) into the relation $\partial\mathfrak{S}_a(\{\boldsymbol{R}_\beta\})/\partial r_{\alpha j} = 0$, and using the definition (9) for $\mathfrak{Q}$, the assumption (10) that it is invertible on the gauge manifold, and the antisymmetry of $(\partial U_{ik}/\partial r_{\alpha j} U_{lk})$ in i and l, we obtain the relation

$$\frac{\partial U_{ik}}{\partial r_{\alpha j}} U_{lk} = \sum_{a=1}^{3} \varepsilon_{ilm} \mathfrak{Q}^{-1}_{ma} m_\alpha \Gamma_{a\alpha n} U_{nj} \tag{16}$$

which expresses $\partial\boldsymbol{U}/\partial r_{\alpha j}\boldsymbol{U}^\dagger$ in terms of $\{\boldsymbol{R}_\gamma\}$ and $\{\theta_b\}$. This expression characterizes the dependence of $\boldsymbol{U}$ on $\{\boldsymbol{r}_\alpha\}$, and will be important below, especially in the discussion of angular momentum (see section 3.1). Unlike the two-dimensional case [1] in which the explicit form of $\boldsymbol{U}$ is easily found, (16) does not give us the explicit information about possible Gribov ambiguities of this gauge. Those ambiguities are analysed below (section 3.4), in connection with the derivation of the Hilbert-space inner product in this gauge.

The Lagrangian in this gauge is given by $\mathcal{L}$ in (3) with $\boldsymbol{r}_\alpha$ and $\widehat{e}$ substituted by $\boldsymbol{R}_\alpha$ and $\widehat{\boldsymbol{E}}$, according to our convention. Due to relation (14) between $\boldsymbol{\xi}$ and $\dot{\theta}_a$, we can use $\{\boldsymbol{R}_\alpha\}, \{\theta_a\}, \widehat{\boldsymbol{E}}$ as dynamical variables, the Lagrangian in terms of them being obtained by substituting $\boldsymbol{\xi} = \dot{\boldsymbol{U}}\boldsymbol{U}^\dagger$ in (3). Formulating the theory in those variables, however, would result in momenta p_{θ_a} conjugate to θ_a which are linearly related to $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$, not just $\boldsymbol{L}$. Furthermore, in the Hamiltonian formulation we have $[L_i, \widehat{\boldsymbol{E}}] \neq 0 = [J_i, \widehat{\boldsymbol{E}}]$. Thus, the gauge transformation (12) 'mixes' the particle degrees of freedom $\{\boldsymbol{R}_\alpha\}$ and $\{\theta_a\}$ with the rotator degrees of freedom $\widehat{\boldsymbol{E}}$. We can avoid such mixing by describing the rigid rotator in terms of its position vector in the lab frame. Once the dynamical variables in (3) have been appropriately capitalized, we set $\boldsymbol{\xi} = \dot{\boldsymbol{U}}\boldsymbol{U}^\dagger$ and $\widehat{\boldsymbol{E}} = \boldsymbol{U}\widehat{e}$ to obtain

$$\mathcal{L} = \mathcal{L}_N + \mathcal{L}_{\mathrm{rt}} \qquad \mathcal{L}_{\mathrm{rt}} = \frac{\mathcal{I}}{2}\dot{\widehat{e}}^2$$

$$\mathcal{L}_N = \frac{1}{2}\sum_{\alpha=1}^{N} m_\alpha \dot{\boldsymbol{R}}_\alpha^2 + \frac{1}{2}\sum_{\alpha=1}^{N} m_\alpha \left(\boldsymbol{R}_\alpha^2 \delta_{ij} - R_{\alpha i} R_{\alpha j}\right) \sum_{c,d=1}^{3} \Lambda_{ci}\Lambda_{dj}\dot{\theta}_c\dot{\theta}_d$$
$$- \sum_{\alpha=1}^{N} m_\alpha \varepsilon_{ijk} R_{\alpha j}\dot{R}_{\alpha k} \sum_{c=1}^{3} \Lambda_{ci}\dot{\theta}_c - \mathcal{V}. \tag{17}$$

This Lagrangian, with the gauge conditions (8) holding as strong (operator) equalities and the constraint $\boldsymbol{J} = 0$ valid as a weak (state space) equality describes the same dynamics as (3). The formulation based on (17), with $\{\boldsymbol{R}_\alpha\}, \{\theta_a\}, \widehat{e}$ as dynamical variables, closely follows the treatment of non-Abelian Yang–Mills theories in non-covariant linear gauges given in [6].

3.1. Angular and linear momenta

In the quantum theory in the gauge $\boldsymbol{\xi} = 0$, as discussed in section 2.1, the angular momentum operator $\boldsymbol{l}$ satisfies the usual commutator algebra. Using (16), the definition (9) of $\mathfrak{Q}$, and the unimodularity of $\boldsymbol{U}$, we obtain

$$[l_i, U_{jk}] = \sum_{\alpha=1}^{N} \varepsilon_{ilm} r_{\alpha l} \frac{1}{\mathrm{i}} \frac{\partial U_{jk}}{\partial r_{\alpha m}} = \mathrm{i}\varepsilon_{ikn} U_{jn}. \tag{18}$$

From (18), using $\boldsymbol{L} = \boldsymbol{U}\boldsymbol{l}$ and $\boldsymbol{R}_\alpha = \boldsymbol{U}\boldsymbol{r}_\alpha$, we get

$$\begin{aligned} &[L_i, U_{jk}] = -\mathrm{i}\varepsilon_{ijn} U_{nk} \qquad [l_i, R_{\alpha j}] = 0 = [L_i, R_{\alpha j}] \\ &[l_i, l_j] = \mathrm{i}\varepsilon_{ijk} l_k \qquad [l_i, L_j] = 0 \qquad [L_i, L_j] = -\mathrm{i}\varepsilon_{ijk} L_k. \end{aligned} \tag{19}$$

As expected, the particle position vectors $\boldsymbol{R}_\alpha$ in this gauge are rotation invariant. The commutators among components of $\boldsymbol{l}$ and $\boldsymbol{L}$ are the same as for a rigid body, with $\boldsymbol{l}$ the angular momentum in the laboratory and $\boldsymbol{L}$ in the body frame. Furthermore, taking into account the commutators (7) for $\boldsymbol{s}$, $[\boldsymbol{s}, \boldsymbol{U}] = 0$, $\boldsymbol{S} = \boldsymbol{U}\boldsymbol{s}$ and $\boldsymbol{J} \equiv \boldsymbol{L} + \boldsymbol{S} = \boldsymbol{U}\boldsymbol{j}$, we have

$$\begin{aligned} &[S_i, S_j] = \mathrm{i}\varepsilon_{ijk} S_k \qquad [L_i, S_j] = -\mathrm{i}\varepsilon_{ijk} S_k \\ &[J_i, J_j] = -\mathrm{i}\varepsilon_{ijk} J_k \qquad [J_i, L_j] = -\mathrm{i}\varepsilon_{ijk} J_k \qquad [J_i, S_j] = 0. \end{aligned} \tag{20}$$

Note that $[\boldsymbol{L}, \boldsymbol{S}] \neq 0$, due to the dependence of $\boldsymbol{S}$ on the angles $\{\theta_a\}$. The classical expressions for $\boldsymbol{L}$ and $p_{\theta a}$ follow immediately from the Lagrangian (17) and (5),

$$p_{\theta a} = -\Lambda_{ai} L_i \qquad L_i = \sum_{\alpha=1}^{N} m_\alpha \varepsilon_{ijk} R_{\alpha j} \dot{R}_{\alpha k} - \sum_{\alpha=1}^{N} m_\alpha \left(\boldsymbol{R}_\alpha^2 \delta_{ij} - R_{\alpha i} R_{\alpha j} \right) \widetilde{\xi}_j \tag{21}$$

with $\widetilde{\boldsymbol{\xi}}$ given by (14). By using the identity $\sum_{c=1}^{3} \partial \Lambda_{ci}/\partial\theta_a \dot{\theta}_c = \dot{\Lambda}_{ai} + \Lambda_{aj}\varepsilon_{ijk} \sum_{c=1}^{3} \dot{\theta}_c \Lambda_{ck}$, which follows from the definition (13) of Λ_{ai}, the equation of motion for θ_a from the Lagrangian (17) can be reduced to the form $D_t \boldsymbol{L} = 0$, in agreement with (6). In the quantum theory,

$$p_{\theta a} = \frac{1}{\mathrm{i}} \frac{\partial}{\partial\theta_a} \qquad L_i = \sum_{a=1}^{3} \Lambda_{ia}^{-1} \mathrm{i} \frac{\partial}{\partial\theta_a}. \tag{22}$$

Similarly, $p_{\theta a} = -\lambda_{ai} l_i$ and $l_i = \sum_{a=1}^{3} \lambda_{ia}^{-1} \mathrm{i}\partial/\partial\theta_a$. Equations (18)–(22) are completely analogous to the relations among colour currents in Yang–Mills theories in non-covariant gauges (see equations (4.44)–(4.48) and (4.55) in [6]).

In the classical theory, we obtain the momenta $\boldsymbol{P}_\alpha$ conjugate to $\boldsymbol{R}_\alpha$ by differentiating (17) (or, equivalently, (3)) with respect to $\dot{\boldsymbol{R}}_\alpha$ under the constraints $\dot{\mathfrak{S}}_a(\{\boldsymbol{R}_\alpha\}) = \mathfrak{S}_a(\{\dot{\boldsymbol{R}}_\alpha\}) = 0$ to obtain

$$P_{\alpha i} = m_\alpha \dot{R}_{\alpha i} - m_\alpha \widetilde{\xi}_j \left(\varepsilon_{ijk} R_{\alpha k} - \sum_{b=1}^{3} \frac{1}{\mathfrak{R}_b^2} \mathfrak{Q}_{bj} \Gamma_{b\alpha i} \right) \tag{23}$$

with $\mathfrak{Q}_{bj}$ and $\mathfrak{R}_b^2$ defined in (9) and (11). These momenta are consistent with the gauge condition, since they satisfy

$$0 = \sum_{\beta=1}^{N} \Gamma_{a\beta j} P_{\beta j} = \mathfrak{S}_a\left(\{\boldsymbol{P}_\alpha/m_\alpha\}\right). \tag{24}$$

From the transformation (12), we can obtain the relation between the velocities $\{\dot{\boldsymbol{r}}_\alpha\}$ in the gauge $\boldsymbol{\xi} = 0$, and those in the gauge $\mathfrak{S}_a = 0$, $\{\dot{\boldsymbol{R}}_\alpha\}$, $\{\dot{\theta}_a\}$. Correspondingly, we can express the momenta $\{\boldsymbol{p}_\alpha\}$ in one gauge in terms of the momenta $\{\boldsymbol{P}_\alpha\}$ and $\boldsymbol{L}$ in the other,

$$p_{\alpha j} = U_{kj}\left(P_{\alpha k} + \sum_{a=1}^{3} m_\alpha \Gamma_{a\alpha k}\mathfrak{Q}^{-1}_{na}(L_n - \Lambda_n)\right) \qquad \text{with} \quad \Lambda_n \equiv \sum_{\gamma=1}^{N} \varepsilon_{npq} R_{\gamma p} P_{\gamma q}. \tag{25}$$

The quantity[4] Λ_n defined by this equation has the appearance of an angular momentum but, as shown below, it does not satisfy the $so(3)$ commutation relations in general. With the transformation (25) for momenta we obtain from $\mathcal{H}_N$ in (7) the classical Hamiltonian for the particle system in this gauge,

$$\mathcal{H}_N = \sum_{\alpha=1}^{N} \frac{1}{2m_\alpha} \boldsymbol{P}_\alpha^2 + \frac{1}{2}\sum_{a=1}^{3} \mathfrak{R}_a^2 \mathfrak{Q}^{-1}_{ia}\mathfrak{Q}^{-1}_{ja}(L_i - \Lambda_i)(L_j - \Lambda_j) + \mathcal{V}. \tag{26}$$

The Hamiltonian $\mathcal{H}_{\rm rt}$ for the rigid rotator is clearly the same as in (7).

The transformations (12) and (25) can be inverted, to express $\boldsymbol{P}_\alpha$, $\boldsymbol{L}$, $\boldsymbol{R}_\alpha$ and θ_a in terms of $\boldsymbol{p}_\alpha$ and $\boldsymbol{r}_\alpha$. Using the Poisson brackets (7), we then get the Poisson brackets in this gauge. Alternatively, they can be found as Dirac brackets [16] relative to the set of second-class constraints $\mathfrak{S}_a(\{\boldsymbol{R}_\alpha\}) = 0 = \mathfrak{S}_a(\{\boldsymbol{P}_\alpha/m_\alpha\})$, $a = 1, 2, 3$. The results, written in the notation of quantum commutators, are

$$[R_{\alpha i}, P_{\beta j}] = \mathrm{i}\left(\delta_{\alpha\beta}\delta_{ij} - \sum_{a=1}^{3} \frac{m_\beta}{\mathfrak{R}_a^2}\Gamma_{a\alpha i}\Gamma_{a\beta j}\right). \tag{27}$$

All other commutators among $\boldsymbol{R}_\alpha$ and $\boldsymbol{P}_\beta$ vanish, and $[\boldsymbol{L}, \boldsymbol{R}_\alpha] = 0 = [\boldsymbol{L}, \boldsymbol{P}_\beta]$. From (27), we get

$$[\mathfrak{S}_a(\{\boldsymbol{R}_\alpha\}), P_{\beta j}] = 0 = [\mathfrak{S}_a(\{\boldsymbol{P}_\alpha/m_\alpha\}), R_{\beta j}] = [\Lambda_n, \mathfrak{S}_a(\{\boldsymbol{R}_\alpha\})] \tag{28a}$$

$$[\Lambda_i, \Lambda_j] = \mathrm{i}\varepsilon_{ijk}\Lambda_k - \mathrm{i}\sum_{\alpha=1}^{N}\sum_{a=1}^{3} \frac{1}{\mathfrak{R}_a^2}\Gamma_{a\alpha m}(\varepsilon_{imn}\mathfrak{Q}_{aj} - \varepsilon_{jmn}\mathfrak{Q}_{ai})P_{\alpha n}. \tag{28b}$$

We see that the gauge conditions (8), as well as (24), are operator equations, which can be evaluated within commutators. We also note that the definition (25) of $\boldsymbol{\Lambda}$ is free of ordering problems, even though the commutators (27) are not canonical, but its components Λ_i in general do not close an angular momentum algebra, as shown by (28*b*).

In the quantum theory, a realization of the commutators (27) is obtained by defining $\boldsymbol{P}_\alpha$ as the projection of the gradient ∇_α on the gauge hyperplane $\mathfrak{S}_a = 0$,

$$P_{\alpha j} = \frac{1}{\mathrm{i}}\frac{\partial}{\partial R_{\alpha j}} - \sum_{a=1}^{3} m_\alpha \Gamma_{a\alpha j}\frac{1}{\mathfrak{R}_a^2}\sum_{\beta=1}^{N}\Gamma_{a\beta k}\frac{1}{\mathrm{i}}\frac{\partial}{\partial R_{\beta k}}. \tag{29}$$

These operators satisfy both (27) and the gauge condition (24). They also satisfy relation (25) which, with $p_{\alpha j} = -\mathrm{i}\partial/\partial r_{\alpha j}$, is simply the chain rule for derivatives with respect to variables related by the transformation (12). Relations exactly analogous to (27) and (29) hold in Yang–Mills theories (compare (29) with equations between (6.13) and (6.14) in [6]).

3.2. Quantum Hamiltonian

The classical Hamiltonian in this gauge, (26), was obtained from $\mathcal{H}_N$ in the gauge $\boldsymbol{\xi} = 0$ by using the transformation (25). The Hamiltonian operator can in principle be computed in a similar fashion, essentially by squaring (25) as an operator equation. That procedure works

[4] There should be no possibility of confusion between the three-component operator $\boldsymbol{\Lambda}$ defined in (25) and the 3×3 matrix Λ_{ai} defined in (13).

satisfactorily in the two-dimensional case [1], but in three dimensions a more systematic approach is needed in order to handle the much larger amount of algebra required. The main difference between the two cases is that in two dimensions the operator Λ analogous to $\mathbf{\Lambda}$ in (25) commutes with the Faddeev–Popov determinant [1], but that is not the case in three dimensions. Following [6] we will first formulate the theory in terms of an appropriate set of independent generalized coordinates and their conjugate momenta. The results obtained in this intermediate step, which are of interest by themselves, will be transformed afterwards to the variables $\{\boldsymbol{R}_\alpha\}$ and $\{\theta_a\}$.

The gauge conditions (8) are defined by $9N$ constants $\Gamma_{a\alpha i}$, $a = 1, 2, 3, \alpha = 1, \ldots, N$, which constitute a set of three vectors $\mathbf{\Gamma}_a$ with $3N$ components $\Gamma_{a\alpha i}$ each, orthogonalized according to (11). We extend the set $\{\mathbf{\Gamma}_a\}_{a=1}^3$ to an orthogonal basis $\{\mathbf{\Gamma}_a\}_{a=1}^{3N}$ of $\mathbb{R}^{3N}$ by arbitrarily choosing $3(N-1)$ additional vectors $\{\mathbf{\Gamma}_b\}_{b=4}^{3N}$ satisfying the orthogonality and completeness relations,

$$\sum_{\alpha=1}^{N} m_\alpha \Gamma_{a\alpha j}\Gamma_{b\alpha j} = \mathfrak{R}_a^2\delta_{ab} \quad 1 \leqslant a, b \leqslant 3N \qquad \sum_{a=1}^{3N} \frac{m_\alpha m_\beta}{\mathfrak{R}_a^2}\Gamma_{a\alpha i}\Gamma_{a\beta j} = m_\alpha\delta_{\alpha\beta}\delta_{ij} \tag{30}$$

which generalize (11). We assume, for simplicity, that $\mathfrak{R}_4^2 = \cdots = \mathfrak{R}_{3N}^2 \equiv \mathfrak{R}^2$, with $\mathfrak{R}^2 > 0$ an arbitrary constant. Furthermore, we choose all $\Gamma_{a\alpha i}$ to have dimensions of length, so that $\mathfrak{S}_a$, $\mathfrak{Q}_{ai}$ and $\mathfrak{R}_a^2$ all have the dimensions of an inertia moment. We define a set of generalized coordinates q_a, $1 \leqslant a \leqslant 3N$, in the laboratory gauge $\boldsymbol{\xi} = 0$ by

$$r_{\alpha i}(t) = \sum_{a=1}^{3N} q_a(t)\frac{\Gamma_{a\alpha i}}{\mathfrak{R}_a} \qquad q_c(t) = \sum_{\alpha=1}^{N}\frac{m_\alpha}{\mathfrak{R}_c}\Gamma_{c\alpha i}r_{\alpha i}(t) \quad 1 \leqslant c \leqslant 3N. \tag{31}$$

Similarly, we introduce $3N-3$ independent generalized coordinates in the gauge (8) by

$$R_{\alpha i}(t) = \sum_{a=4}^{3N} Q_a(t)\Gamma_{a\alpha i} \qquad Q_c(t) = \sum_{\alpha=1}^{N}\frac{m_\alpha}{\mathfrak{R}^2}\Gamma_{c\alpha i}R_{\alpha i}(t) \quad 4 \leqslant c \leqslant 3N. \tag{32}$$

Due to the orthogonality relations (30), expression (32) for $\boldsymbol{R}_\alpha$ satisfies the gauge conditions (8). The dynamics in this gauge are completely specified by the $3N$ independent variables $\{\theta_a\}_{a=1}^3$ and $\{Q_a\}_{a=4}^{3N}$, and their conjugate momenta. Note that the normalization of the coordinates q_a and Q_a is different. In (32), the Q_a are chosen to be dimensionless, for later convenience, whereas in (31) the q_a are defined so that the kinetic energy operator takes the simplest possible form, that of a Laplacian in Cartesian coordinates.

The Hamiltonian $\mathcal{H}_N$ in the laboratory frame, (7), is given in terms of q_a by

$$\mathcal{H}_N = -\frac{1}{2}\sum_{a=1}^{3N}\frac{\partial^2}{\partial q_a^2} + \mathcal{V}$$

from whence the expression for $\mathcal{H}_N$ in terms of $\{\theta_a\}$ and $\{Q_a\}$ follows by means of a coordinate transformation. The kinetic energy operator then takes the standard form of a Laplacian in curvilinear coordinates in configuration space. As shown in appendix A, the result can be written as

$$\mathcal{H}_N = -\frac{1}{2\mathfrak{R}^2\mathcal{J}}\sum_{a=4}^{3N}\frac{\partial}{\partial Q_a}\mathcal{J}\frac{\partial}{\partial Q_a} - \frac{1}{2|\Lambda|\mathcal{J}}\left(\frac{1}{\mathfrak{R}^2}\sum_{a=4}^{3N}\frac{\partial}{\partial Q_a}\mathfrak{Q}_{ai} + \sum_{b=1}^{3}\frac{\partial}{\partial\theta_b}\Lambda_{ib}^{-1}\right)\mathcal{N}_{ij}^{-1}|\Lambda|\mathcal{J}$$
$$\times\left(\frac{1}{\mathfrak{R}^2}\sum_{c=4}^{3N}\mathfrak{Q}_{cj}\frac{\partial}{\partial Q_c} + \sum_{d=1}^{3}\Lambda_{jd}^{-1}\frac{\partial}{\partial\theta_d}\right) + \mathcal{V} \tag{33}$$

where $|\Lambda| = \det(\Lambda_{ai})$ with Λ_{ai} defined in (13) and $\mathcal{J} = \det(\mathcal{N})^{1/2}$ with

$$\mathcal{N}_{hi} = \sum_{c=1}^{3} \frac{1}{\mathfrak{R}_c^2} \mathfrak{Q}_{ch} \mathfrak{Q}_{ci} \qquad \mathcal{N}_{jk}^{-1} = \sum_{d=1}^{3} \mathfrak{R}_d^2 \mathfrak{Q}_{jd}^{-1} \mathfrak{Q}_{kd}^{-1}. \tag{34}$$

The quantities $\mathfrak{Q}_{ai}$ with $4 \leqslant a \leqslant 3N$ appearing in (33) are defined as in equation (9), of which they are an extension to $a \geqslant 4$. The inverse matrix $\mathfrak{Q}_{ia}^{-1}$, however, is defined only for $a \leqslant 3$. Expression (33) for $\mathcal{H}_N$ depends explicitly on the constants $\Gamma_{\alpha\alpha i}$ with $a \geqslant 4$ through $\mathfrak{Q}_{ai}$ with $a \geqslant 4$ and on the parametrization of $\boldsymbol{U}(\{\theta_a\})$ through Λ_{kc}^{-1}, both of which are largely arbitrary. Those dependences will disappear once we recast $\mathcal{H}_N$ in terms of $\boldsymbol{P}_\alpha$ and $\boldsymbol{L}$.

Using the relation, valid for any matrix depending on a parameter,

$$\frac{\partial|\Lambda|}{\partial\theta_a} = |\Lambda| \sum_{b=1}^{3} \Lambda_{nb}^{-1} \frac{\partial\Lambda_{bn}}{\partial\theta_a} \tag{35}$$

we obtain (compare (4.48) of [6])

$$\sum_{b=1}^{3} \left[p_{\theta_b}, |\Lambda|\Lambda_{jb}^{-1}\right] = \sum_{b=1}^{3} \frac{1}{\mathrm{i}} \frac{\partial\left(|\Lambda|\Lambda_{jb}^{-1}\right)}{\partial\theta_b} = 0 \tag{36}$$

and hence, using (22),

$$\frac{1}{|\Lambda|} \sum_{b=1}^{3} \frac{\partial}{\partial\theta_b} |\Lambda|\Lambda_{jb}^{-1} = \sum_{b=1}^{3} \Lambda_{jb}^{-1} \frac{\partial}{\partial\theta_b} = -\mathrm{i}L_j. \tag{37}$$

Therefore, we can rewrite $\mathcal{H}_N$ in terms of $\boldsymbol{L}$ as

$$\mathcal{H}_N = -\frac{1}{2\mathfrak{R}^2\mathcal{J}} \sum_{a=4}^{3N} \frac{\partial}{\partial Q_a} \mathcal{J} \frac{\partial}{\partial Q_a} - \frac{1}{2\mathcal{J}} \left(\frac{1}{\mathfrak{R}^2} \sum_{a=4}^{3N} \frac{\partial}{\partial Q_a} \mathfrak{Q}_{ai} - \mathrm{i}L_i \right) \mathcal{N}_{ij}^{-1} \mathcal{J} \left(\frac{1}{\mathfrak{R}^2} \sum_{c=4}^{3N} \mathfrak{Q}_{cj} \frac{\partial}{\partial Q_c} - \mathrm{i}L_j \right) + \mathcal{V} \tag{38}$$

thus eliminating all explicit dependence of $\mathcal{H}_N$ on Λ_{ia}^{-1} and the parametrization of $\boldsymbol{U}(\{\theta_a\})$. Applying the chain rule, from (32) we have

$$\frac{\partial}{\partial Q_c} = \sum_{\alpha=1}^{N} \Gamma_{c\alpha i} \frac{\partial}{\partial R_{\alpha i}} \qquad 4 \leqslant c \leqslant 3N. \tag{39}$$

The fact that the $\boldsymbol{R}_\alpha$ are not independent, being related by (8), does not affect (39) because of the orthogonality relations (30). Using the definition (29) of $\boldsymbol{P}_\alpha$ and the completeness relation (30), we get

$$P_{\beta j} = \sum_{c=4}^{3N} \frac{m_\beta}{\mathfrak{R}^2} \Gamma_{c\beta j} \frac{1}{\mathrm{i}} \frac{\partial}{\partial Q_c} \qquad \frac{1}{\mathrm{i}} \frac{\partial}{\partial Q_d} = \sum_{\beta=1}^{N} \Gamma_{d\beta j} P_{\beta j} \quad 4 \leqslant d \leqslant 3N \tag{40}$$

and from (40) and completeness,

$$\frac{1}{\mathfrak{R}^2} \sum_{a=4}^{3N} \frac{1}{\mathrm{i}} \frac{\partial}{\partial Q_a} \mathfrak{Q}_{ai} = \frac{1}{\mathfrak{R}^2} \sum_{c=4}^{3N} \mathfrak{Q}_{ci} \frac{1}{\mathrm{i}} \frac{\partial}{\partial Q_c} = \Lambda_i \tag{41}$$

with Λ_i given by (25). Substituting (40) and (41) into $\mathcal{H}_N$ in (38), we finally obtain

$$\mathcal{H}_N = \sum_{\alpha=1}^{N} \frac{1}{2m_\alpha\mathcal{J}} P_{\alpha i} \mathcal{J} P_{\alpha i} + \frac{1}{2\mathcal{J}} (L_i - \Lambda_i) \mathcal{N}_{ij}^{-1} \mathcal{J} (L_j - \Lambda_j) + \mathcal{V} \tag{42}$$

in which all dependence on $\{\Gamma_{a\alpha i}\}_{a=4}^{3N}$ has disappeared. The total Hamiltonian in this gauge is $\mathcal{H} = \mathcal{H}_N + \mathcal{H}_{\rm rt}$, with $\mathcal{H}_{\rm rt}$ from (7). Since $\boldsymbol{s}$ is a constant of the motion we can let $\mathcal{I} \to \infty$ with $\boldsymbol{s}$ fixed, so that $\mathcal{H}_{\rm rt}$ vanishes. We are then left with an N-body system described by $\mathcal{H}_N$ and the constraint $\boldsymbol{L}|\,\rangle = -\boldsymbol{S}|\,\rangle = -\boldsymbol{U}(\{\theta_a\})\boldsymbol{s}|\,\rangle$ on the state space, with $\dot{\boldsymbol{s}} = [\mathcal{H}_N, \boldsymbol{s}] = 0$. We now turn to this constraint equation.

3.3. Constraint and physical Hilbert space

The wavefunction in this gauge $\psi(\{\boldsymbol{R}_\alpha\}, \{\theta_a\}, \widehat{\boldsymbol{e}})$ is required to satisfy the constraint $\boldsymbol{J}|\psi\rangle = (\boldsymbol{L} + \boldsymbol{S})|\psi\rangle = 0$, originating in the equation of motion (4*c*). Expressing $\boldsymbol{L}$ in terms of $p_{\theta a}$ as in (22), and using $\boldsymbol{S} = \boldsymbol{U}\boldsymbol{s}$ and (13), we can write the constraint explicitly as

$$\left(\mathrm{i}\frac{\partial}{\partial\theta_a} + \lambda_{ak}s_k\right)\psi(\{\boldsymbol{R}_\alpha\}, \{\theta_a\}, \widehat{\boldsymbol{e}}) = 0 \qquad a = 1, 2, 3. \tag{43}$$

We introduce the unitary operator $\mathcal{U}(\{\theta_a\})$ [6], depending on $\{\theta_a\}$ and acting on the Hilbert space of the rigid rotator, which satisfies the analogue in that Hilbert space of (13),

$$\frac{\partial\mathcal{U}}{\partial\theta_a}\mathcal{U}^\dagger = \mathrm{i}\lambda_{ak}s_k \qquad a = 1, 2, 3. \tag{44}$$

The matrix elements of $\mathcal{U}(\{\theta_a\})$ in the basis of eigenfuntions of $\boldsymbol{s}^2$, s_z, $\langle\widehat{\boldsymbol{e}}|s, s_z\rangle = Y_{ss_z}(\widehat{\boldsymbol{e}})$ are the matrices $D^s_{s_z's_z}(\{\theta_a\})$ (given, e.g., in [20] in terms of Euler angles). Defining the physical wavefunction $\widehat{\psi}(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{e}})$

$$\psi(\{\boldsymbol{R}_\alpha\}, \{\theta_a\}, \widehat{\boldsymbol{e}}) = \mathcal{U}(\{\theta_a\})\widehat{\psi}(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{e}}) \tag{45}$$

we see by direct substitution that (45) is a solution to the constraint equation (43) [6]. The wavefunctions $\widehat{\psi}(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{e}})$ span the physical Hilbert space of the system.

Some remarks about the form of the solution (45) to the constraint are in order. By definition $\widehat{\boldsymbol{E}} = \boldsymbol{U}(\{\theta_a\})\widehat{\boldsymbol{e}}$ and $\boldsymbol{S} = \boldsymbol{U}(\{\theta_a\})\boldsymbol{s}$. Since $[s_i, (\widehat{\boldsymbol{e}})_j] = \mathrm{i}\varepsilon_{ijk}(\widehat{\boldsymbol{e}})_k$, we have $[S_i, (\widehat{\boldsymbol{E}})_j] = \mathrm{i}\varepsilon_{ijk}(\widehat{\boldsymbol{E}})_k$ and from (18), $[L_k, (\widehat{\boldsymbol{E}})_l] = -\mathrm{i}\varepsilon_{kln}(\widehat{\boldsymbol{E}})_n$. From these relations, and taking into account that $\boldsymbol{s}$ is a differential operator on the Hilbert space of the rigid rotator, we obtain $\mathcal{U}(\{\theta_a\})\chi(\widehat{\boldsymbol{e}}) = \chi(\widehat{\boldsymbol{E}})$ for any $\chi(\widehat{\boldsymbol{e}})$. Thus, (45) can be rewritten as $\psi(\{\boldsymbol{R}_\alpha\}, \{\theta_a\}, \widehat{\boldsymbol{e}}) = \widehat{\psi}(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{E}})$. Had we formulated the theory in terms of $\{\boldsymbol{R}_\alpha\}$, $\{\theta_a\}$ and $\widehat{\boldsymbol{E}}$, the momenta conjugate to θ_a would have been $p_{\theta a} = -\Lambda_{ai}J_i$, instead of (21), and the constraint $\boldsymbol{J}\psi = 0$ would have led to ψ not depending on $\{\theta_a\}$, $\psi(\{\boldsymbol{R}_\alpha\}, \{\theta_a\}, \widehat{\boldsymbol{E}}) = \widehat{\psi}(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{E}})$, the same result as (45).

From (44) we obtain $[L_k, \mathcal{U}] = -S_k\mathcal{U}$, which leads to $\mathcal{U}^\dagger L_k\mathcal{U} = L_k - \mathcal{U}^\dagger S_k\mathcal{U}$. Either from this last equation or from the constraint, on the physical wavefunctions we have $\mathcal{U}^\dagger L_k\mathcal{U}\widehat{\psi} = -\mathcal{U}^\dagger S_k\mathcal{U}\widehat{\psi} = -s_k\widehat{\psi}$. Therefore, in the physical Hilbert space, the Hamiltonian (42) acquires the form

$$\widehat{\mathcal{H}}_N \equiv \mathcal{U}^\dagger\mathcal{H}_N\mathcal{U} = \sum_{\alpha=1}^{N}\frac{1}{2m_\alpha\mathcal{J}}P_{\alpha i}\mathcal{J}P_{\alpha i} + \frac{1}{2\mathcal{J}}(s_i + \Lambda_i)\mathcal{N}^{-1}_{ij}\mathcal{J}(s_j + \Lambda_j) + \mathcal{V}. \tag{46}$$

Similarly, we can write $\widehat{\mathcal{H}}_N$ in terms of the independent coordinates $\{Q_a\}$ and their conjugate momenta, by just substituting $-\boldsymbol{s}$ for $\boldsymbol{L}$ in (38). Thus, once the constraint has been solved the angular variables enter the dynamics only through the dependence of $\widehat{\mathcal{H}}_N$ on $\boldsymbol{s}$, the angular momentum of the rigid rotator in the lab frame. Note that although $\boldsymbol{s}$ is a constant of motion in the full Hilbert space of the theory, in general $[\boldsymbol{s}, \widehat{\mathcal{H}}_N] \neq 0$ because $[\boldsymbol{s}, \mathcal{U}] \neq 0$. Thus, although $\boldsymbol{s}^2$ can always be diagonalized simultaneously with $\widehat{\mathcal{H}}_N$ within the physical subspace, s_z in general cannot be diagonalized. The physical reason is that within the physical subspace the matrix elements of $\boldsymbol{s}$ are equal to those of $-\boldsymbol{L}$, which is not conserved.

3.4. Inner product in Hilbert space

In order to find the inner product in the gauge $\mathfrak{S}_a = 0$, we transform its expression (7) in the gauge $\boldsymbol{\xi} = 0$ by means of the Faddeev–Popov technique [19]. For that purpose, we first find an appropriate resolution of the identity over the group $SO(3)$, fixing on the way any Gribov ambiguities [11, 2] inherent in the gauge conditions. The invariant integration over $SO(3)$ is given by (see, e.g., [21])

$$\int_{SO(3)} \mathrm{d}g\, f(g) = \int \prod_{a=1}^{3} \mathrm{d}\theta_a |\Lambda| f(g(\{\theta_a\})) \tag{47}$$

where on the lhs the integration variable g takes values in $SO(3)$ and $f : SO(3) \to \mathbb{C}$. On the rhs of (47) the integration extends over all of parameter space and $|\Lambda| \equiv \det(\Lambda_{ai})$ with Λ_{ai} defined in (13). From (36) and (47), the operators $\boldsymbol{L}$ defined in (22) are Hermitian, $\int \prod_{a=1}^{3} \mathrm{d}\theta_a |\Lambda| \psi^* L_k \phi = \left(\int \prod_{a=1}^{3} \mathrm{d}\theta_a |\Lambda| \phi^* L_k \psi\right)^*$.

3.4.1. Resolution of the identity: singularities of the coordinate frame (Gribov ambiguities). With the integration measure (47), the resolution of the identity for the gauge (10) takes the form

$$1 = \int \prod_{a=1}^{3} \mathrm{d}\theta_a |\Lambda| \prod_{b=1}^{3} \delta\left(\frac{1}{\mathfrak{R}_b}\mathfrak{S}_b(\{\boldsymbol{U}(\theta)\boldsymbol{r}_\alpha\})\right) \mathcal{J}(\{\boldsymbol{U}(\theta)\boldsymbol{r}_\alpha\}) \Theta\left(\mathcal{J}(\{\boldsymbol{U}(\theta)\boldsymbol{r}_\alpha\})\right) \Theta(\mathcal{F}) \tag{48}$$

where the gauge conditions are conventionally written as $\mathfrak{S}_b/\mathfrak{R}_b$, and $\mathcal{J}(\{\boldsymbol{r}_\alpha\})$ is defined after (33). To obtain (48), let $\theta_0 = \{\theta_{0a}\}$ be a root to $\mathfrak{S}_b(\{\boldsymbol{U}(\theta_0)\boldsymbol{r}_\alpha\}) = 0$, $b = 1, 2, 3$, for some fixed $\{\boldsymbol{r}_\alpha\}$. Then,

$$\begin{aligned} \mathfrak{S}_b(\{\boldsymbol{U}(\theta_0 + \delta\theta)\boldsymbol{r}_\alpha\}) &= \sum_{\alpha=1}^{N} m_\alpha \Gamma_{b\alpha j} \delta r_{\alpha j} \\ \delta r_{\alpha j} = \sum_{c=1}^{3} \delta\theta_c \frac{\partial U_{jk}}{\delta\theta_c}(\theta_0) r_{\alpha k} &= \sum_{c=1}^{3} \delta\theta_c \Lambda_{cn} \varepsilon_{jnl} U_{lm}(\theta_0) r_{\alpha m} \end{aligned} \tag{49}$$

where for the last equality we used (13). Using (9), we rewrite (49) as

$$\frac{1}{\mathfrak{R}_b}\mathfrak{S}_b\left(\{\boldsymbol{U}(\theta_0 + \delta\theta)\boldsymbol{r}_\alpha\}\right) = \sum_{c=1}^{3} \delta\theta_c \frac{1}{\mathfrak{R}_b} \Lambda_{cn} \mathfrak{Q}_{bn}(\{\boldsymbol{U}(\theta_0)\boldsymbol{r}_\alpha\}) \tag{50}$$

so that

$$\begin{aligned} \det\left(\frac{\delta(\mathfrak{S}_b/\mathfrak{R}_b)}{\delta\theta_c}\right)_{\theta_0} &= |\Lambda| \det\left(\frac{1}{\mathfrak{R}_b}\mathfrak{Q}_{bn}(\{\boldsymbol{U}(\theta_0)\boldsymbol{r}_\alpha\})\right) \\ &= \frac{1}{\prod_{c=1}^{3} \mathfrak{R}_c} |\Lambda| \det(\mathfrak{Q}_{bn}(\{\boldsymbol{U}(\theta_0)\boldsymbol{r}_\alpha\})) \end{aligned} \tag{51}$$

and therefore

$$\prod_{b=1}^{3} \delta\left(\frac{1}{\mathfrak{R}_b}\mathfrak{S}_b(\{\boldsymbol{U}(\theta_0)\boldsymbol{r}_\alpha\})\right) = \sum_{\theta_0} \frac{\prod_{c=1}^{3} \mathfrak{R}_c}{|\Lambda| |\det(\mathfrak{Q})|} \prod_{a=1}^{3} \delta(\theta_a - \theta_{0a}) \tag{52}$$

where the sum extends over all roots θ_0. In order for the lhs of (48) to be 1, θ_0 must be unique. The linear gauge conditions, however, have in general Gribov ambiguities leading to a discrete set of roots θ_0. We assume that we have chosen the parametrization $\boldsymbol{U}(\{\theta_a\})$ so that $|\Lambda| > 0$. But $\det(\boldsymbol{\mathfrak{Q}})$ can vanish at some configurations $\{\boldsymbol{r}_\alpha\}$ at which the gauge conditions are singular. Given a configuration $\{\boldsymbol{R}'_\alpha = \boldsymbol{U}(\{\theta'_a\})\boldsymbol{r}_\alpha, \theta'_a\}$ with $\det(\boldsymbol{\mathfrak{Q}}) < 0$, we can always find a gauge-equivalent one $\{\boldsymbol{R}_\alpha = \boldsymbol{U}(\{\theta_a\})\boldsymbol{r}_\alpha, \theta_a\}$ with $\det(\boldsymbol{\mathfrak{Q}}) > 0$. Thus, we restrict ourselves to those configurations satisfying

$$0 < \frac{\det(\boldsymbol{\mathfrak{Q}})}{\prod_{c=1}^{3} \mathfrak{R}_c} = (\det(\boldsymbol{\mathcal{N}}))^{1/2} \equiv \mathcal{J}. \tag{53}$$

If this supplementary condition were enough to remove all ambiguities, together with (52) it would lead to (48). Unlike the two-dimensional case [1], however, choosing the sign of the Faddeev–Popov determinant $\mathcal{J}$ is in general not enough to remove the ambiguities. Further supplementary conditions may be required which are of the form $F_1 > 0, \ldots, F_r > 0$, where the F_j are r functions of the particle coordinates (as many as necessary to fix the gauge), such that for each j it is true that $F_j = 0$ implies $\mathcal{J} = 0$. This set of additional supplementary conditions is symbolized by the factor $\Theta(\mathcal{F})$ in (48).

A simple example will illustrate the previous discussion. Assume that for a system of $N \geqslant 3$ particles we want to choose a coordinate frame rotating so that particle 1 is on the X-axis and particle 2 is on the X–Z plane for all t. That frame is not well defined if particle 1 is at the origin or particle 2 is on the X-axis. The gauge conditions defining the frame are $\mathfrak{S}_1 \equiv R_{1Y} = 0$, $\mathfrak{S}_2 \equiv R_{1Z} = 0$, $\mathfrak{S}_3 \equiv R_{2Y} = 0$, leading to $\det(\boldsymbol{\mathfrak{Q}}) = -R_{1X}^2 R_{2Z}$. As expected, $\det(\boldsymbol{\mathfrak{Q}}) = 0$ if $R_{1X} = 0$ (1 is at the origin) or $R_{2Z} = 0$ (2 is on the X-axis). These singularities stem from the fact that there are four ways to choose the rotating frame, depending on whether we choose $R_{1X} \gtrless 0$, $R_{2Z} \gtrless 0$ for all t. By requiring $\mathcal{J} > 0$ we must have $R_{2Z} < 0$, which fixes the ambiguity only partially. In order to completely fix the gauge we have to impose a supplementary condition such as $F_1 \equiv R_{1X} > 0$. Clearly, $F_1 = 0$ implies $\det(\boldsymbol{\mathfrak{Q}}) = 0 = \mathcal{J}$. Alternatively, we may exploit the fact that if we do not impose the condition $R_{1X} > 0$ every configuration is counted twice (except for those with $R_{1X} = 0$ which are counted once, but they have zero measure and do not contribute to (48)). Thus, in this example, we may omit the factor $\Theta(\mathcal{F})$ on the rhs of (48) and set the lhs to 2.

The general case is analogous to the simple example above. We either have to include in (48) the factor $\Theta(\mathcal{F})$ appropriate to the gauge conditions, or replace it by a factor $1/(1 + N(\{\boldsymbol{R}_\alpha\}))$ with $N(\{\boldsymbol{R}_\alpha\})$ the number of gauge-equivalent copies of each configuration $\{\boldsymbol{R}_\alpha\}$ satisfying the gauge conditions and $\mathcal{J} > 0$ [11]. In those cases in which $N(\{\boldsymbol{R}_\alpha\})$ is a constant over all of configuration space (except maybe for a zero-measure set) we can omit those factors, absorbing them in the normalization of the inner product.

3.4.2. Inner product in Hilbert space. The inner product in this gauge is straightforward to obtain from (7) by using the Faddeev–Popov trick with the resolution of the identity (48). We briefly sketch the derivation in order to highlight the relationship among wavefunctions in the gauge $\boldsymbol{\xi} = 0$ and those in this gauge. We rewrite (7) as

$$\langle\phi|\psi\rangle = \kappa \int \prod_{\beta=1}^{N} \mathrm{d}^3\boldsymbol{r}'_\beta \, \mathrm{d}^2\widehat{\boldsymbol{e}} (\phi_0^*\psi_0)(\{\boldsymbol{U}(\theta_a)\boldsymbol{r}'_\beta\}, \widehat{\boldsymbol{e}}) \tag{54}$$

where $\kappa > 0$ is a normalization constant to be chosen later (in (7), $\kappa = 1$), and we performed a change of variables $\boldsymbol{r}'_\beta = \boldsymbol{U}(\theta_a)\boldsymbol{r}_\beta$ with $\boldsymbol{U}(\theta_a)$ an orthogonal matrix. (In (54) we temporarily introduced the notation ψ_0 for wavefunctions in the gauge $\boldsymbol{\xi} = 0$ for convenience.) Inserting (48) in (54), exchanging the order of integration, and changing variables back to $\boldsymbol{r}_\beta$, we get

$$\langle\phi|\psi\rangle = \kappa \int \prod_{a=1}^{3} \mathrm{d}\theta_a |\Lambda| \int \prod_{\beta=1}^{N} \mathrm{d}^3\boldsymbol{r}_\beta \, \mathrm{d}^2\widehat{\boldsymbol{e}} \prod_{b=1}^{3} \delta\left(\frac{1}{\mathfrak{R}_b}\mathfrak{S}_b\right) \mathcal{J}\Theta(\mathcal{J})\Theta(\mathcal{F})(\phi_0^*\psi_0)(\{\boldsymbol{r}_\beta\}, \widehat{\boldsymbol{e}}) \tag{55}$$

where we omitted the argument $\{\boldsymbol{r}_\beta\}$ in $\mathfrak{S}_b$ and $\mathcal{J}$ for brevity. We can now choose κ to be the reciprocal of the volume of the rotation group. Identifying, up to a phase factor, the physical wavefunction $\widehat{\psi}(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{e}}) = \psi_0(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{e}})$ for $\{\boldsymbol{R}_\alpha\}$ satisfying the gauge condition, we finally obtain

$$\langle\phi|\psi\rangle = \int \prod_{\beta=1}^{N} \mathrm{d}^3\boldsymbol{R}_\beta \, \mathrm{d}^2\widehat{\boldsymbol{e}} \prod_{b=1}^{3} \delta\left(\frac{1}{\mathfrak{R}_b}\mathfrak{S}_b\right) \mathcal{J}\Theta(\mathcal{J})\Theta(\mathcal{F})(\widehat{\phi}^*\widehat{\psi})(\{\boldsymbol{R}_\beta\}, \widehat{\boldsymbol{e}}). \tag{56}$$

This gives the inner product in the physical Hilbert space of the system. The matrix elements for the Hamiltonian can be computed with the operator $\widehat{\mathcal{H}}_N$ of (46) and the inner product (56). The Hermiticity of $\widehat{\mathcal{H}}_N$ with respect to (56) follows by partial integration, taking into account that $P_{\alpha i}$ and Λ_i are homogeneous first-order differential operators, with constant coefficients, satisfying $[P_{\alpha i}, \mathfrak{S}_b] = 0 = [\Lambda_i, \mathfrak{S}_b]$, and that $\mathcal{J}\delta(F_j) = 0$ since, as mentioned above, $F_j = 0$ implies $\mathcal{J} = 0$.

We also remark that for states satisfying the constraint $(\boldsymbol{L} + \boldsymbol{S})|\psi\rangle = 0$, using the definition (45) of the physical wavefunction and $\mathcal{U}^\dagger \boldsymbol{S}\mathcal{U} = \boldsymbol{s}$ we get the equality

$$\int \prod_{a=1}^{3} \mathrm{d}\theta_a |\Lambda| \int \mathrm{d}\mu\, \phi^*(\{\boldsymbol{R}_\alpha\}, \{\theta_a\}), \widehat{\boldsymbol{e}}) L_i \psi(\{\boldsymbol{R}_\alpha\}, \{\theta_a\}), \widehat{\boldsymbol{e}})$$
$$= \frac{1}{\kappa} \int \mathrm{d}\mu\, \widehat{\phi}^*(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{e}})(-s_i)\widehat{\psi}(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{e}}) \tag{57}$$

where we denoted by $\mathrm{d}\mu$ the measure appearing in (56). The factor $1/\kappa$ appears in (57) due to the normalization we chose for the inner product in the physical subspace. From (57), we see that for physical wavefunctions the operator $-\boldsymbol{s}$ gives the matrix elements of $\boldsymbol{L}$.

3.5. Reduced Hamiltonian and Weyl ordering: quantum potential

When working in curvilinear coordinates it is often convenient to redefine the state space by absorbing the Jacobian in the wavefunctions, thus eliminating it from the integration measure in the inner product and from the kinetic energy operator. That is the case, for instance, when a perturbative expansion of $\mathcal{J}$ contains terms of many different orders. Furthermore, the reduced Hamiltonian is easier to cast into Weyl-ordered form, in which the relation between the operator and path-integral approaches is straightforward.

The Hamiltonian (46) has been simplified by restricting it to the physical Hilbert space of gauge-invariant wavefunctions $\widehat{\psi}$, so it is not of the form of a Laplacian in curvilinear coordinates. Thus, we go back to the form (33) for $\mathcal{H}_N$, in which the angles $\{\theta_a\}$ and their conjugate momenta $p_{\theta a} = -\mathrm{i}\partial/\partial\theta_a$ appear explicitly. From (33) and (A.17), we get

$$\begin{aligned}\widetilde{\mathcal{H}}_N &\equiv |\Lambda|^{\frac{1}{2}}\mathcal{J}^{\frac{1}{2}}\mathcal{H}_N|\Lambda|^{-\frac{1}{2}}\mathcal{J}^{-\frac{1}{2}} \\ &= -\frac{1}{2\mathfrak{R}^2}\sum_{a=4}^{3N}\frac{\partial}{\partial Q_a}\frac{\partial}{\partial Q_a} - \frac{1}{2\mathfrak{R}^4}\sum_{a,b=4}^{3N}\left(\mathfrak{Q}_{aj}\mathfrak{Q}_{bk}\mathcal{N}_{jk}^{-1}\frac{\partial}{\partial Q_a}\frac{\partial}{\partial Q_b}\right)_W \\ &\quad - \frac{1}{2\mathfrak{R}^2}\sum_{a=4}^{3N}\sum_{b=1}^{3}\left(\mathfrak{Q}_{aj}\Lambda_{kb}^{-1}\mathcal{N}_{jk}^{-1}\frac{\partial}{\partial Q_a}\frac{\partial}{\partial\theta_b}\right)_W \\ &\quad - \frac{1}{2\mathfrak{R}^2}\sum_{a=1}^{3}\sum_{b=4}^{3N}\left(\Lambda_{ja}^{-1}\mathfrak{Q}_{bk}\mathcal{N}_{jk}^{-1}\frac{\partial}{\partial\theta_a}\frac{\partial}{\partial Q_b}\right)_W \\ &\quad - \frac{1}{2}\sum_{a,b=1}^{3}\left(\Lambda_{ja}^{-1}\Lambda_{kb}^{-1}\mathcal{N}_{jk}^{-1}\frac{\partial}{\partial\theta_a}\frac{\partial}{\partial\theta_b}\right)_W + V_Q + \mathcal{V}\end{aligned} \tag{58}$$

where V_Q is the quantum potential given below (see (65)) and $(\cdots)_W$ indicates Weyl ordering (e.g., (A.11)). Let us introduce the notation

$$\mathcal{D}^{\alpha}_{ij} \equiv \varepsilon_{ijk} R_{\alpha k} = \sum_{a=1}^{3N} \frac{1}{\mathfrak{R}_a^2} \Gamma_{a\alpha i} \mathfrak{Q}_{aj} \tag{59}$$

where the second equality follows from (9) and (30). With this definition and relations (40) and (24), we can rewrite (58) in terms of $\boldsymbol{P}_\alpha$ operators as

$$\begin{aligned}\widetilde{\mathcal{H}}_N = \sum_{\alpha=1}^{N} \frac{1}{2m_\alpha} \boldsymbol{P}_\alpha^2 + \frac{1}{2} \sum_{\alpha,\beta=1}^{N} \left(\mathcal{D}^{\alpha}_{ij} \mathcal{D}^{\beta}_{lk} \mathcal{N}^{-1}_{jk} P_{\alpha i} P_{\beta l}\right)_W + \sum_{b=1}^{3} \frac{1}{2} \left(\Lambda^{-1}_{kb} \frac{1}{\mathrm{i}} \frac{\partial}{\partial\theta_b} + \frac{1}{\mathrm{i}} \frac{\partial}{\partial\theta_b} \Lambda^{-1}_{kb}\right) \\ \times \sum_{\alpha=1}^{N} \frac{1}{2}\left(\mathcal{N}^{-1}_{jk} \mathcal{D}^{\alpha}_{ij} P_{\alpha i} + P_{\alpha i} \mathcal{N}^{-1}_{jk} \mathcal{D}^{\alpha}_{ij}\right) + \frac{1}{2} \mathcal{N}^{-1}_{jk} \sum_{a,b=1}^{3} \left(\Lambda^{-1}_{ja} \Lambda^{-1}_{kb} \frac{1}{\mathrm{i}} \frac{\partial}{\partial\theta_a} \frac{1}{\mathrm{i}} \frac{\partial}{\partial\theta_b}\right)_W + V_Q + \mathcal{V}.\end{aligned} \tag{60}$$

This operator is to be applied to wavefunctions of the form $\widetilde{\psi}(\{\boldsymbol{R}_\alpha\}, \{\theta_a\}, \widehat{\boldsymbol{e}}) = |\Lambda|^{1/2} \mathcal{J}^{1/2} \psi(\{\boldsymbol{R}_\alpha\}, \{\theta_a\}, \widehat{\boldsymbol{e}})$ or, using (45),

$$\widetilde{\psi}(\{\boldsymbol{R}_\alpha\}, \{\theta_a\}, \widehat{\boldsymbol{e}}) = |\Lambda|^{\frac{1}{2}} \mathcal{U}(\{\theta_a\}) \widehat{\widetilde{\psi}}(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{e}}) \qquad \text{with} \quad \widehat{\widetilde{\psi}}(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{e}}) \equiv \mathcal{J}^{\frac{1}{2}} \widehat{\psi}(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{e}}). \tag{61}$$

$\widehat{\widetilde{\psi}}$ is the reduced form of the physical wavefunction $\widehat{\psi}$ of (45).

From (36), we obtain the form of the angular momentum operator on the first line of (60) when applied to wavefunctions of the form (61)

$$\sum_{b=1}^{3} \frac{1}{2} \left(\Lambda^{-1}_{kb} \frac{1}{\mathrm{i}} \frac{\partial}{\partial\theta_b} + \frac{1}{\mathrm{i}} \frac{\partial}{\partial\theta_b} \Lambda^{-1}_{kb}\right) \widetilde{\psi} = -|\Lambda|^{\frac{1}{2}} L_k \mathcal{U}(\{\theta_a\}) \widehat{\widetilde{\psi}} = |\Lambda|^{\frac{1}{2}} \mathcal{U}(\{\theta_a\}) s_k \widehat{\widetilde{\psi}} \tag{62}$$

the second equality following from the discussion immediately above (46). After appropriately rearranging the angular operator on the second line of (60) we can apply (62) to it as well and, taking into account that $\mathcal{N}^{-1}_{ij}$ is symmetric, we get

$$\begin{aligned}\frac{1}{2} \mathcal{N}^{-1}_{jk} \sum_{a,b=1}^{3} \left(\Lambda^{-1}_{ja} \Lambda^{-1}_{kb} \frac{1}{\mathrm{i}} \frac{\partial}{\partial\theta_a} \frac{1}{\mathrm{i}} \frac{\partial}{\partial\theta_b}\right)_W \widetilde{\psi} &= -\frac{1}{8} \mathcal{N}^{-1}_{jk} \sum_{a,b=1}^{3} \left\{ \frac{\partial \Lambda^{-1}_{ja}}{\partial\theta_b} \frac{\partial \Lambda^{-1}_{kb}}{\partial\theta_a} \right. \\ &\quad \left. + \left(\Lambda^{-1}_{ja} \frac{\partial}{\partial\theta_a} + \frac{\partial}{\partial\theta_a} \Lambda^{-1}_{ja}\right) \left(\Lambda^{-1}_{kb} \frac{\partial}{\partial\theta_b} + \frac{\partial}{\partial\theta_b} \Lambda^{-1}_{kb}\right) \right\} \widetilde{\psi} \\ &= -\frac{1}{8} |\Lambda|^{\frac{1}{2}} \mathcal{U} \mathcal{N}^{-1}_{jk} \sum_{a,b=1}^{3} \frac{\partial \Lambda^{-1}_{ja}}{\partial\theta_b} \frac{\partial \Lambda^{-1}_{kb}}{\partial\theta_a} \widehat{\widetilde{\psi}} + \frac{1}{2} |\Lambda|^{\frac{1}{2}} \mathcal{U} \mathcal{N}^{-1}_{jk} s_j s_k \widehat{\widetilde{\psi}}.\end{aligned} \tag{63}$$

Thus, combining (60), (62) and (63) we obtain

$$\begin{aligned}\widetilde{\mathcal{H}}_N \widetilde{\psi} = |\Lambda|^{\frac{1}{2}} \mathcal{U}(\{\theta_a\}) \left\{ \sum_{\alpha=1}^{N} \frac{1}{2m_\alpha} \boldsymbol{P}_\alpha^2 + \frac{1}{2} \sum_{\alpha,\beta=1}^{N} \left(\mathcal{N}^{-1}_{jk} \mathcal{D}^{\alpha}_{lj} \mathcal{D}^{\beta}_{mk} P_{\alpha l} P_{\beta m}\right)_W \right. \\ + \frac{1}{2} \sum_{\alpha=1}^{N} \left(\mathcal{N}^{-1}_{jk} \mathcal{D}^{\alpha}_{lj} P_{\alpha l} + P_{\alpha l} \mathcal{N}^{-1}_{jk} \mathcal{D}^{\alpha}_{lj}\right) s_k \\ \left. + \frac{1}{2} \mathcal{N}^{-1}_{jk} s_j s_k - \frac{1}{8} \mathcal{N}^{-1}_{jk} \sum_{a,b=1}^{3} \frac{\partial \Lambda^{-1}_{ja}}{\partial\theta_b} \frac{\partial \Lambda^{-1}_{kb}}{\partial\theta_a} + V_Q + \mathcal{V} \right\} \widehat{\widetilde{\psi}}.\end{aligned} \tag{64}$$

The quantum potential is computed in appendix A.2, with the result

$$V_Q = \frac{1}{8}\mathcal{N}^{-1}_{jk}\sum_{a,b=1}^{3}\frac{\partial\Lambda^{-1}_{ja}}{\partial\theta_b}\frac{\partial\Lambda^{-1}_{kb}}{\partial\theta_a} + \mathcal{V}_1 + \mathcal{V}_2$$

$$\mathcal{V}_1 = -\frac{1}{8}\sum_{\alpha=1}^{N}\sum_{c,d=1}^{3} m_\alpha \mathfrak{Q}^{-1}_{l'c}\Gamma_{c\alpha l}\mathfrak{Q}^{-1}_{md}\Gamma_{d\alpha k}\varepsilon_{kl'p}\varepsilon_{plm}$$

$$\mathcal{V}_2 = \frac{-1}{8}\sum_{\beta,\gamma=1}^{N}\varepsilon_{nlk}\mathcal{N}^{-1}_{kh}\varepsilon_{hl'n'}\left(\delta_{\beta\gamma}\delta_{l'n} - \varepsilon_{l'gs}R_{\gamma s}\sum_{a=1}^{3}\mathfrak{Q}^{-1}_{ga}m_\beta\Gamma_{a\beta n}\right)$$
$$\times\left(\delta_{\beta\gamma}\delta_{n'l} - \varepsilon_{lmp}R_{\beta p}\sum_{b=1}^{3}\mathfrak{Q}^{-1}_{mb}m_\gamma\Gamma_{b\gamma n'}\right). \tag{65}$$

(Note that both $\mathcal{V}_{1,2}$ are $\mathcal{O}(|\boldsymbol{R}_\alpha|^{-2})$ as $|\boldsymbol{R}_\alpha| \to \infty$.) Thus, the Weyl-ordered, reduced Hamiltonian $\widehat{\widetilde{\mathcal{H}}}_N = \mathcal{J}^{1/2}\widehat{\mathcal{H}}_N\mathcal{J}^{-1/2} = \mathcal{U}^\dagger\widetilde{\mathcal{H}}_N\mathcal{U}$ acting on the space of reduced physical wavefunctions $\widehat{\widetilde{\psi}}(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{e}})$ is given by

$$\widehat{\widetilde{\mathcal{H}}}_N = \sum_{\alpha=1}^{N}\frac{1}{2m_\alpha}\boldsymbol{P}^2_\alpha + \frac{1}{2}\left(\left(\sum_{\beta=1}^{N}P_{\beta l}\mathcal{D}^{\beta}_{lj} + s_j\right)\mathcal{N}^{-1}_{jk}\left(\sum_{\gamma=1}^{N}\mathcal{D}^{\gamma}_{mk}P_{\gamma m} + s_k\right)\right)_W + \mathcal{V}_1 + \mathcal{V}_2 + \mathcal{V} \tag{66}$$

where the second term is, explicitly,

$$\frac{1}{2}(\cdots)_W = \frac{1}{8}\sum_{\beta,\gamma=1}^{N}\left(\mathcal{D}^{\beta}_{rj}\mathcal{N}^{-1}_{jk}\mathcal{D}^{\gamma}_{sk}P_{\beta r}P_{\gamma s} + 2P_{\beta r}\mathcal{D}^{\beta}_{rj}\mathcal{N}^{-1}_{jk}\mathcal{D}^{\gamma}_{sk}P_{\gamma s} + P_{\beta r}P_{\gamma s}\mathcal{D}^{\beta}_{rj}\mathcal{N}^{-1}_{jk}\mathcal{D}^{\gamma}_{sk}\right)$$
$$+ \frac{1}{4}\sum_{\beta=1}^{N}\left(\mathcal{N}^{-1}_{jk}\mathcal{D}^{\beta}_{rj}P_{\beta r} + P_{\beta r}\mathcal{N}^{-1}_{jk}\mathcal{D}^{\beta}_{rj}\right)s_k + \frac{1}{2}\mathcal{N}^{-1}_{jk}s_j s_k. \tag{67}$$

Given two states $|\phi\rangle$ and $|\psi\rangle$ represented by the reduced, physical wavefunctions $\widehat{\widetilde{\phi}}$, $\widehat{\widetilde{\psi}}$, their inner product is, according to (56) and (61),

$$\langle\phi|\psi\rangle = \int\prod_{\beta=1}^{N}\mathrm{d}^3\boldsymbol{R}_\beta\,\mathrm{d}^2\widehat{\boldsymbol{e}}\prod_{b=1}^{3}\delta\left(\frac{1}{\mathfrak{R}_b}\mathfrak{S}_b\right)\Theta(\mathcal{J})\Theta(\mathcal{F})\widehat{\widetilde{\phi}}^*(\{\boldsymbol{R}_\beta\},\widehat{\boldsymbol{e}})\widehat{\widetilde{\psi}}(\{\boldsymbol{R}_\beta\},\widehat{\boldsymbol{e}}). \tag{68}$$

The matrix elements of $\widehat{\widetilde{\mathcal{H}}}_N$ computed with this inner product are, of course, identical to those of the operator $\widehat{\mathcal{H}}_N$ of (46) computed with the inner product (56).

As pointed out before, there is a close formal analogy between the results given above for the quantum theory in reference frames defined by linear conditions and the corresponding results in Yang–Mills theories in non-covariant linear gauges. The derivation of the Hamiltonian given here parallels that of [6]. Thus, the quantum potentials $\mathcal{V}_{1,2}$ from (65) are formally analogous to the corresponding expressions (6.12) and (6.14) in [6]. The kinetic energy operator in (46) and in the Weyl-ordered form (66) are formally equivalent to (4.62) and (6.15) of [6], respectively. In order to make the formal analogy clear, we note that the space derivatives appearing in field-theoretic expressions must be mapped to zero in the mechanical case considered here. Thus, $\mathfrak{Q}_{ai}$ from (9) is the analogue of the expression $\Gamma_k\mathfrak{D}_k$ in the notation of [6]. From (25) and (59), $\Lambda_l = -\sum_{\alpha=1}^{N}m_\alpha\mathcal{D}^{\alpha}_{lj}P_{\alpha j}$, which is the analogue of $\mathfrak{D}_i P^l_i \sim -P^l_i\mathfrak{D}_i$ and, similarly, $\mathcal{N}^{-1}_{ij}$ from (34) is identified with $(\Gamma_k\mathfrak{D}_k)^{-1}\left(\Gamma_j\Gamma^\dagger_j\right)\left(\mathfrak{D}^\dagger_k\Gamma^\dagger_k\right)^{-1}$ in [6].

4. Centre of mass motion

In this section and the next one, we set $U = 0$ in the Lagrangian and take into account the translation invariance of (1) in order to separate the centre of mass degrees of freedom. Since the centre of mass motion is dynamically trivial, we restrict our treatment to dynamical states with vanishing total momentum.

The Lagrangian (1) is invariant under time-independent transformations of the Euclidean group,

$$\boldsymbol{r}'_\alpha = \boldsymbol{U}\boldsymbol{r}_\alpha + \boldsymbol{u} \qquad \widehat{\boldsymbol{e}}\,' = \boldsymbol{U}\widehat{\boldsymbol{e}} \tag{69}$$

with $\boldsymbol{U}$ an orthogonal matrix. We define the covariant derivatives

$$D_t\boldsymbol{r}_\alpha = \dot{\boldsymbol{r}}_\alpha - \boldsymbol{\xi}\boldsymbol{r}_\alpha - \boldsymbol{\rho} \qquad D_t\widehat{\boldsymbol{e}} = \dot{\widehat{\boldsymbol{e}}} - \boldsymbol{\xi}\widehat{\boldsymbol{e}}. \tag{70}$$

Under time-dependent transformations $\boldsymbol{r}_\alpha$ and $\widehat{\boldsymbol{e}}$ transform as in (69), and

$$\begin{aligned} &\boldsymbol{\xi}' = \boldsymbol{U}\boldsymbol{\xi}\boldsymbol{U}^\dagger + \dot{\boldsymbol{U}}\boldsymbol{U}^\dagger \qquad && \boldsymbol{\rho}' = \boldsymbol{U}\boldsymbol{\rho} + \dot{\boldsymbol{u}} - \boldsymbol{\xi}'\boldsymbol{u} \\ &(D_t\boldsymbol{r}_\alpha)' = \boldsymbol{U}D_t\boldsymbol{r}_\alpha && (D_t\widehat{\boldsymbol{e}})' = \boldsymbol{U}D_t\widehat{\boldsymbol{e}}. \end{aligned} \tag{71}$$

Substituting time derivatives by covariant ones in (1) we obtain a Lagrangian invariant under the time-dependent transformations (69) and (71),

$$\mathcal{L} = \mathcal{L}_N + \mathcal{L}_{\mathrm{rt}} + \mathcal{L}_{\mathrm{cm}} \qquad \mathcal{L}_{\mathrm{cm}} = \frac{1}{2}\sum_{\alpha=1}^{N} m_\alpha \boldsymbol{\rho}^2 - \boldsymbol{\rho}\cdot\sum_{\alpha=1}^{N} m_\alpha(\dot{\boldsymbol{r}}_\alpha - \boldsymbol{\xi}\boldsymbol{r}_\alpha) \tag{72}$$

where $\mathcal{L}_N$ and $\mathcal{L}_{\mathrm{rt}}$ have the same form as in (3). The equations of motion for $\boldsymbol{r}_\alpha$ and $\widehat{\boldsymbol{e}}$ take the form (4) when expressed in terms of covariant derivatives, but in this case the derivation is slightly more involved because now $D_t\boldsymbol{r}_\alpha$ as given by (70) does not depend linearly on $\boldsymbol{r}_\alpha$ but, rather, affinely (see appendix B). The angular momenta $\boldsymbol{l}$ and $\boldsymbol{s}$ are still given by (5), with $D_t\boldsymbol{r}_\alpha$ from (70). We define $\boldsymbol{l}_{\mathrm{cm}} = M\boldsymbol{r}_{\mathrm{cm}} \wedge D_t\boldsymbol{r}_{\mathrm{cm}}$, where $\boldsymbol{r}_{\mathrm{cm}}$ is the centre of mass position, $D_t\boldsymbol{r}_{\mathrm{cm}} = \dot{\boldsymbol{r}}_{\mathrm{cm}} - \boldsymbol{\xi}\boldsymbol{r}_{\mathrm{cm}} - \boldsymbol{\rho}$, and $M = \sum_{\alpha=1}^N m_\alpha$. As shown in appendix B, the equations of motion lead to

$$\left(\frac{\mathrm{d}}{\mathrm{d}t} - \boldsymbol{\xi}\right)(\boldsymbol{l} - \boldsymbol{l}_{\mathrm{cm}}) = 0 = \left(\frac{\mathrm{d}}{\mathrm{d}t} - \boldsymbol{\xi}\right)\boldsymbol{s} \tag{73}$$

which is the same as (6), with $(\boldsymbol{l} - \boldsymbol{l}_{\mathrm{cm}})$ instead of $\boldsymbol{l}$. Thus, the magnitudes of $(\boldsymbol{l} - \boldsymbol{l}_{\mathrm{cm}})$ and $\boldsymbol{s}$ are both conserved and frame independent. Due to the fact that we are now including (time-dependent) translations as symmetries of the system, the role played by $\boldsymbol{l}$ in sections 2 and 3 is now played by $(\boldsymbol{l} - \boldsymbol{l}_{\mathrm{cm}})$. The equations of motion for $\boldsymbol{\xi}$ and $\boldsymbol{\rho}$ are now of the form $\boldsymbol{l} + \boldsymbol{s} = 0$ and $\boldsymbol{p}_{\mathrm{cm}} = 0$ (with $\boldsymbol{p}_{\mathrm{cm}} = MD_t\boldsymbol{r}_{\mathrm{cm}}$). Thus, in particular $\boldsymbol{l}_{\mathrm{cm}} = 0$ and, like in section 2, the total angular momentum of the system vanishes.

If we choose the gauge conditions $\boldsymbol{\xi} = 0 = \boldsymbol{\rho}$, corresponding to the laboratory frame, we recover the Lagrangian (1), constrained by the equations of motion for $\boldsymbol{\xi}$ and $\boldsymbol{\rho}$ in this gauge,

$$\sum_{\alpha=1}^{N} m_\alpha \boldsymbol{r}_\alpha \wedge \dot{\boldsymbol{r}}_\alpha + \mathcal{I}\widehat{\boldsymbol{e}} \wedge \dot{\widehat{\boldsymbol{e}}} \equiv \boldsymbol{l} + \boldsymbol{s} = 0 \qquad \sum_{\alpha=1}^{N} m_\alpha \dot{\boldsymbol{r}}_\alpha = 0. \tag{74}$$

These constraints are first class. In the quantum theory they restrict the state space, $(\boldsymbol{l} + \boldsymbol{s})\psi = 0$, $\sum_{\alpha=1}^N \nabla_\alpha\psi = 0$, analogous to the Gauss law in Yang–Mills theories [6]. Except for the additional constraint on the centre of mass momentum, the quantization in this gauge is carried out exactly as in section 2.1.

We can now proceed along the same lines as in section 3, imposing on the system the gauge conditions

$$\mathfrak{S}_a(\{\boldsymbol{R}_\alpha\}) = 0 \quad a = 1, 2, 3 \qquad \mathfrak{C}(\{\boldsymbol{R}_\alpha\}) \equiv \frac{1}{M}\sum_{\beta=1}^{N} m_\beta \boldsymbol{R}_\beta = 0 \tag{75}$$

with $\mathfrak{S}_a$ defined in (8). Equation (75) defines a reference frame in a particular state of rotation, with origin at the centre of mass. Like in section 3, in the rest of this section we denote vectors referred to this frame by capital letters, while lower-case symbols denote lab frame quantities. The gauge conditions (75) are not mutually consistent unless $\mathfrak{S}_a$ are translation invariant,

$$\sum_{\alpha=1}^{N} m_\alpha \Gamma_{a\alpha j} = 0 \qquad a = 1, 2, 3 \tag{76}$$

the condition $\mathfrak{C} = 0$ being clearly rotationally invariant. Furthermore, we assume that $\mathfrak{S}_a$ satisfy (10) and (11). The gauge transformation from the gauge $\boldsymbol{\xi} = 0 = \boldsymbol{\rho}$ is of the form (69)–(71), with parameter $\boldsymbol{u} = -\boldsymbol{U}\boldsymbol{r}_{\mathrm{cm}}$, where $\boldsymbol{r}_{\mathrm{cm}} = \sum_{\alpha=1}^{N} m_\alpha/M\boldsymbol{r}_\alpha$ is the centre of mass in the lab frame,

$$\boldsymbol{R}_\alpha = \boldsymbol{U}(\boldsymbol{r}_\alpha - \boldsymbol{r}_{\mathrm{cm}}) \qquad \widehat{\boldsymbol{E}} = \boldsymbol{U}\widehat{\boldsymbol{e}} \qquad \boldsymbol{\xi} = \dot{\boldsymbol{U}}\boldsymbol{U}^\dagger \qquad \boldsymbol{\rho} = -\boldsymbol{U}\dot{\boldsymbol{r}}_{\mathrm{cm}}. \tag{77}$$

The transformation (77) mixes the particle degrees of freedom $\boldsymbol{R}_\alpha$ with those of the centre of mass and the rigid rotator, just like (12) did in the non-translation-invariant case. In particular, in these variables p_{θ_a} is not linearly related to $\boldsymbol{L}$. That mixing is avoided, as in section 3, by trading the dynamical variables $\{\boldsymbol{R}_\alpha\}$, $\widehat{\boldsymbol{E}}$, $\boldsymbol{\xi}$, $\boldsymbol{\rho}$ for $\{\boldsymbol{R}_\alpha\}$, $\widehat{\boldsymbol{e}}$, $\{\theta_a\}$, $\boldsymbol{r}_{\mathrm{cm}}$. Substituting the last three of (77) into the Lagrangian (72) we get

$$\mathcal{L} = \mathcal{L}_N + \mathcal{L}_{\mathrm{rt}} + \mathcal{L}_{\mathrm{cm}} \qquad \mathcal{L}_{\mathrm{cm}} = \tfrac{1}{2}M\dot{\boldsymbol{r}}_{\mathrm{cm}}^2 \tag{78}$$

with $\mathcal{L}_N$ and $\mathcal{L}_{\mathrm{rt}}$ now given by (17). The Lagrangian (78) is supplemented by the gauge conditions (75) holding as strong (operator) equations, and the constraints $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S} = 0$ and $\boldsymbol{p}_{\mathrm{cm}} \equiv M\dot{\boldsymbol{r}}_{\mathrm{cm}} = 0$ valid as weak (state space) equalities.

We keep the definitions (13) of Λ_{ai} and λ_{ai} from section 3. Expression (14) of $\boldsymbol{\xi}$ in terms of $\{\dot{\theta}_a\}$ then holds unchanged since $\boldsymbol{\xi} = \dot{\boldsymbol{U}}\boldsymbol{U}^\dagger$ just like in section 3. From $\mathcal{L}$ in (78), we can then derive relations (21) for p_{θ_a} and the angular momentum $\boldsymbol{L}$ in this gauge. The classical expression (21) for $\boldsymbol{L}$, in turn, together with the transformation law (77), leads to the relation

$$\boldsymbol{L} = \boldsymbol{U}(\boldsymbol{l} - \boldsymbol{l}_{\mathrm{cm}}) \tag{79}$$

where the centre of mass angular momentum in the lab frame is defined as $\boldsymbol{l}_{\mathrm{cm}} = \boldsymbol{r}_{\mathrm{cm}} \wedge \boldsymbol{p}_{\mathrm{cm}} = M\boldsymbol{r}_{\mathrm{cm}} \wedge \dot{\boldsymbol{r}}_{\mathrm{cm}}$. From relation (77) between $\boldsymbol{R}_\alpha$ and $\boldsymbol{r}_\alpha$ we can derive an expression for $\partial\boldsymbol{U}/\partial r_{\alpha j}\boldsymbol{U}^\dagger$ by following the same steps leading to (16) in section 3. The result is that (16) remains valid without modifications and that, due to the translation invariance condition (76) for $\mathfrak{S}_a$, $\boldsymbol{U}$ does not depend on $\boldsymbol{r}_{\mathrm{cm}}$,

$$\sum_{\alpha=1}^{N} \frac{\partial \boldsymbol{U}}{\partial \boldsymbol{r}_\alpha} = 0. \tag{80}$$

In particular, $[\boldsymbol{l}_{\mathrm{cm}}, \boldsymbol{U}] = 0$. From (16), in turn, the commutator (18) of $\boldsymbol{l}$ with $\boldsymbol{U}$ follows. Thus, with the commutator (18), the transformation relations (77) and (79) and (80), we recover all of the commutators (19) and also

$$\begin{aligned} &[l_{\mathrm{cm}i}, l_{\mathrm{cm}j}] = \mathrm{i}\varepsilon_{ijk} l_{\mathrm{cm}k} \qquad && [l_i, l_{\mathrm{cm}j}] = \mathrm{i}\varepsilon_{ijk} l_{\mathrm{cm}k} \\ &[l_{\mathrm{cm}i}, U_{jk}] = 0 && [l_{\mathrm{cm}i}, L_j] = 0. \end{aligned} \tag{81}$$

Furthermore, $[l_{\mathrm{cm}i}, s_j] = 0$. Thus, since $\boldsymbol{J} \equiv \boldsymbol{L} + \boldsymbol{S} = \boldsymbol{U}(\boldsymbol{l} - \boldsymbol{l}_{\mathrm{cm}} + \boldsymbol{s})$, with (81) we find $[l_{\mathrm{cm}i}, S_j] = 0 = [l_{\mathrm{cm}i}, J_j]$ and then all of the commutators (20) follow. In summary, with the exception of equation (79), all of the results of section 3.1 remain valid in this case.

The relation among linear momenta in the gauge $\boldsymbol{\xi} = 0 = \boldsymbol{\rho}$ and the gauge $\mathfrak{S}_a = 0 = \mathfrak{C}$ analogous to (25) takes the form

$$p_{\alpha j} = U_{kj}\left(P_{\alpha k} + \sum_{a=1}^{3} m_\alpha \Gamma_{a\alpha k} \mathfrak{Q}^{-1}_{na}(L_n - \Lambda_n)\right) + \frac{m_\alpha}{M} p_{\mathrm{cm}\, j} \tag{82}$$

with $\boldsymbol{\Lambda}$ defined as in (25). Correspondingly, the classical Hamiltonian is given by (26) with the addition of the centre of mass kinetic energy $\boldsymbol{p}_{\mathrm{cm}}^2\big/(2M)$. Due to the additional gauge conditions $\mathfrak{C} = 0$, the fundamental commutators (27) become

$$[R_{\alpha i}, P_{\beta j}] = \mathrm{i}\left(\delta_{\alpha\beta}\delta_{ij} - \frac{m_\beta}{M}\delta_{ij} - \sum_{a=1}^{3} \frac{m_\beta}{\mathfrak{R}_a^2} \Gamma_{a\alpha i}\Gamma_{a\beta j}\right) \tag{83}$$

and $[P_{\alpha i}, \mathfrak{S}_a(\{\boldsymbol{R}_\beta\})] = 0 = [P_{\alpha i}, \mathfrak{C}(\{\boldsymbol{R}_\beta\})]$. The differential operators realizing this algebra are obtained in the same way as those in (29), which is now modified to

$$P_{\alpha i} = \frac{1}{\mathrm{i}}\frac{\partial}{\partial R_{\alpha i}} - \sum_{a=1}^{3} \frac{m_\alpha}{\mathfrak{R}_a^2}\Gamma_{a\alpha i} \sum_{\beta=1}^{N} \Gamma_{a\beta j}\frac{1}{\mathrm{i}}\frac{\partial}{\partial R_{\beta j}} - \frac{m_\alpha}{M}\sum_{\beta=1}^{N}\frac{1}{\mathrm{i}}\frac{\partial}{\partial R_{\beta i}}. \tag{84}$$

These operators satisfy $\mathfrak{S}_a(\{\boldsymbol{P}_\alpha/m_\alpha\}) = 0 = \sum_{\alpha=1}^{N} \boldsymbol{P}_\alpha$. They also satisfy (82), with $p_{\alpha j} = 1/\mathrm{i}\partial/\partial r_{\alpha j}$. The additional term in (84) with respect to (29) does not modify the form of $\boldsymbol{\Lambda}$ as a differential operator. Clearly, the commutators of $\boldsymbol{R}_\alpha$ and $\boldsymbol{P}_\alpha$ with $\boldsymbol{r}_{\mathrm{cm}}$ and $\boldsymbol{p}_{\mathrm{cm}} = 1/\mathrm{i}\partial/\partial\boldsymbol{r}_{\mathrm{cm}}$ vanish strongly.

4.1. Quantum Hamiltonian

The Hamiltonian operator is obtained by the same procedure as in section 3.2, with obvious modifications. We omit all calculational details and quote the results only, after establishing the appropriate notation.

Like in section 3.2, we extend the gauge coefficients $\Gamma_{a\alpha i}$, $a = 1, 2, 3$, $\alpha = 1, \ldots, N$, to an orthogonal basis of $\mathbb{R}^{3N}$. That is, we consider an extended set of coefficients $\Gamma_{a\alpha i}$ with $1 \leqslant a \leqslant 3N$, $\alpha = 1, \ldots, N$, $i = 1, \ldots, 3$, satisfying the orthogonality and completeness relations (30). For simplicity, like in section 3.2, we set the normalization constants in (30) to be independent of a for $4 \leqslant a \leqslant 3N$, $\mathfrak{R}_a^2 = \mathfrak{R}^2 > 0$ with $\mathfrak{R}^2$ a constant at our disposal. Furthermore, for $3N - 2 \leqslant a \leqslant 3N$ we choose the coefficients $\Gamma_{a\alpha j}$ to be independent of α. Specifically, we set

$$\Gamma_{a\alpha i} = \frac{\mathfrak{R}}{\sqrt{M}}\delta_{(a-3N+3)i} \qquad 3N-2 \leqslant a \leqslant 3N \quad 1 \leqslant \alpha \leqslant N. \tag{85}$$

With this choice the orthogonality relations (30) with $3N-2 \leqslant a \leqslant 3N$ and $1 \leqslant b \leqslant 3N-3$ read

$$\sum_{\alpha=1}^{N} m_\alpha \Gamma_{b\alpha j} = 0 \qquad 1 \leqslant b \leqslant 3N-3. \tag{86}$$

In particular, (86) contains the translation invariance conditions (76) for $\mathfrak{S}_b$.

We can now define the generalized coordinates $\{q_a\}_{a=1}^{3N}$ by (31). We see that for $3N - 2 \leqslant a \leqslant 3N, q_a = \sqrt{M} r_{\text{cm}(a-3N+3)}$, i.e., up to a normalization constant the last three q_a are the components of $\boldsymbol{r}_{\text{cm}}$. The analogue of (31) is now

$$R_{\alpha i}(t) = \sum_{a=4}^{3N-3} Q_a(t)\Gamma_{a\alpha i} \qquad Q_c(t) = \sum_{\alpha=1}^{N} \frac{m_\alpha}{\mathfrak{R}^2}\Gamma_{c\alpha i}R_{\alpha i}(t) \quad 4 \leqslant c \leqslant 3N - 3. \tag{87}$$

From (30) and (85), expression (87) for $\boldsymbol{R}_\alpha$ satisfies the gauge conditions (75). The dynamics in this gauge is then completely specified by the $3N$ independent variables $\{\theta_a\}_{a=1}^{3}$, $\{Q_a\}_{a=4}^{3N-3}$ and $\boldsymbol{r}_{\text{cm}}$, and their conjugate momenta. In those variables $\mathcal{H}_N$ is given by (33) with only two modifications: first, the sums over indices running up to $3N$ now run only up to $3N - 3$, and second, the addition of the term $-1/(2M)\partial^2/\partial {r_{\text{cm}}}_j^2$. The definitions (34) of $\mathcal{N}_{ij}$ and its inverse, and of $\mathcal{J}$ and $|\Lambda|$ remain unchanged. Similarly, $\mathcal{H}_N$ is expressed in terms of $\boldsymbol{R}_\alpha$, their conjugate momenta $\boldsymbol{P}_\alpha$, and $\boldsymbol{L}$ by (42), but now with the momentum operators $\boldsymbol{P}_\alpha$ from (84), and with the addition of the centre of mass kinetic energy term.

4.2. Physical Hilbert space, inner product, Weyl-ordered Hamiltonian

The wavefunction in this gauge $\psi(\{\boldsymbol{R}_\alpha\}, \{\theta_a\}, \widehat{\boldsymbol{e}}, \boldsymbol{r}_{\text{cm}})$ is required to satisfy the constraints $\boldsymbol{p}_{\text{cm}}\psi = 0$ and $(\boldsymbol{L} + \boldsymbol{S})\psi = 0$ originating in the equations of motion for $\boldsymbol{\rho}$ and $\boldsymbol{\xi}$ from the Lagrangian (72). The first constraint is trivial to solve. Considering wavefunctions ψ independent of $\boldsymbol{r}_{\text{cm}}$, we are left with the constraint on the angular variables which, since $[\boldsymbol{p}_{\text{cm}}, \boldsymbol{L}] = 0 = [\boldsymbol{p}_{\text{cm}}, \boldsymbol{S}]$, can now be treated exactly as in section 3.3. Using the same notation as in (45), the solution to the constraint equations is of the form

$$\psi(\{\boldsymbol{R}_\alpha\}, \{\theta_a\}, \widehat{\boldsymbol{e}}, \boldsymbol{r}_{\text{cm}}) = \mathcal{U}(\{\theta_a\})\widehat{\psi}(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{e}}). \tag{88}$$

Within the subspace of physical wavefunctions $\widehat{\psi}(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{e}})$, the Hamiltonian $\widehat{\mathcal{H}}_N \equiv \mathcal{U}^\dagger\mathcal{H}_N\mathcal{U}$ is given by (46), with the momentum operators $\boldsymbol{P}_\alpha$ from (84).

The discussion of the inner product from section 3.4 requires only minor changes in order to adapt it to the translation-invariant case. Besides the resolution of the identity (48) for the rotational gauge conditions $\mathfrak{S}_a = 0$, we have to fix the translational gauge by means of a resolution of the form

$$1 = \int d^3u \prod_{i=1}^{3} \delta\left(\mathfrak{C}_i(\{\boldsymbol{r}_\alpha\}) + u_i\right). \tag{89}$$

Inserting this factor of 1 together with (48) into the canonical inner product (7), we obtain $\langle\phi|\psi\rangle$ in terms of wavefunctions in this gauge. A technical detail is that, after applying the Faddeev–Popov procedure, the volume of the symmetry group appears as a prefactor in $\langle\phi|\psi\rangle$ (see (55)). In this case, the volume of the translation group is infinite, so an appropriate limiting or regularization procedure must be applied. Assuming that has been done, the resulting inner product in terms of physical wavefunctions analogous to (56) is

$$\langle\phi|\psi\rangle = \int \prod_{\alpha=1}^{N} d^3\boldsymbol{R}_\alpha\, d^2\widehat{\boldsymbol{e}} \prod_{a=1}^{3} \delta\left(\frac{1}{\mathfrak{R}_a}\mathfrak{S}_a\right) \delta^{(3)}\left(\boldsymbol{\mathfrak{C}}\right) \Theta(\mathcal{F})\Theta(\mathcal{J})\mathcal{J}(\widehat{\phi}^*\widehat{\psi})(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{e}}). \tag{90}$$

The factor $\Theta(\mathcal{F})$ is exactly as discussed in section 3.4.1, since the centre of mass condition does not introduce further Gribov ambiguities.

We consider, finally, the form of the Weyl-ordered reduced Hamiltonian. Taking proper account of translation invariance as described above, the analysis of section 3.5 remains valid *mutatis-mutandis*. Defining the reduced physical wavefunctions

$$\widehat{\widehat{\psi}}(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{e}}) \equiv \mathcal{J}^{\frac{1}{2}}\widehat{\psi}(\{\boldsymbol{R}_\alpha\}, \widehat{\boldsymbol{e}}) \tag{91}$$

with $\widehat{\psi}$ as defined in (88), the reduced Hamiltonian $\widehat{\widetilde{\mathcal{H}}}_N = \mathcal{J}^{1/2}\widehat{\mathcal{H}}_N\mathcal{J}^{-1/2} = \mathcal{J}^{1/2}\mathcal{U}^\dagger\widetilde{\mathcal{H}}_N\mathcal{U}\mathcal{J}^{-1/2}$ is given in Weyl-ordered form by (66), with $\boldsymbol{P}_\alpha$ given by (84). The quantum potentials $\mathcal{V}_{1,2}$, in particular, are still defined as in (65). The reduced inner product is immediately obtained from (90) and (91).

5. Quasi-rigid systems in the Eckart frame

We assume now that the potential energy $\mathcal{V}$ (with $U = 0$) has a minimum for some configuration $\{\boldsymbol{z}_\alpha\}$ of the system, such that $\mathcal{V}_0 \equiv \mathcal{V}(\{\boldsymbol{z}_\alpha\}) \leqslant \mathcal{V}(\{\boldsymbol{r}_\gamma\})$ for all configurations $\{\boldsymbol{r}_\gamma\}$. Due to the invariance of $\mathcal{V}$ under the Euclidean group E_3 any configuration $\{\boldsymbol{z}'_\alpha\}$ related to $\{\boldsymbol{z}_\alpha\}$ by a transformation of the form (69) is also a minimum. Denoting by $\mathcal{M}_\mathcal{V}$ the manifold of configuration space defined by $\mathcal{V}(\{\boldsymbol{r}_\gamma\}) = \mathcal{V}_0$, we assume that the quotient $\mathcal{M}_\mathcal{V}/E_2$ is a discrete set. The configurations of minimal potential energy are therefore rigid. In this section, we discuss the quantization of the small oscillations of the system about these rigid equilibrium configurations. We will denote by $\{\boldsymbol{Z}_\alpha\}$ the unique (up to discrete degeneracy) minimum of $\mathcal{V}$ satisfying

$$\sum_{\alpha=1}^{N} m_\alpha Z_{\alpha i} Z_{\alpha j} = 0 \quad i \neq j \qquad \sum_{\alpha=1}^{N} m_\alpha \boldsymbol{Z}_\alpha = 0. \tag{92}$$

We will restrict ourselves to considering only systems for which the inertia tensor for the equilibrium configuration $\{\boldsymbol{Z}_\alpha\}$ is non-singular. The small oscillations of the system are described by trajectories of the form

$$\boldsymbol{r}_\alpha(t) = \boldsymbol{z}_\alpha(t) + \boldsymbol{\delta r}_\alpha(t) \qquad \text{with} \quad \boldsymbol{z}_\alpha(t) = \boldsymbol{U}(t)\boldsymbol{Z}_\alpha + \boldsymbol{u} \tag{93}$$

for some orthogonal matrix $\boldsymbol{U}(t)$ and $\boldsymbol{u}$ appropriately chosen so that $\boldsymbol{\delta r}_\alpha(t)$ are small with respect to their characteristic scale for all t. Since we restrict ourselves to states with vanishing total momentum, the translation vector $\boldsymbol{u}$ in (93) must be time independent.

It is convenient to apply the inverse of the gauge transformation defined by the second equation in (93) in order to switch to a reference frame, the 'body frame' of the rigid equilibrium configuration, so that

$$\boldsymbol{r}_\alpha(t) = \boldsymbol{Z}_\alpha + \boldsymbol{\delta r}_\alpha(t). \tag{94}$$

This fixes the gauge only to leading order in $\boldsymbol{\delta r}_\alpha$. We fix the residual gauge freedom by imposing a gauge condition on $\boldsymbol{\delta r}_\alpha$, which amounts to correcting the definitions (92)–(94) of the reference frame by small quantities of first order. We choose the origin of the reference frame at the centre of mass, so to first order in $\boldsymbol{\delta r}_\alpha$ the gauge conditions must be of the form (75). The choice of the coefficients $\Gamma_{a\alpha i}$ is arbitrary as long as (76) is satisfied. We then have

$$\boldsymbol{R}_\alpha(t) = \boldsymbol{Z}_\alpha + \boldsymbol{\delta R}_\alpha(t) \qquad \mathfrak{S}_a(\{\boldsymbol{\delta R}_\alpha\}) = 0 \qquad \mathfrak{C}(\{\boldsymbol{\delta R}_\alpha\}) = 0. \tag{95}$$

The Eckart frame corresponds to choosing $\Gamma_{a\alpha i} = \varepsilon_{aji} Z_{\alpha j}$, $a = 1, 2, 3$ [12, 9]. With this choice the normalization constants $\mathfrak{R}_a^2$, $a = 1, 2, 3$, of (11) (and also (30) and (86)) are given by the inertia moments of the equilibrium configuration, and the matrix $\mathfrak{Q}(\{\boldsymbol{R}_{\alpha i}\})$ of (9) is

$$\begin{aligned} \mathfrak{Q}_{ai}(\{\boldsymbol{\delta R}_\alpha\}) &= \mathfrak{R}_a^2\delta_{ai} + \delta\mathfrak{Q}_{ai}(\{\boldsymbol{\delta R}_\alpha\}) \\ \delta\mathfrak{Q}_{ai}(\{\boldsymbol{\delta R}_\alpha\}) &= \sum_{\gamma=1}^{N} m_\gamma(\boldsymbol{Z}_\gamma \cdot \boldsymbol{\delta R}_\gamma\delta_{ai} - \delta R_{\gamma a} Z_{\gamma i}) \qquad a = 1, 2, 3. \end{aligned} \tag{96}$$

Thus, since $\mathfrak{R}_a^2 \neq 0$ by assumption, for small $\boldsymbol{\delta R}_\alpha$ the condition $\det(\mathfrak{Q}_{ai}(\{\boldsymbol{R}_\alpha\})) \neq 0$ is satisfied.

The momentum operators $\boldsymbol{P}_\alpha$ and their fundamental commutators are as given in (83) and (84), with the replacement of $\partial/\partial R_{\alpha i}$ by $\partial/\partial\delta R_{\alpha i}$. The operator $\boldsymbol{\Lambda}$ defined in (25) can be rewritten in the form

$$\Lambda_i = \sum_{\alpha=1}^{N} \varepsilon_{ijk}\delta R_{\alpha j}\frac{1}{\mathrm{i}}\frac{\partial}{\partial\delta R_{\alpha k}} - \sum_{a=1}^{3}\frac{\delta\mathfrak{Q}_{ai}}{\mathfrak{R}_a^2}\sum_{\alpha=1}^{N}\varepsilon_{ajk}Z_{\alpha j}\frac{1}{\mathrm{i}}\frac{\partial}{\partial\delta R_{\alpha k}}. \tag{97}$$

As expected in this gauge [12, 1], its coefficients are of $\mathcal{O}(\boldsymbol{\delta R}_\alpha)$. Similarly, the operators $\sum_{\alpha=1}^{N}\mathcal{D}_{ij}^{\alpha}P_{\alpha i}$ and $\sum_{\alpha=1}^{N}P_{\alpha i}\mathcal{D}_{ij}^{\alpha}$ appearing in $\widehat{\widetilde{\mathcal{H}}}_N$ are of $\mathcal{O}(\boldsymbol{\delta R}_\alpha)$. The Hamiltonian $\widehat{\widetilde{\mathcal{H}}}_N$, given by (66) with $\boldsymbol{P}_\alpha$ from (84), is obtained perturbatively by expanding (66) in powers of $\boldsymbol{\delta R}_\alpha$. From this point of view, the elimination of the Jacobian $\mathcal{J}$ from the kinetic energy, as indicated in sections 3.5 and 4.2, is particularly convenient in perturbation theory. The inner product, finally, is given by (90) with the modification (91), and with $\boldsymbol{\delta R}_\alpha$ as the integration variable. Once the equilibrium configuration $\{\boldsymbol{Z}_\alpha\}$ has been chosen, its body frame is uniquely fixed. The Eckart frame is then equally well defined as long as $\{\boldsymbol{\delta R}_\alpha\}$ are small. Thus, except in those cases in which the equilibrium configuration $\{\boldsymbol{Z}_\alpha\}$ is exceptionally close to a zero of $\mathcal{J}$, we can neglect the factor $\Theta(\mathcal{J})$ in (90) since large displacements $\boldsymbol{\delta R}_\alpha$ which could drive $\mathcal{J}$ to zero should be exponentially suppressed by the wavefunction. Similarly, we also expect to be able to neglect $\Theta(\mathcal{F})$ in (90) in perturbation theory.

As a minimal illustration and consistency check of the formalism we analyse below a simple example with $N = 3$, and briefly comment on the $N = 4$ case. The natural variables for quasi-rigid systems are normal coordinates, so below we recast the Hamiltonian in terms of those coordinates. We remark, however, that the results of the previous sections are more general than the simple examples considered here, and can be applied to non-quasi-rigid N-body systems, both in the operator and path integral formalism.

5.1. A simple example with N = 3

The simplest possible model, within our assumptions, consists of three particles of equal mass m interacting through a two-body potential $\mathcal{V}$ as in (1), with $U = 0$ and $V_{\alpha\beta} = V$ independent of α, β. $V(r)$ is assumed to have an absolute minimum at $r = a > 0$. The classical equilibrium configurations are then those in which the particles lie at relative rest on the vertices of an equilateral triangle of side a. An equilibrium configuration satisfying (92), unique up to permutations of the particles and discrete rotations of the coordinate axes, is

$$\boldsymbol{Z}_1 = a\left(-\tfrac{1}{2}, -\tfrac{1}{2\sqrt{3}}, 0\right) \qquad \boldsymbol{Z}_2 = a\left(\tfrac{1}{2}, -\tfrac{1}{2\sqrt{3}}, 0\right) \qquad \boldsymbol{Z}_3 = a\left(0, \tfrac{1}{\sqrt{3}}, 0\right) \tag{98}$$

with the inertia tensor $ma^2/2\,\mathrm{diag}(1, 1, 2)$.

The Eckart gauge is defined by (75) with $\Gamma_{a\alpha i} = \varepsilon_{aji}Z_{\alpha j}, a = 1, 2, 3$, which are normalized to $\mathfrak{R}_1^2 = ma^2/2 = \mathfrak{R}_2^2, \mathfrak{R}_3^2 = ma^2$. Those gauge conditions make the planar nature of the problem apparent, since they imply that $\delta R_{\alpha 3} = 0 = P_{\alpha 3}, \alpha = 1, 2, 3$, as operators. This leads, in particular, to the operator $\boldsymbol{\Lambda}$ of (25) having two null components $\Lambda_1 = 0 = \Lambda_2$ (as operators), with Λ_3 being conserved and having integer eigenvalues, as shown below. Thus, in this example $\boldsymbol{\Lambda}$ is an angular momentum operator, though two- rather than three-dimensional, and can be rightfully termed 'residual' angular momentum as in [1]. The three-dimensional rotations of the system are taken into account by the total angular momentum operator $\boldsymbol{s}$.

Setting $V''(a) \equiv m\omega^2$, the quadratic terms in an expansion of $\mathcal{V}$ about $\{\boldsymbol{Z}_\alpha\}$ are

$$\mathcal{V}_{(2)} = \frac{m\omega^2}{2}\sum_{\alpha<\beta=1}^{3}\left(\frac{1}{a}(\boldsymbol{Z}_\alpha - \boldsymbol{Z}_\beta)\cdot(\boldsymbol{\delta R}_\alpha - \boldsymbol{\delta R}_\beta)\right)^2. \tag{99}$$

Using the gauge conditions we could eliminate six degrees of freedom, describing the system in terms of, e.g., $\delta R_{1X}, \delta R_{2X}, \delta R_{2Y}$ and their conjugate momenta. A better approach is to use a set of normal coordinates $\{\delta Q_a\}_{a=4}^{6}$ as discussed in sections 3.2 and 4.1. Thus, with $\Gamma_{a\alpha i}$, $a = 1, 2, 3$, as defined above and $\Gamma_{a\alpha i}$, $a = 7, 8, 9$, as defined by (85), we can choose $\Gamma_{a\alpha i}$, $a = 4, 5, 6$, to be those eigenvectors of the quadratic form associated with $\mathcal{V}_{(2)}$ which satisfy the orthogonality conditions (30) (in particular, (86)), and normalized[5] to $\mathfrak{R}^2 = \hbar/\omega$. Those $\Gamma_{a\alpha i}$, $a = 4, 5, 6$, are the vibrational normal modes of $\mathcal{V}_{(2)}$, whose associated normal coordinates δQ_a are given by (87),

$$\begin{aligned}
\delta Q_4 &= \sqrt{\frac{m\omega}{\hbar}}\left(\frac{1}{2}\delta R_{1X} - \frac{1}{2\sqrt{3}}\delta R_{1Y} - \frac{1}{2}\delta R_{2X} - \frac{1}{2\sqrt{3}}\delta R_{2Y} + \frac{1}{\sqrt{3}}\delta R_{3Y}\right)\\
\delta Q_5 &= \sqrt{\frac{m\omega}{\hbar}}\left(-\frac{1}{2\sqrt{3}}\delta R_{1X} - \frac{1}{2}\delta R_{1Y} - \frac{1}{2\sqrt{3}}\delta R_{2X} + \frac{1}{2}\delta R_{2Y} + \frac{1}{\sqrt{3}}\delta R_{3X}\right)\\
\delta Q_6 &= \sqrt{\frac{m\omega}{\hbar}}\left(-\frac{1}{2}\delta R_{1X} - \frac{1}{2\sqrt{3}}\delta R_{1Y} + \frac{1}{2}\delta R_{2X} - \frac{1}{2\sqrt{3}}\delta R_{2Y} + \frac{1}{\sqrt{3}}\delta R_{3Y}\right).
\end{aligned} \tag{100}$$

Similarly, from (39), (40) (with $3N-3$ instead of $3N$) we obtain the relation between $\partial/\partial\delta Q_a$ and either $\partial/\partial\delta R_{\alpha i}$ or $P_{\alpha i}$. The result is given by (100) with δQ_a substituted by $1/\mathrm{i}\partial/\partial\delta Q_a$ on the lhs, and $\delta R_{\alpha i}$ substituted by either $\hbar/(m\omega)1/\mathrm{i}\partial/\partial R_{\alpha i}$ or $1/(m\omega)P_{\alpha i}$, respectively, on the rhs.

The quadratic piece of the Hamiltonian $\widehat{\widetilde{\mathcal{H}}}_N$ (henceforth $\widehat{\widetilde{\mathcal{H}}}$) of section 4.2 can be written as

$$\widehat{\widetilde{\mathcal{H}}}_0 \equiv \frac{1}{2m}\sum_{\beta=1}^{3}\boldsymbol{P}_\beta^2 + \mathcal{V}_{(2)} = \frac{\hbar\omega}{2}\sum_{a=4}^{6}\left(-\frac{\partial^2}{\partial\delta Q_a^2} + \sigma_a^2\delta Q_a^2\right) \qquad \sigma_4^2 = \frac{3}{2} = \sigma_5^2 \quad \sigma_6^2 = 3. \tag{101}$$

$\widehat{\widetilde{\mathcal{H}}}_0$ is the lowest-order Hamiltonian in a perturbative expansion in powers of $\epsilon = \sqrt{\hbar/(m\omega a^2)} \ll 1$. From the definition (25), or equivalently from (97), we find the residual angular momentum as

$$\Lambda_i = \sum_{a=4}^{3N-3}\frac{\delta\mathfrak{Q}_{ai}}{\mathfrak{R}^2}\frac{1}{\mathrm{i}}\frac{\partial}{\partial\delta Q_a}$$

and therefore

$$\Lambda_1 = 0 = \Lambda_2 \quad \Lambda_3 = \frac{1}{\mathrm{i}}\left(\delta Q_5\frac{\partial}{\partial\delta Q_4} - \delta Q_4\frac{\partial}{\partial\delta Q_5}\right) \tag{102}$$

with $\delta\mathfrak{Q}_{ai}$ defined in (96). To $\mathcal{O}(\epsilon^2)$ the quantities entering $\widehat{\widetilde{\mathcal{H}}}$ are $\mathfrak{R}_1^2 = \mathfrak{R}_2^2 = \mathfrak{R}_3^2/2 = \hbar/(2\omega\epsilon^2)$, $\mathcal{N}_{ij}^{-1} = 1/\mathfrak{R}_{(i)}^2\delta_{(i)j} + \mathcal{O}(\epsilon^3)$, $\mathcal{V}_1 = \mathcal{O}(\epsilon^3)$, and the anharmonic terms in $\mathcal{V}$, which are $\mathcal{O}(\epsilon^3)$. The expansion of $\mathcal{V}_2 = \text{const} + \mathcal{O}(\epsilon^3)$ starts at $\mathcal{O}(\epsilon^2)$ but the lowest-order term is a constant, which we drop. Retaining only terms through $\mathcal{O}(\epsilon^2)$ in $\widehat{\widetilde{\mathcal{H}}}$, and expressing them in terms of normal coordinates, we obtain

$$\widehat{\widetilde{\mathcal{H}}} = \widehat{\widetilde{\mathcal{H}}}_0 + \widehat{\widetilde{\mathcal{H}}}_1 \qquad \widehat{\widetilde{\mathcal{H}}}_1 = \frac{\omega\epsilon^2}{\hbar}\left(\boldsymbol{s}^2 - s_3^2 + \frac{1}{2}(s_3 + \Lambda_3)^2\right) + \mathcal{O}(\epsilon^3) \tag{103}$$

where we used Λ_3 as defined in (102), and dropped all constant terms. The operators $\boldsymbol{s}^2, s_3$ and Λ_3 all commute with each other and with the Hamiltonian. The physical meaning of the Hamiltonian (103) is apparent from (57): for physical wavefunctions the

[5] In this section and the following, we restore $\hbar$ in all expressions.

operator $\boldsymbol{s}$ gives the matrix elements of $-\boldsymbol{L}$ so that, to this order, (103) corresponds to $\widetilde{\mathcal{H}}_1 = 1/2\mathcal{N}_{ij}^{-1}(L_i - \Lambda_i)(L_j - \Lambda_j)$, with $\mathcal{N}_{ij}^{-1}$ the inverse of the equilibrium inertia tensor and $\boldsymbol{L} - \boldsymbol{\Lambda}$ the difference of the total and residual angular momenta in the Eckart frame.

Since we are not going to compute beyond $\mathcal{O}(\epsilon^2)$ in perturbation theory, it is easier (to this order) to solve the eigenvalue problem for (103) exactly rather than as a perturbation about the Hamiltonian (101). We introduce cylindrical coordinates in the space of $\delta Q_{4,5,6}$

$$\rho = \sqrt{\delta Q_4^2 + \delta Q_5^2} \qquad \varphi = \arctan\left(\frac{\delta Q_4}{\delta Q_5}\right) \qquad \zeta = \delta Q_6 \tag{104}$$

and classify the Hamiltonian eigenfunctions and eigenvalues according to the eigenvalues of $\widehat{\widetilde{\mathcal{H}}}_0$, Λ_3, $\boldsymbol{s}^2$ and s_3 (with quantum numbers denoted by (n, n_ζ), λ, ℓ, m, respectively). The wavefunctions are

$$\begin{aligned}
&\widehat{\widetilde{\psi}}{}^{\ell m}_{n\lambda n_\zeta}(\rho, \varphi, \zeta; \widehat{e}) = R_{n|\lambda|}(\rho)\Phi_\lambda(\varphi)Z_{n_\zeta}(\zeta)Y_{\ell m}(\widehat{e}) \\
&R_{n|\lambda|}(\rho) = \rho^{|\lambda|}L_n^{|\lambda|}\left(\sqrt{\frac{3}{2}}\rho^2\right)\mathrm{e}^{-\sqrt{3/2}\rho^2/2} \qquad \Phi_\lambda(\varphi) = \mathrm{e}^{\mathrm{i}\lambda\varphi} \\
&Z_{n_\zeta}(\zeta) = H_{n_\zeta}(\sqrt{3}\zeta)\,\mathrm{e}^{-3\zeta^2/2}
\end{aligned} \tag{105}$$

where we omitted a normalization constant, n, n_ζ and ℓ are non-negative integers, λ and m are integers, and the spherical harmonics $Y_{\ell m}$, associated Laguerre polynomials L_n^k and Hermite polynomials H_n are defined in the standard way in quantum mechanics [20]. The dependence of the wavefunction (105) on $\widehat{e}$ only carries the representation of the rotation group appropriate to a state of angular momentum ℓ. We could as well suppress the dependence on $\widehat{e}$ and define the wavefunction to be a column with $2\ell + 1$ components, depending only on the three vibrational variables ρ, φ, ζ. The energy eigenvalues are

$$\begin{aligned}
&E^{\ell m}_{n\lambda n_\zeta} = E^{(0)}_{n\lambda n_\zeta} + E^{(1)}_{\lambda\ell m} \qquad E^{(0)}_{n\lambda n_\zeta} = \hbar\omega\left(\sqrt{3}\left(n_\zeta + \tfrac{1}{2}\right) + \sqrt{\tfrac{3}{2}}(2n + |\lambda| + 1)\right) \\
&E^{(1)}_{\lambda\ell m} = \hbar\omega\epsilon^2\left(\ell(\ell+1) - m^2 + \tfrac{1}{2}(m+\lambda)^2\right).
\end{aligned} \tag{106}$$

In the vibrational ground state $n = n_\zeta = \lambda = 0$, (106) reduces to the spectrum of an axis-symmetric top.

5.2. *A simple example with $N = 4$*

Adding one more particle of the same mass to the model of the previous section, we obtain a system whose classical equilibria are those configurations with the particles lying at relative rest on the vertices of a regular tetrahedron of side a. The inertia tensor of the equilibrium configuration is now $ma^2\,\mathrm{diag}(1, 1, 1)$. The constants $\Gamma_{a\alpha i} = \varepsilon_{aji}Z_{\alpha j}$, $a = 1, 2, 3$, defining the Eckart gauge are then normalized to $\mathfrak{R}^2_{1,2,3} = ma^2$.

This system, unlike that of the previous section, is fully three-dimensional. With $\epsilon = \sqrt{\hbar/(m\omega a^2)}$, the $\mathcal{O}(\epsilon^2)$ perturbation $\widehat{\widetilde{\mathcal{H}}}_1$ does not commute with the zeroth-order quadratic Hamiltonian, so the $\mathcal{O}(\epsilon^2)$ corrections to the unperturbed energies must be computed perturbatively. Diagonalizing $\widehat{\widetilde{\mathcal{H}}}_1$ within eigenspaces of $\widehat{\widetilde{\mathcal{H}}}_0$ is best done numerically, due to the large accidental degeneracies of the unperturbed levels beyond the ground state. For that reason, we will restrict ourselves to making only some remarks on the form of the $\mathcal{O}(\epsilon^2)$ Hamiltonian.

We have six vibrational normal modes, with normal coordinates $\{\delta Q_a\}_{a=4}^9$ whose expressions in terms of the position vectors $\{\boldsymbol{\delta R}_\alpha\}$ we omit for brevity. The unperturbed

Hamiltonian is given by (101), with β now running up to 4, a up to 9, and with $\sigma_4^2 = \sigma_5^2 = 1$, $\sigma_6^2 = \sigma_7^2 = \sigma_8^2 = 2$ and $\sigma_9^2 = 4$. We have $\mathcal{N}_{ij}^{-1} = 1/(ma^2)\delta_{ij} + \mathcal{O}(\epsilon^3)$, and the quantum potentials $\mathcal{V}_{1,2}$ and the anharmonic corrections to $\mathcal{V}_{(2)}$ starting at $\mathcal{O}(\epsilon^3)$ up to constant terms. Thus, to $\mathcal{O}(\epsilon^2)$ the perturbation Hamiltonian is given by the second term in (66), with the momentum operators of (84). Dropping constant terms, the $\mathcal{O}(\epsilon^2)$ perturbation can be arranged in the form

$$\widehat{\widetilde{\mathcal{H}}}_1 = \frac{\omega\epsilon^2}{\hbar}(\boldsymbol{s} + \boldsymbol{\Lambda})^2 + \mathcal{O}(\epsilon^3) \qquad \Lambda_i = \frac{\hbar}{\mathrm{i}} \sum_{c=4}^{9} \frac{1}{\mathfrak{R}^2} \delta\mathfrak{Q}_{ci} \frac{\partial}{\partial \delta Q_c}. \tag{107}$$

The normal coordinate we call δQ_9 corresponds to a vibrational mode $\boldsymbol{\Gamma}_9$ with $\Gamma_{9\alpha i} \propto Z_{\alpha i}$, i.e., a dilatation mode. Explicit computation shows that $\delta\mathfrak{Q}_{9i} = 0$, and then $[\boldsymbol{\Lambda}, \delta Q_9] = 0$. We obtain also $\left[\Lambda_i, \sum_{a=4}^{8} \delta Q_a^2\right] = 0$, but $[\Lambda_i, \mathcal{V}_{(2)}] \neq 0$. The operator $\boldsymbol{\Lambda}$ is not an angular momentum operator, as expected on general grounds from (28b), but it turns out to be proportional to one, $[2\Lambda_i, 2\Lambda_j] = \mathrm{i}\varepsilon_{ijk} 2\Lambda_k$. We cannot give at present necessary and sufficient conditions a many-body system and a rotating frame must satisfy for $\boldsymbol{\Lambda}$, or a multiple thereof, to be an angular momentum operator.

6. Final remarks

The gauge-invariant approach presented here leads to a general and systematic framework for the quantization of many-body systems in rotating frames. Our approach naturally incorporates the notions of time-dependent symmetry transformations (i.e., gauge transformations), body-frame time-derivatives (covariant derivatives), moving reference frames defined as functions of the particle positions (gauge conditions) and of reference-frame singularities (Gribov ambiguities) in a most economical way. It is not, therefore, a superfluous formal structure imposed on the physics. The amount of formalism that has been introduced is in fact minimal. Rather, we put all those notions within a consistent mathematical framework.

We have shown that the rotational symmetry of an N-body system is a gauge symmetry, if we restrict ourselves to a fixed angular momentum sector (equation (3)). Using gauge invariance, we formulated both the classical and quantum theory (in the operator approach) in rotating frames defined by linear gauge conditions. In particular, we explicitly obtained the Hamiltonian operator (42) in terms of position vectors referred to the rotating frame, therefore constrained by the gauge conditions. We also showed that the orientational degrees of freedom can be eliminated from the formalism, and computed the Hamiltonian operator and the inner product within the corresponding reduced Hilbert space (equations (46) and (56), respectively). A further simplification is obtained by eliminating the Jacobian from the kinetic energy and the inner product, leading to the form (66) for the Hamiltonian, including the quantum potentials $\mathcal{V}_{1,2}$ of (65), and (68) for the inner product. The Hamiltonian (66), being Weyl ordered, can be associated with a generating functional in the path-integral approach with mid-point discretization. Those results were extended in section 4 to the translation-invariant case, where the system is further reduced by eliminating the centre of mass degrees of freedom. The particular case of quasi-rigid systems was discussed in section 5.

The results given in the foregoing apply to a very general class of models comprising all N-particle systems in the three-dimensional Euclidean space with rotation-invariant potentials. The fact that we computed the Hamiltonian operator in terms of position vectors referred to a rotating frame amounts to a purely conventional choice of coordinates. Once the Hamiltonian has been given in those coordinates it is straightforward to transform it to any other coordinate set, as done in sections 5.1 and 5.2, there being no need to compute it again. For simplicity, however, we restricted ourselves to systems with spin-independent interactions. The extension of the formalism to include dynamical spin degrees of freedom should in principle be straightforward. We note, in this respect, that in order to obtain half-integer values for the total angular momentum of the N-particle system, when appropriate, we should substitute the rigid rotator in (1) by a 'rotator' with a half-integer angular momentum. We did not consider, either, those cases in which it is not possible, or desirable, to impose three gauge conditions depending only on particle coordinates. Among those are, e.g., one-particle systems (including translation-invariant two-particle systems), for which the gauge conditions $R_Y = R_Z = 0 = \widetilde{\xi}_X$ lead to a description in spherical coordinates, and the conditions $R_Y = 0 = \widetilde{\xi}_X = \widetilde{\xi}_Y$ to cylindrical coordinates. The case of reference frames defined by gauge conditions of a more general form than those considered in the previous sections can also be treated by the methods discussed in this paper.

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Appendix A. The Laplacian in configuration space

The kinetic energy of the system of particles considered in section 3 is proportional to the Laplacian in the configuration space $\nabla_q^2 = \sum_{a=1}^{3N} \partial^2/\partial q_a^2$, with the generalized coordinates $\{q_a\}_{a=1}^{3N}$ defined in (31). In this appendix, we compute the expression for ∇_q^2 in curvilinear coordinates $\{Q_a\}_{a=1}^{3N}$ defined as follows. For $1 \leqslant a \leqslant 3$, $Q_a \equiv \theta_a$, with θ_a parametrizing $\boldsymbol{U}$ in (12), and $\{Q_a\}_{a=4}^{3N}$ defined by (32). The relation between the two sets of coordinates is given implicitly by (31) and (32). ∇_q^2 is then given by the standard expression

$$\nabla_q^2 = \sum_{a,b=1}^{3N} \frac{1}{J} \frac{\partial}{\partial Q_a} M_{ab}^{-1} J \frac{\partial}{\partial Q_b} \qquad M_{ab} \equiv \sum_{c=1}^{3N} \frac{\partial q_c}{\partial Q_a} \frac{\partial q_c}{\partial Q_b}$$
$$M_{ab}^{-1} = \sum_{c=1}^{3N} \frac{\partial Q_a}{\partial q_c} \frac{\partial Q_b}{\partial q_c} \qquad J \equiv \det\left(\frac{\partial q}{\partial Q}\right) = (\det(\boldsymbol{M}))^{1/2}. \tag{A.1}$$

In order to obtain an explicit expression for ∇_q^2 we have to build the matrix M_{ab}^{-1}.

For $1 \leqslant a \leqslant 3$ we have $\partial Q_a/\partial q_c \equiv \partial\theta_a/\partial q_c = \sum_{\alpha=1}^{N} (\partial r_{\alpha j}/\partial q_c)(\partial\theta_a/\partial r_{\alpha j})$. From (13), we have

$$\frac{\partial\theta_a}{\partial r_{\alpha j}} = \frac{1}{2} \Lambda_{ia}^{-1} \varepsilon_{mik} \frac{\partial U_{ml}}{\partial r_{\alpha j}} U_{kl} = -\Lambda_{ia}^{-1} \sum_{b=1}^{3} \mathfrak{Q}_{ib}^{-1} m_\alpha \Gamma_{b\alpha k} U_{kj} \tag{A.2}$$

where in the second equality we used (16). Thus,

$$\frac{\partial\theta_a}{\partial q_c} = -\sum_{\alpha=1}^{N} \sum_{b=1}^{3} \frac{m_\alpha}{\mathfrak{R}_c} \Gamma_{c\alpha j} \Gamma_{b\alpha k} \Lambda_{ia}^{-1} \mathfrak{Q}_{ib}^{-1} U_{kj}. \tag{A.3}$$

For $4 \leqslant a \leqslant 3N$ we have, from (31),

$$\frac{\partial Q_a}{\partial r_{\alpha j}} = \sum_{\beta=1}^{N} \frac{m_\alpha}{\mathfrak{R}^2} \Gamma_{a\beta i} \frac{\partial R_{\beta i}}{\partial r_{\alpha j}} = \frac{m_\alpha}{\mathfrak{R}^2} \Gamma_{a\alpha i} U_{ij} - \sum_{d=1}^{3} \mathfrak{Q}_{ai} \mathfrak{Q}_{id}^{-1} \frac{m_\alpha}{\mathfrak{R}^2} \Gamma_{d\alpha k} U_{kj} \tag{A.4}$$

where the last equality follows directly from (15) and (16). Note that, by definition, $\mathfrak{Q}^{-1}_{id}$ is a 3×3 matrix inverse to $\mathfrak{Q}_{ai}$ with $1 \leqslant a \leqslant 3$, but in general $\mathfrak{Q}_{ai}\mathfrak{Q}^{-1}_{id} \neq \delta_{ad}$ if $4 \leqslant a \leqslant 3N$ like in the last term in (A.4). With (A.4) and (31), we obtain

$$\frac{\partial Q_a}{\partial q_c} = \sum_{\alpha=1}^{N} \frac{m_\alpha}{\mathfrak{R}^2}\Gamma_{a\alpha i}U_{ij}\frac{\Gamma_{c\alpha j}}{\mathfrak{R}_c} - \sum_{\alpha=1}^{N}\sum_{d=1}^{3}\mathfrak{Q}_{ak}\mathfrak{Q}^{-1}_{kd}\frac{m_\alpha}{\mathfrak{R}^2}\Gamma_{d\alpha i}U_{ij}\frac{\Gamma_{c\alpha j}}{\mathfrak{R}_c}. \tag{A.5}$$

The matrix elements M^{-1}_{ab} can now be computed, starting with their definition (A.1), and using the orthogonality and completeness relations (30), and the definition (9) of $\mathfrak{Q}_{ai}$.

For $1 \leqslant a, b \leqslant 3$, we get

$$M^{-1}_{ab} = \sum_{c=1}^{3N}\frac{\partial\theta_a}{\partial q_c}\frac{\partial\theta_b}{\partial q_c} = \Lambda^{-1}_{ia}\Lambda^{-1}_{jb}\sum_{d=1}^{3}\mathfrak{R}^2_d\mathfrak{Q}^{-1}_{id}\mathfrak{Q}^{-1}_{jd} = \Lambda^{-1}_{ia}\Lambda^{-1}_{jb}\mathcal{N}^{-1}_{ij} \tag{A.6}$$

with $\boldsymbol{\mathcal{N}}^{-1}$ defined by the last equality (compare (34)). For $1 \leqslant a \leqslant 3$, $4 \leqslant b \leqslant 3N$, we get

$$M^{-1}_{ab} = \sum_{c=1}^{3N}\frac{\partial\theta_a}{\partial q_c}\frac{\partial Q_b}{\partial q_c} = \frac{1}{\mathfrak{R}^2}\Lambda^{-1}_{ia}\mathfrak{Q}_{bj}\mathcal{N}^{-1}_{ij}. \tag{A.7}$$

The case $4 \leqslant a \leqslant 3N$, $1 \leqslant b \leqslant 3$ follows from (A.7) by the symmetry of M^{-1}_{ab}. Finally, for $4 \leqslant a, b \leqslant 3N$

$$M^{-1}_{ab} = \sum_{c=1}^{3N}\frac{\partial Q_a}{\partial q_c}\frac{\partial Q_b}{\partial q_c} = \frac{1}{\mathfrak{R}^2}\delta_{ab} + \frac{1}{\mathfrak{R}^4}\mathfrak{Q}_{ai}\mathfrak{Q}_{bj}\mathcal{N}^{-1}_{ij}. \tag{A.8}$$

M^{-1}_{ab} is given by (A.6)–(A.8) in four blocks $\left(\begin{array}{c|c} {\scriptstyle 3\times 3} & {\scriptstyle 3\times(3N-3)} \\ \hline {\scriptstyle (3N-3)\times 3} & {\scriptstyle (3N-3)\times(3N-3)}\end{array}\right)$

$$\begin{aligned} \boldsymbol{M}^{-1} &= \left(\begin{array}{c|c} \boldsymbol{\Lambda}^{-1t}\boldsymbol{\mathcal{N}}^{-1}\boldsymbol{\Lambda}^{-1} & \boldsymbol{\Lambda}^{-1t}\boldsymbol{\mathcal{N}}^{-1}\boldsymbol{\mathfrak{Q}}^t/\mathfrak{R}^2 \\ \hline \boldsymbol{\mathfrak{Q}}\boldsymbol{\mathcal{N}}^{-1}\boldsymbol{\Lambda}^{-1}/\mathfrak{R}^2 & \mathbf{1}/\mathfrak{R}^2 + \boldsymbol{\mathfrak{Q}}\boldsymbol{\mathcal{N}}^{-1}\boldsymbol{\mathfrak{Q}}^t/\mathfrak{R}^4 \end{array}\right) \\ &= \left(\begin{array}{c|c} \boldsymbol{\Lambda}^{-1t} & \mathbf{0} \\ \hline \boldsymbol{\mathfrak{Q}}/\mathfrak{R}^2 & \boldsymbol{\mathcal{N}}^{\frac{1}{2}} \end{array}\right)\left(\begin{array}{c|c} \boldsymbol{\mathcal{N}}^{-1} & \mathbf{0} \\ \hline \mathbf{0} & \boldsymbol{\mathcal{N}}^{-1}/\mathfrak{R}^2 \end{array}\right)\left(\begin{array}{c|c} \boldsymbol{\Lambda}^{-1} & \boldsymbol{\mathfrak{Q}}^t/\mathfrak{R}^2 \\ \hline \mathbf{0} & \boldsymbol{\mathcal{N}}^{\frac{1}{2}} \end{array}\right). \end{aligned} \tag{A.9}$$

From the last equality we obtain $J = \mathfrak{R}^3|\Lambda|\mathcal{J}$, with $|\Lambda| = \det(\boldsymbol{\Lambda})$ and $\mathcal{J} = (\det(\boldsymbol{\mathcal{N}}))^{1/2}$. Substituting (A.9) and J into (A.1) we obtain $\nabla^2_q = -2(\mathcal{H}_N - \mathcal{V})$, with $\mathcal{H}_N$ given by (33).

A.1. Reduced Laplacian and Weyl ordering

In order to eliminate the factors of J from ∇^2_q in (A.1), and to Weyl order it, we write

$$\begin{aligned} \widetilde{\nabla}^2_q &\equiv J^{1/2}\nabla^2_q J^{-1/2} \\ &= \sum_{a,b=1}^{3N}\left(M^{-1}_{ab}\frac{\partial^2}{\partial Q_a\partial Q_b} + \frac{\partial M^{-1}_{ab}}{\partial Q_a}\frac{\partial}{\partial Q_b}\right) - \frac{1}{J^{1/2}}\sum_{a,b=1}^{3N}\left(\frac{\partial}{\partial Q_a}\left(M^{-1}_{ab}\frac{\partial J^{1/2}}{\partial Q_b}\right)\right). \end{aligned} \tag{A.10}$$

Defining the Weyl-ordered differential operator,

$$\begin{aligned} \left(M^{-1}_{ab}\frac{\partial}{\partial Q_a}\frac{\partial}{\partial Q_b}\right)_W &= \frac{1}{4}M^{-1}_{ab}\frac{\partial}{\partial Q_a}\frac{\partial}{\partial Q_b} + \frac{1}{4}\frac{\partial}{\partial Q_a}M^{-1}_{ab}\frac{\partial}{\partial Q_b} \\ &\quad + \frac{1}{4}\frac{\partial}{\partial Q_b}M^{-1}_{ab}\frac{\partial}{\partial Q_a} + \frac{1}{4}\frac{\partial}{\partial Q_a}\frac{\partial}{\partial Q_b}M^{-1}_{ab} \end{aligned} \tag{A.11}$$

(A.10) becomes

$$\widetilde{\nabla}_q^2 = \sum_{a,b=1}^{3N} \left(M_{ab}^{-1} \frac{\partial}{\partial Q_a} \frac{\partial}{\partial Q_b} \right)_W - \frac{1}{4} \sum_{a,b=1}^{3N} \frac{\partial^2 M_{ab}^{-1}}{\partial Q_a \partial Q_b} - \sum_{a,b=1}^{3N} \frac{1}{J^{1/2}} \left(\frac{\partial}{\partial Q_a} \left(M_{ab}^{-1} \frac{\partial J^{1/2}}{\partial Q_b} \right) \right). \tag{A.12}$$

The last two terms on the rhs are multiplicative operators which, up to a constant factor, constitute the quantum potential. The last one can be considerably simplified by using the second line of (A.1) to write

$$\begin{aligned} -\sum_{a,b=1}^{3N} \frac{1}{J^{1/2}} \left(\frac{\partial}{\partial Q_a} \left(M_{ab}^{-1} \frac{\partial J^{1/2}}{\partial Q_b} \right) \right) &= \frac{1}{2} \sum_{a,b,c=1}^{3N} \frac{1}{J^{1/2}} \frac{\partial}{\partial Q_a} \left(\frac{\partial Q_a}{\partial q_c} J^{1/2} \left(\frac{\partial}{\partial Q_b} \frac{\partial Q_b}{\partial q_c} \right) \right) \\ &= \sum_{a,b,c=1}^{3N} \left(\frac{1}{2} \left(\frac{\partial}{\partial Q_a} \frac{\partial Q_a}{\partial q_c} \right) \left(\frac{\partial}{\partial Q_b} \frac{\partial Q_b}{\partial q_c} \right) + \frac{1}{2} \frac{\partial Q_a}{\partial q_c} \left(\frac{\partial^2}{\partial Q_a \partial Q_b} \frac{\partial Q_b}{\partial q_c} \right) \right. \\ &\quad \left. + \frac{1}{4} \frac{\partial Q_a}{\partial q_c} \left(\frac{\partial}{\partial Q_b} \frac{\partial Q_b}{\partial q_c} \right) \sum_{c',d=1}^{3N} \frac{\partial Q_d}{\partial q_{c'}} \left(\frac{\partial}{\partial Q_a} \frac{\partial q_{c'}}{\partial Q_d} \right) \right) \end{aligned} \tag{A.13}$$

where for the last equality we used the analogue of (35),

$$\frac{\partial J}{\partial Q_a} = J \sum_{c,d=1}^{3N} \frac{\partial Q_d}{\partial q_c} \left(\frac{\partial}{\partial Q_a} \frac{\partial q_c}{\partial Q_d} \right). \tag{A.14}$$

The last term in (A.13) can be simplified using

$$\sum_{c',d=1}^{3N} \frac{\partial Q_d}{\partial q_{c'}} \left(\frac{\partial}{\partial Q_a} \frac{\partial q_{c'}}{\partial Q_d} \right) = -\sum_{c',d=1}^{3N} \left(\frac{\partial}{\partial Q_a} \frac{\partial Q_d}{\partial q_{c'}} \right) \frac{\partial q_{c'}}{\partial Q_d}$$

and

$$\sum_{a=1}^{3N} \frac{\partial Q_a}{\partial q_c} \left(\frac{\partial}{\partial Q_a} \frac{\partial Q_d}{\partial q_{c'}} \right) = \sum_{a=1}^{3N} \frac{\partial Q_a}{\partial q_{c'}} \left(\frac{\partial}{\partial Q_a} \frac{\partial Q_d}{\partial q_c} \right)$$

to obtain

$$(\mathrm{A.13}) = \sum_{a,b,c=1}^{3N} \left(\frac{1}{4} \left(\frac{\partial}{\partial Q_a} \frac{\partial Q_a}{\partial q_c} \right) \left(\frac{\partial}{\partial Q_b} \frac{\partial Q_b}{\partial q_c} \right) + \frac{1}{2} \frac{\partial Q_a}{\partial q_c} \left(\frac{\partial^2}{\partial Q_a \partial Q_b} \frac{\partial Q_b}{\partial q_c} \right) \right). \tag{A.15}$$

The second term on the rhs of (A.12) can be rewritten as

$$\begin{aligned} -\frac{1}{4} \sum_{a,b=1}^{3N} \frac{\partial^2 M_{ab}^{-1}}{\partial Q_a \partial Q_b} = -\frac{1}{4} \sum_{a,b,c=1}^{3N} & \left(2 \left(\frac{\partial^2}{\partial Q_a \partial Q_b} \frac{\partial Q_a}{\partial q_c} \right) \frac{\partial Q_b}{\partial q_c} + \left(\frac{\partial}{\partial Q_b} \frac{\partial Q_a}{\partial q_c} \right) \left(\frac{\partial}{\partial Q_a} \frac{\partial Q_b}{\partial q_c} \right) \right. \\ & \left. + \left(\frac{\partial}{\partial Q_a} \frac{\partial Q_a}{\partial q_c} \right) \left(\frac{\partial}{\partial Q_b} \frac{\partial Q_b}{\partial q_c} \right) \right). \end{aligned} \tag{A.16}$$

Thus, finally, substituting (A.15) and (A.16) into (A.12),

$$\widetilde{\nabla}_q^2 = \sum_{a,b=1}^{3N} \left(M_{ab}^{-1} \frac{\partial}{\partial Q_a} \frac{\partial}{\partial Q_b} \right)_W - \frac{1}{4} \sum_{a,b,c=1}^{3N} \left(\frac{\partial}{\partial Q_b} \frac{\partial Q_a}{\partial q_c} \right) \left(\frac{\partial}{\partial Q_a} \frac{\partial Q_b}{\partial q_c} \right). \tag{A.17}$$

A.2. The quantum potential

The kinetic energy in (58) is $-1/2\widetilde{\nabla}_q^2$. Thus, from (A.17) we have

$$V_Q = \frac{1}{8}\sum_{a,b,c=1}^{3N}\left(\frac{\partial}{\partial Q_b}\frac{\partial Q_a}{\partial q_c}\right)\left(\frac{\partial}{\partial Q_a}\frac{\partial Q_b}{\partial q_c}\right). \tag{A.18}$$

The evaluation of V_Q is straightforward, though rather laborious. We closely follow the analogous computation of [6], which leads to a compact expression for V_Q. In order to compute V_Q we split it into three terms,

$$\begin{aligned} V_Q &= V_{Q_0} + V_{Q_1} + V_{Q_2} \qquad V_{Q_0} = \frac{1}{8}\sum_{a,b=4}^{3N}\sum_{c=1}^{3N}\left(\frac{\partial}{\partial Q_a}\frac{\partial Q_b}{\partial q_c}\right)\left(\frac{\partial}{\partial Q_b}\frac{\partial Q_a}{\partial q_c}\right) \\ V_{Q_1} &= \frac{1}{4}\sum_{a=1}^{3}\sum_{b=4}^{3N}\sum_{c=1}^{3N}\left(\frac{\partial}{\partial\theta_a}\frac{\partial Q_b}{\partial q_c}\right)\left(\frac{\partial}{\partial Q_b}\frac{\partial\theta_a}{\partial q_c}\right) \\ V_{Q_2} &= \frac{1}{8}\sum_{a,b=1}^{3}\sum_{c=1}^{3N}\left(\frac{\partial}{\partial\theta_a}\frac{\partial\theta_b}{\partial q_c}\right)\left(\frac{\partial}{\partial\theta_b}\frac{\partial\theta_a}{\partial q_c}\right) \end{aligned} \tag{A.19}$$

which we consider separately.

A.2.1. V_{Q_0}. From (A.5), we get $\partial Q_b/\partial q_c$ and thence,

$$\left(\frac{\partial}{\partial Q_a}\frac{\partial Q_b}{\partial q_c}\right) = -\sum_{\beta=1}^{N}\frac{\Gamma_{c\beta n}}{\mathfrak{R}_c}\sum_{d=1}^{3}\frac{m_\beta}{\mathfrak{R}^2}\Gamma_{d\beta s}U_{sn}\left(\frac{\partial}{\partial Q_a}\mathfrak{Q}_{bg}\mathfrak{Q}^{-1}_{gd}\right). \tag{A.20}$$

Substituting this expression, and the corresponding one with a, b interchanged, into V_{Q_0} and using the completeness and orthogonality relations (30) and (40), we get

$$V_{Q_0} = -\frac{1}{8}\sum_{a,b=4}^{3N}\sum_{\beta,\gamma=1}^{N}\sum_{d=1}^{3}\frac{\mathfrak{R}_d^2}{\mathfrak{R}^4}\Gamma_{a\beta l}\Gamma_{b\gamma l'}\left(P_{\beta l}\mathfrak{Q}_{bg}\mathfrak{Q}^{-1}_{gd}\right)\left(P_{\gamma l'}\mathfrak{Q}_{am}\mathfrak{Q}^{-1}_{md}\right). \tag{A.21}$$

In (A.21), we can extend the summations over a and b down to 1, due to (24). Expanding the definitions (9) of $\mathfrak{Q}_{bg}$ and $\mathfrak{Q}_{am}$ and using completeness (30)

$$V_{Q_0} = -\frac{1}{8}\sum_{\beta,\gamma=1}^{N}\sum_{d=1}^{3}\mathfrak{R}_d^2\varepsilon_{l'gs}\varepsilon_{lmp}\left(P_{\beta l}R_{\gamma s}\mathfrak{Q}^{-1}_{gd}\right)\left(P_{\gamma l'}R_{\beta p}\mathfrak{Q}^{-1}_{md}\right). \tag{A.22}$$

It is not difficult to check that if in this equation we expand expression (29) for $P_{\beta l}$ and $P_{\gamma l'}$, the contribution due to the second term in (29) vanishes, and we get

$$V_{Q_0} = \frac{1}{8}\sum_{\beta,\gamma=1}^{N}\sum_{d=1}^{3}\mathfrak{R}_d^2\varepsilon_{l'gs}\varepsilon_{lmp}\left(\frac{\partial}{\partial R_{\beta l}}R_{\gamma s}\mathfrak{Q}^{-1}_{gd}\right)\left(\frac{\partial}{\partial R_{\gamma l'}}R_{\beta p}\mathfrak{Q}^{-1}_{md}\right). \tag{A.23}$$

Using the definition (9) of $\mathfrak{Q}_{ai}$, the derivatives can be evaluated to give

$$\left(\frac{\partial}{\partial R_{\beta l}} R_{\gamma s} \mathfrak{Q}_{gd}^{-1}\right) = \left(\delta_{\beta\gamma}\delta_{sl}\delta_{gk} - R_{\gamma s} \sum_{a=1}^{3} \mathfrak{Q}_{ga}^{-1} m_\beta \Gamma_{a\beta n} \varepsilon_{nkl}\right) \mathfrak{Q}_{kd}^{-1} \qquad \text{(A.24)}$$

and similarly $\left(\partial/\partial R_{\gamma l'} R_{\beta p} \mathfrak{Q}_{md}^{-1}\right)$. Thus,

$$V_{Q_0} = \frac{1}{8} \sum_{\beta,\gamma=1}^{N} \left(\sum_{d=1}^{3} \mathfrak{R}_d^2 \mathfrak{Q}_{kd}^{-1} \mathfrak{Q}_{hd}^{-1}\right) \varepsilon_{l'gs} \varepsilon_{lmp} \left(\delta_{\beta\gamma}\delta_{sl}\delta_{gk} - R_{\gamma s} \sum_{a=1}^{3} \mathfrak{Q}_{ga}^{-1} m_\beta \Gamma_{a\beta n} \varepsilon_{nkl}\right)$$
$$\times \left(\delta_{\beta\gamma}\delta_{pl'}\delta_{mh} - R_{\beta p} \sum_{b=1}^{3} \mathfrak{Q}_{mb}^{-1} m_\gamma \Gamma_{b\gamma n'} \varepsilon_{n'hl'}\right). \qquad \text{(A.25)}$$

Identifying the first parenthesis in this expression with $\mathcal{N}_{kh}^{-1}$ as defined in (34), it is straightforward to rearrange the factors to obtain $V_{Q_0} = \mathcal{V}_2$, with $\mathcal{V}_2$ given in (65).

A.2.2. V_{Q_1} and V_{Q_2}. With the derivatives $\partial\theta_a/\partial q_c$ given in (A.3), using the completeness relation (30) we easily get

$$V_{Q_2} = \frac{1}{8} \sum_{a,b=1}^{3} \sum_{\alpha=1}^{N} \sum_{d_1,d_2=1}^{3} m_\alpha \Gamma_{d_1\alpha k} \Gamma_{d_2\alpha p} \mathfrak{Q}_{ld_1}^{-1} \mathfrak{Q}_{qd_2}^{-1} \left(\frac{\partial}{\partial\theta_a} \Lambda_{qb}^{-1} U_{pj}\right) \left(\frac{\partial}{\partial\theta_b} \Lambda_{la}^{-1} U_{kj}\right). \qquad \text{(A.26)}$$

We can write the derivatives $\partial \boldsymbol{U}/\partial\theta_a$ in terms of Λ_{ai} using (13) to obtain the expanded form

$$V_{Q_2} = \frac{1}{8} \sum_{a,b=1}^{3} \left(\sum_{d=1}^{3} \mathfrak{R}_d^2 \mathfrak{Q}_{ld}^{-1} \mathfrak{Q}_{qd}^{-1}\right) \frac{\partial \Lambda_{qb}^{-1}}{\partial\theta_a} \frac{\partial \Lambda_{la}^{-1}}{\partial\theta_b} + \frac{1}{8} \sum_{a,b=1}^{3} \sum_{\alpha=1}^{N}$$
$$\times \sum_{d_1,d_2=1}^{3} m_\alpha \Gamma_{d_1\alpha k} \Gamma_{d_2\alpha p} \mathfrak{Q}_{ld_1}^{-1} \mathfrak{Q}_{qd_2}^{-1} \varepsilon_{ksp} \left(\frac{\partial \Lambda_{qb}^{-1}}{\partial\theta_a} \Lambda_{la}^{-1} \Lambda_{bs} - \frac{\partial \Lambda_{la}^{-1}}{\partial\theta_b} \Lambda_{qb}^{-1} \Lambda_{as}\right)$$
$$+ \frac{1}{8} \sum_{\alpha=1}^{N} \sum_{d_1,d_2=1}^{3} m_\alpha \Gamma_{d_1\alpha k} \Gamma_{d_2\alpha p} \mathfrak{Q}_{ld_1}^{-1} \mathfrak{Q}_{qd_2}^{-1} \varepsilon_{plr} \varepsilon_{kqr}. \qquad \text{(A.27)}$$

The second line can be evaluated from the commutators (19), $[L_i, L_j] = -\mathrm{i}\varepsilon_{ijk} L_k$. Substituting into these commutators expression (22) for L_i, we are led to

$$\sum_{d=1}^{3} \left(\Lambda_{jd}^{-1} \frac{\partial \Lambda_{ic}^{-1}}{\partial\theta_d} - \Lambda_{id}^{-1} \frac{\partial \Lambda_{jc}^{-1}}{\partial\theta_d}\right) = \varepsilon_{ijk} \Lambda_{kc}^{-1}. \qquad \text{(A.28)}$$

Thus, (A.27) can be rewritten as

$$V_{Q_2} = \frac{1}{8} \sum_{a,b=1}^{3} \mathcal{N}_{lq}^{-1} \frac{\partial \Lambda_{qb}^{-1}}{\partial\theta_a} \frac{\partial \Lambda_{la}^{-1}}{\partial\theta_b}$$
$$+ \frac{1}{8} \sum_{\alpha=1}^{N} \sum_{d_1,d_2=1}^{3} m_\alpha \Gamma_{d_2\alpha n} \mathfrak{Q}_{qd_2}^{-1} (\varepsilon_{nlr} \varepsilon_{kqr} + \varepsilon_{qll'} \varepsilon_{kl'n}) \mathfrak{Q}_{ld_1}^{-1} \Gamma_{d_1\alpha k}. \qquad \text{(A.29)}$$

The factor in parenthesis in the second term equals $\varepsilon_{nql'} \varepsilon_{kll'}$, but we will refrain from simplifying it. After renaming dummy indices, we can rewrite (A.29) as

$$V_{Q_2} = \frac{1}{8} \sum_{a,a'=1}^{3} \mathcal{N}_{ll'}^{-1} \frac{\partial \Lambda_{l'a'}^{-1}}{\partial\theta_a} \frac{\partial \Lambda_{la}^{-1}}{\partial\theta_{a'}}$$
$$+ \frac{1}{8} \sum_{\alpha=1}^{N} m_\alpha \sum_{d_1,d_2=1}^{3} \left(\mathfrak{Q}_{l'd_2}^{-1} \Gamma_{d_2\alpha q} \varepsilon_{qln} - \varepsilon_{l'lq} \mathfrak{Q}_{qd_2}^{-1} \Gamma_{d_2\alpha n}\right) \mathfrak{Q}_{ld_1}^{-1} \Gamma_{d_1\alpha k} \varepsilon_{kl'n} \qquad \text{(A.30)}$$

which is exactly analogous to (6.8) of [6].

With the derivatives (A.3) and (A.5), and using completeness (30), we can write

$$V_{Q_1} = -\frac{1}{4}\sum_{a=1}^{3}\sum_{b=4}^{3N}\sum_{\alpha=1}^{N}\frac{m_\alpha}{\mathfrak{R}^2}\left(\Gamma_{b\alpha r} - \sum_{d_2=1}^{3}\mathfrak{Q}_{bq}\mathfrak{Q}^{-1}_{qd_2}\Gamma_{d_2\alpha r}\right)\frac{\partial U_{rl}}{\partial\theta_a}\sum_{d_1=1}^{3}\Gamma_{d_1\alpha n}\Lambda^{-1}_{l'a}U_{nl}\frac{\partial\mathfrak{Q}^{-1}_{l'd_1}}{\partial Q_b}. \tag{A.31}$$

The derivative $\partial U_{rl}/\partial\theta_a$ can be written in terms of Λ_{ai} with (13). On the other hand, using (39) to write $\partial\mathfrak{Q}^{-1}_{l'd_1}/\partial Q_b$ in terms of $\partial\mathfrak{Q}^{-1}_{l'd_1}/\partial R_{\beta l}$ and evaluating the latter from (9), we arrive at

$$V_{Q_1} = -\frac{1}{4}\sum_{\alpha,\beta=1}^{N}\left(\sum_{c,d_1=1}^{3}\mathfrak{Q}^{-1}_{l'c}\Gamma_{c\beta p}\varepsilon_{plm}\right)\left(\mathfrak{Q}^{-1}_{md_1}\Gamma_{d_1\alpha n}\right)\sum_{b=4}^{3N}\frac{m_\alpha m_\beta}{\mathfrak{R}^2}\Gamma_{b\beta l}$$
$$\times\left(\Gamma_{b\alpha r} - \sum_{d_2=1}^{3}\mathfrak{Q}_{bq}\mathfrak{Q}^{-1}_{qd_2}\Gamma_{d_2\alpha r}\right)\varepsilon_{rl'n}. \tag{A.32}$$

Expanding $\mathfrak{Q}_{bq}$ and using completeness to evaluate the sum over b, with $\mathcal{D}^{\beta}_{lq}$ defined in (59) we get

$$V_{Q_1} = -\frac{1}{4}\sum_{\alpha,\beta=1}^{N}m_\alpha\sum_{c,d_1=1}^{3}\left(\mathfrak{Q}^{-1}_{l'c}\Gamma_{c\beta p}\varepsilon_{plm}\right)\left(\mathfrak{Q}^{-1}_{md_1}\Gamma_{d_1\alpha n}\right)\left(\delta_{\alpha\beta}\delta_{lr} - \sum_{d_2=1}^{3}m_\beta\mathcal{D}^{\beta}_{lq}\mathfrak{Q}^{-1}_{qd_2}\Gamma_{d_2\alpha r}\right)\varepsilon_{rl'n} \tag{A.33}$$

an expression which is exactly analogous to equation (6.10) of [6]. Combining this last expression for V_{Q1} and (A.29) for V_{Q2}, we can write

$$V_{Q_1}+V_{Q_2} = \frac{1}{8}\sum_{a,a'=1}^{3}\mathcal{N}^{-1}_{ll'}\frac{\partial\Lambda^{-1}_{l'a'}}{\partial\theta_a}\frac{\partial\Lambda^{-1}_{la}}{\partial\theta_{a'}} - \frac{1}{8}\sum_{\alpha=1}^{N}m_\alpha\sum_{c,d=1}^{3}\mathfrak{Q}^{-1}_{l'c}\Gamma_{c\alpha l}\mathfrak{Q}^{-1}_{md}\Gamma_{d\alpha n}(\varepsilon_{nl'p}\varepsilon_{plm} + \varepsilon_{nlp}\varepsilon_{pl'm})$$
$$-\frac{1}{4}\sum_{\alpha,\beta=1}^{N}m_\alpha m_\beta\sum_{c,d_1=1}^{3}\mathfrak{Q}^{-1}_{l'c}\Gamma_{c\beta p}\varepsilon_{plm}\mathfrak{Q}^{-1}_{md_1}\Gamma_{d_1\alpha r}\varepsilon_{rl'n}\sum_{d_2=1}^{3}\mathcal{D}^{\beta}_{lq}\mathfrak{Q}^{-1}_{qd_2}\Gamma_{d_2\alpha n}. \tag{A.34}$$

The summand on the second line of this equation is the product of $\left(\varepsilon_{plm}\mathcal{D}^{\beta}_{lq}\right)$ times an expression antisymmetric in m and q. Thus, we can replace $\left(\varepsilon_{plm}\mathcal{D}^{\beta}_{lq}\right) \to 1/2\left(\varepsilon_{plm}\mathcal{D}^{\beta}_{lq} - \varepsilon_{plq}\mathcal{D}^{\beta}_{lm}\right) = 1/2\varepsilon_{qlm}\mathcal{D}^{\beta}_{lp}$, and the second line of (A.34) becomes

$$-\frac{1}{8}\left(\sum_{\beta=1}^{N}m_\beta\sum_{c=1}^{3}\mathfrak{Q}^{-1}_{l'c}\Gamma_{c\beta p}\mathcal{D}^{\beta}_{lp}\right)\varepsilon_{qlm}\sum_{\alpha=1}^{N}m_\alpha\sum_{d_1,d_2=1}^{3}\mathfrak{Q}^{-1}_{md_1}\Gamma_{d_1\alpha r}\varepsilon_{rl'n}\mathfrak{Q}^{-1}_{qd_2}\Gamma_{d_2\alpha n}. \tag{A.35}$$

From the definitions (59) and (9), we see that the factor within parentheses in (A.35) reduces to $(-\delta_{ll'})$. Making that simplification in (A.35) and substituting the result for the second line of (A.34), we finally get

$$V_{Q_1} + V_{Q_2} = \frac{1}{8}\sum_{a,a'=1}^{3}\mathcal{N}^{-1}_{ll'}\frac{\partial\Lambda^{-1}_{l'a'}}{\partial\theta_a}\frac{\partial\Lambda^{-1}_{la}}{\partial\theta_{a'}} + \mathcal{V}_1 \tag{A.36}$$

with $\mathcal{V}_1$ given by (65).

Appendix B. Affine transformations and covariant derivatives

The transformations (69) do not depend on $\boldsymbol{r}_\alpha$ linearly but affinely, i.e., $(c_1\boldsymbol{r}_\alpha + c_2\boldsymbol{r}_\beta)' = c_1\boldsymbol{r}_\alpha{}' + c_2\boldsymbol{r}_\beta{}'$ iff $c_1 + c_2 = 1$. Covariant derivatives are defined so that they transform under time-dependent transformations in the same way as ordinary derivatives transform under time-independent transformations. Thus, we define $D_t\boldsymbol{r}_\alpha$ as in (70), so that $(D_t\boldsymbol{r}_\alpha)' = \boldsymbol{U}D_t\boldsymbol{r}_\alpha$, but $D_t(c_1\boldsymbol{r}_\alpha + c_2\boldsymbol{r}_\beta) = c_1D_t\boldsymbol{r}_\alpha + c_2D_t\boldsymbol{r}_\beta$ iff $c_1 + c_2 = 1$. Similarly, the rule for the derivative of a vector product is not the usual one, $D_t(\boldsymbol{r}_\alpha \wedge \boldsymbol{r}_\beta) = (D_t\boldsymbol{r}_\alpha) \wedge \boldsymbol{r}_\beta + \boldsymbol{r}_\alpha \wedge (D_t\boldsymbol{r}_\beta) + (\boldsymbol{r}_\alpha - \boldsymbol{r}_\beta) \wedge \boldsymbol{\rho} - \boldsymbol{\rho}$. Since $D_t\boldsymbol{r}_\alpha$ transforms linearly under gauge transformations, we define

$$D_tD_t\boldsymbol{r}_\alpha \equiv \frac{\mathrm{d}}{\mathrm{d}t}(D_t\boldsymbol{r}_\alpha) - \boldsymbol{\xi}(D_t\boldsymbol{r}_\alpha) \qquad (D_tD_t\boldsymbol{r}_\alpha)' = \boldsymbol{U}D_tD_t\boldsymbol{r}_\alpha. \tag{B.1}$$

With (70) and (B.1), the equations of motion from Lagrangian (72) take the form $m_\alpha D_tD_t\boldsymbol{r}_\alpha = -\nabla_\alpha\mathcal{V}$ as in (4).

With the definition (5) for the angular momentum $\boldsymbol{l}$ and the transformation law (69) we have $\boldsymbol{l}' = \boldsymbol{U}\boldsymbol{l} + M\boldsymbol{u} \wedge (\boldsymbol{U}D_t\boldsymbol{r}_{\mathrm{cm}})$, with $\boldsymbol{r}_{\mathrm{cm}}$ the centre of mass position vector. Thus, we define

$$D_t\boldsymbol{l} \equiv \dot{\boldsymbol{l}} - \boldsymbol{\xi}\boldsymbol{l} - M\boldsymbol{\rho} \wedge (D_t\boldsymbol{r}_{\mathrm{cm}}) \tag{B.2}$$

so that $(D_t\boldsymbol{l})' = \boldsymbol{U}D_t\boldsymbol{l} + M\boldsymbol{u} \wedge (\boldsymbol{U}D_tD_t\boldsymbol{r}_{\mathrm{cm}})$ with $D_tD_t\boldsymbol{r}_{\mathrm{cm}}$ defined as in (B.1) and (70). The centre of mass angular momentum $\boldsymbol{l}_{\mathrm{cm}} = M\boldsymbol{r}_{\mathrm{cm}} \wedge D_t\boldsymbol{r}_{\mathrm{cm}}$ transforms in the same way as $\boldsymbol{l}$, and its covariant derivative is defined as in (B.2). From the equations of motion for $\boldsymbol{r}_\alpha$, we then get

$$D_t\boldsymbol{l} = 0 \qquad D_tD_t\boldsymbol{r}_{\mathrm{cm}} = 0 \qquad D_t\boldsymbol{l}_{\mathrm{cm}} = 0. \tag{B.3}$$

Therefore, $D_t\boldsymbol{l} - D_t\boldsymbol{l}_{\mathrm{cm}} = (\mathrm{d}/\mathrm{d}t - \boldsymbol{\xi})(\boldsymbol{l} - \boldsymbol{l}_{\mathrm{cm}}) = 0$, which is (73) and which, together with the antisymmetry of $\boldsymbol{\xi}$, immediately leads to $\mathrm{d}/\mathrm{d}t(\boldsymbol{l} - \boldsymbol{l}_{\mathrm{cm}})^2 = 0$. Furthermore, $(\boldsymbol{l} - \boldsymbol{l}_{\mathrm{cm}})' = \boldsymbol{U}(\boldsymbol{l} - \boldsymbol{l}_{\mathrm{cm}})$ so that $(\boldsymbol{l} - \boldsymbol{l}_{\mathrm{cm}})^2$ is invariant under gauge transformations, i.e., frame independent.

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