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

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Abstract
We study the quantization of many-body systems in two dimensions in rotating coordinate frames using a gauge-invariant formulation of the dynamics. We consider reference frames defined by linear and quadratic gauge conditions. In both cases we discuss their Gribov ambiguities and commutator algebra. We construct the momentum operators, inner product and Hamiltonian in both types of gauges, for systems with and without translation invariance. The analogy with the quantization of QED in non-covariant gauges is emphasized. Our results are applied to quasi-rigid systems in the Eckart frame.

PACS numbers: 31.15.−p, 03.65.Ca, 11.15.Kc, 24.10.Cn

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. When the underlying dynamics are rotationally symmetric, which is the only case we consider, the coordinate transformation from a space-fixed reference frame to a rotating one with the same origin is a time-dependent symmetry transformation. It is thus appropriate to formulate the theory in such a way that it is invariant under symmetry transformations whose parameters depend on time, or gauge transformations [1]. 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 reference frame. Gauge invariance guarantees that both theories are physically equivalent.

Whereas formulating a quantum theory in a rotating frame is a mathematical problem, the choice of the particular frame in which to formulate the theory is dictated by the physics of the specific system under consideration. It is often the case that the relevant rotating frame is

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]. In quantum electrodynamics (QED), for instance, the degrees of freedom are the components of the vector potential $A(t, x)$, which may be required to satisfy such relations as $\nabla \cdot A = 0$ (Coulomb gauge), or $x \cdot A = 0$ (multipolar gauge) [3], at all times t.

In this paper we study the quantization of many-body systems in two dimensions in rotating coordinate frames, using a gauge-invariant formulation. We consider systems of N spinless particles in the plane, interacting through two-body central potentials. We focus on developing the formalism, which is a necessary step before considering applications to realistic models. By restricting ourselves to the two-dimensional rotation group, we separate the treatment of the gauge-invariant formalism from the technical intricacies of non-Abelian groups such as the three-dimensional rotation group, which we will consider elsewhere.

Our treatment closely follows the approach of [2, 4] to Yang–Mills theories. Previous treatments of the quantization of two- and three-dimensional N-body systems in rotating frames within a gauge-invariant approach have been given in [5–7] (and references therein). In [6] the gauge symmetry is implemented within the Hamiltonian BRST formalism [8]. In [7] a point of view based on the shape-space theory of deformable bodies is adopted. Non-gauge-invariant treatments can be found in, e.g., [9] in the context of nuclear physics, and in [10] in molecular physics. Our goals are to establish a formal framework with the most direct geometrical and physical interpretation, and to provide careful and systematic derivations of our results. Furthermore, the results we obtain are different from previous ones.

In the following section we describe the class of models considered throughout the paper, and their gauge-invariant formulation. Their quantization in a space-fixed frame is given, and shown to be equivalent to the original, non-gauge-invariant system. In the remaining sections we obtain the quantized theory in rotating frames by means of a gauge transformation from the space-fixed frame. In section 3 we consider rotating frames defined by linear gauge conditions. Such gauges are the most important ones for practical applications. We discuss the Gribov ambiguities [11] of these gauges, which are important for the construction of the inner product in Hilbert space. The algebra of commutators is discussed in detail, and an explicit realization of this algebra in terms of differential operators is given. We then use these operators to construct the Hamiltonian. The equivalence of the quantum theory in these and other gauges with the theory formulated in a non-rotating reference frame is kept manifest at every step. We emphasize that by describing the system from a rotating reference frame defined by imposing restrictions on the coordinates, we are in fact introducing orthogonal curvilinear coordinates in configuration space.

In section 4 we go through the same steps, though more briefly, to obtain the theory in the instantaneous principal axes frame as an example of a gauge condition depending quadratically on the coordinates. Although the treatment is straightforward, the results are technically much more complicated than in the linear case. This fact makes the practical usefulness of this gauge condition doubtful. The quantization in linear gauges in section 3 is extended in section 5 to translationally invariant systems in rotating frames with origin at the centre of mass. These results are then applied to the case of quasi-rigid systems in section 6, where we discuss the Eckart gauge and recover some of the classic results of [12]. In section 7 we give our final remarks. Throughout the paper we try to manifest the similarity between our approach and the quantization of QED in non-covariant gauges. In appendix A we give a brief summary

of those aspects of QED which are relevant to the analysis presented in the main body of the paper. In appendix B we derive some technical results needed in the following.

2. *N*-particle system

We consider a system of N particles in two dimensions interacting through a two-body central potential, described by the Lagrangian

$$\mathcal{L} = \frac{1}{2} \sum_{\alpha=1}^{N} m_\alpha \dot{r}_\alpha^2 - \sum_{\alpha<\beta=1}^{N} V(|r_\alpha - r_\beta|) - \sum_{\alpha=1}^{N} U(r_\alpha). \tag{1}$$

If the one-body potential $U = 0$, $\mathcal{L}$ is invariant under the group of Euclidean motions of the plane. In this and the following sections, we consider $U \neq 0$ and focus on the Abelian group of two-dimensional rotations, deferring the discussion of translation invariance until section 5.

We adopt the passive point of view for coordinate transformations. $\mathcal{L}$ 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 usual Yang–Mills construction [13] to (1). We add a new degree of freedom ξ to the system, and postulate the following transformation law under infinitesimal rotations of the coordinate frame,

$$\delta r_\alpha = -\delta\theta \hat{z} \wedge r_\alpha \qquad \delta\xi = -\delta\dot{\theta} \tag{2}$$

with $\delta\theta = \delta\theta(t)$ being an arbitrary function of t, and $\hat{z}$ is a unit vector orthogonal to the plane. These are the infinitesimal gauge transformations of the system. We define the covariant derivative $D_t r_\alpha \equiv \dot{r}_\alpha - \xi \hat{z} \wedge r_\alpha$, which transforms as a vector under gauge transformations, $\delta(D_t r_\alpha) = -\delta\theta \hat{z} \wedge D_t r_\alpha$. Substituting time derivatives in (1) by covariant derivatives, we obtain a Lagrangian invariant under time-dependent rotations of the coordinate frame. Explicitly, we write

$$\mathcal{L} = \frac{1}{2} \sum_{\alpha=1}^{N} m_\alpha (D_t r_\alpha)^2 - \mathcal{V} + \ell_z \xi = \frac{1}{2} \sum_{\alpha=1}^{N} m_\alpha \dot{r}_\alpha^2 + \frac{\xi^2}{2} \sum_{\alpha=1}^{N} m_\alpha r_\alpha^2$$

$$- \xi \hat{z} \cdot \sum_{\alpha=1}^{N} m_\alpha (r_\alpha \wedge \dot{r}_\alpha) - \mathcal{V} + \ell_z \xi \tag{3}$$

where we have denoted by $\mathcal{V}$ the potential energy for brevity. In (3) we added an extra term $\ell_z \xi$ to $\mathcal{L}$ which fixes the value of the angular momentum through the equation of motion for ξ. This term plays a role analogous to the source term $j^0(x)A^0(t, x)$ in electrodynamics[1], as discussed in appendix A. $\mathcal{L}$ is invariant under gauge transformations if the constant $\ell_z = 0$, and quasi-invariant otherwise, $\delta\mathcal{L} = -\ell_z \delta\dot{\theta}$.

$\mathcal{L}$ in (3) describes the same dynamics as (1), but from a coordinate frame rotating with angular velocity $-\xi$ with respect to the laboratory frame [14]. Note, however, that ξ is a dynamical variable describing the coupling of the particles to inertial forces. The equations of motion for r_α are $m_\alpha D_t D_t r_\alpha + \nabla_\alpha \mathcal{V} = 0$ or, more explicitly,

$$m_\beta \ddot{r}_\beta = 2m_\beta \xi \hat{z} \wedge \dot{r}_\beta + m_\beta \dot{\xi} \hat{z} \wedge r_\beta + m_\beta \xi^2 \hat{z} \wedge (r_\beta \wedge \hat{z}) - \nabla_\beta \mathcal{V} \tag{4}$$

---

[1] We remark that external source terms break gauge invariance when the gauge symmetry is non-Abelian. In that case, in order to preserve gauge invariance and, at the same time, have a non-homogeneous Gauss law, we must incorporate the source into the theory as a dynamical degree of freedom.

where the terms corresponding to the Coriolis, azimuthal and centrifugal forces are apparent [15]. A consequence of rotational symmetry is the conservation of the system's total angular momentum

$$L_z = \hat{z} \cdot \sum_{\alpha=1}^{N} m_\alpha (r_\alpha \wedge D_t r_\alpha).$$

The equation of motion for ξ is then $L_z - \ell_z = 0$.

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

2.1. The laboratory frame

Given any trajectory of the system $(\{r_\alpha(t)\}, \xi(t))$ by means of a finite gauge transformation $r'_\alpha = U(\theta(t))r_\alpha, \xi'(t) = \xi(t) - \dot{\theta}(t)$, with U being an orthogonal 2×2 matrix and $\theta(t) = \int_{t_0}^{t} d\tau \xi(\tau)$, we can obtain a physically equivalent trajectory with $\xi'(t) = 0$. The gauge condition $\xi = 0$ corresponds to choosing a non-rotating reference frame, the laboratory frame. In this gauge the Lagrangian (3) reduces to (1). The equation of motion for ξ, $\sum_{\alpha=1}^{N} m_\alpha r_\alpha \wedge \dot{r}_\alpha - \ell_z = 0$, which cannot be obtained from (1), must be imposed on the system as a constraint [2]. In the Hamiltonian formulation in this gauge, this constraint is first class [16], not leading to further secondary constraints.

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

$$
\begin{aligned}
&\mathcal{H} = \sum_{\alpha=1}^{N} \frac{1}{2m_\alpha} p_\alpha^2 + \mathcal{V} \qquad\qquad [r_{\alpha i}, p_{\beta j}] = i\delta_{\alpha\beta}\delta_{ij} \\
&\langle \phi|\psi \rangle = \int \prod_{\beta=1}^{N} d^2 r_\beta \phi^*(\{r_\alpha\})\psi(\{r_\alpha\})
\end{aligned}
\tag{5}
$$

with $p_\alpha = 1/i\nabla_\alpha$. The first-class constraint is imposed on the state space [16], $L_z|\psi\rangle = \ell_z|\psi\rangle$. The constant ℓ_z can only take integer values in the quantum theory. We see that both the classical and quantum theories for this model in the gauge $\xi = 0$ are completely analogous to electrodynamics in Weyl gauge [2, 17] (see appendix A). The constraint fixing the value of L_z, in particular, plays the same role as Gauss law in QED.

3. Linear gauge conditions

The simplest form of gauge condition involving the coordinates is a linear relation among them. As discussed in section 6 this kind of gauge condition is relevant in the context of perturbative or semiclassical expansions. The following notation will be used throughout this paper:

$$\mathfrak{G}(\{r_\alpha\}) = \sum_{\beta=1}^{N} m_\beta (A_\beta x_\beta + B_\beta y_\beta) \tag{6a}$$

$$\mathfrak{Q}(\{r_\alpha\}) = \sum_{\alpha=1}^{N} m_\alpha(B_\alpha x_\alpha - A_\alpha y_\alpha) \qquad \mathfrak{R}^2 \equiv \sum_{\alpha=1}^{N} m_\alpha\left(A_\alpha^2 + B_\alpha^2\right). \qquad (6b)$$

The general linear gauge condition is of the form $\mathfrak{S} = 0$, with $\mathfrak{R}^2 \neq 0$. We denote position vectors $\boldsymbol{R}_\alpha$ and their components X_α, Y_α in this gauge by capital letters, as opposed to vectors in the gauge $\xi = 0$ (the laboratory frame) denoted by $\boldsymbol{r}_\alpha$. Thus $\mathfrak{S}(\{\boldsymbol{R}_\alpha\}) = 0$ but, in general, $\mathfrak{S}(\{\boldsymbol{r}_\alpha\}) \neq 0$. This gauge condition selects a reference frame rotating in such a way that the linear combination of coordinates $\mathfrak{S}$ vanishes for all t. If we choose, for instance, all coefficients in (6a) vanishing except for B_1, the coordinate frame must rotate together with particle 1 so that particle stays on the X axis for all t. The formalism in these linear gauges is entirely analogous to that of electrodynamics in Coulomb gauge (appendix A), in which the fields are also constrained by a linear relation.

The transformation from the gauge $\xi = 0$ to the gauge $\mathfrak{S} = 0$ is given by

$$\boldsymbol{R}_\alpha(t) = \boldsymbol{U}(\theta(t))\boldsymbol{r}_\alpha(t) \qquad \xi(t) = -\dot{\theta}(t) \qquad \text{with} \qquad \theta(t) = \arctan\left(\frac{\mathfrak{s}}{\mathfrak{q}}\right) + n\pi \qquad (7)$$

where we denoted $\mathfrak{s} \equiv \mathfrak{S}(\{r_\alpha\})$, $\mathfrak{q} \equiv \mathfrak{Q}(\{r_\alpha\})$ for brevity. The indetermination in θ up to addition of π is a Gribov ambiguity [11] (see also [2, 4]), related to the two possible choices $\mathfrak{Q} = \pm\sqrt{\mathfrak{q}^2 + \mathfrak{s}^2}$. We fix the ambiguity by requiring $\mathfrak{Q} \geqslant 0$ and $-\pi < \theta \leqslant \pi$. Due to the relation $\xi = -\dot{\theta}$ for all t in this gauge, with θ from (7), we can use $\{\boldsymbol{R}_\alpha, \theta\}$ as dynamical variables instead of $\{\boldsymbol{R}_\alpha, \xi\}$. The former set of variables is preferable in the operator approach we espouse in this paper, whereas in the path integral formulation switching from one set to the other amounts to a mere change of integration variables. The inverse to the transformation (7) is then

$$\boldsymbol{r}_\alpha(t) = \boldsymbol{U}(-\theta(t))\boldsymbol{R}_\alpha(t) \qquad (8)$$

with θ being an independent variable. (If we choose ξ as a dynamical variable instead of θ, then in (8) $\theta(t) = -\int_{t_0}^{t} d\tau \xi(\tau)$.)

Solving the equation of motion for ξ, we get

$$\xi = -\dot{\theta} = \frac{1}{\sum_{\beta=1}^{N} m_\beta \boldsymbol{R}_\beta^2}\left(\hat{\boldsymbol{z}} \cdot \sum_{\alpha=1}^{N} m_\alpha \boldsymbol{R}_\alpha \wedge \dot{\boldsymbol{R}}_\alpha - \ell_z\right). \qquad (9)$$

Since the gauge has already been completely fixed, we can substitute (9) back into the Lagrangian (3). Note that the vector product appearing in (9) is not the total angular momentum of the system. In the classical theory we obtain the momenta $\boldsymbol{\Pi}_\alpha$ conjugate to $\boldsymbol{R}_\alpha$ by differentiating $\mathcal{L}$ in (3) with respect to $\dot{\boldsymbol{R}}_\alpha$ under the constraint $\dot{\mathfrak{S}}(\{\boldsymbol{R}_\alpha\}) = \mathfrak{S}(\{\dot{\boldsymbol{R}}_\alpha\}) = 0$ to obtain

$$\Pi_{X_\alpha} = m_\alpha \dot{X}_\alpha + m_\alpha\xi\left(Y_\alpha + \frac{A_\alpha\mathfrak{Q}}{\mathfrak{R}^2}\right) \qquad \Pi_{Y_\alpha} = m_\alpha \dot{Y}_\alpha - m_\alpha\xi\left(X_\alpha - \frac{B_\alpha\mathfrak{Q}}{\mathfrak{R}^2}\right) \qquad (10)$$

where ξ is given by (9). These momenta are consistent with the gauge condition, since they satisfy

$$0 = \sum_{\beta=1}^{N} \frac{1}{m_\beta}\frac{\partial\mathfrak{S}}{\partial\boldsymbol{R}_\beta} \cdot \boldsymbol{\Pi}_\beta = \mathfrak{S}(\{\boldsymbol{\Pi}_\alpha/m_\alpha\}) \qquad (11)$$

the last equality following from the linearity of $\mathfrak{S}$. Relation (11) is analogous to the condition that the momentum conjugate to the potential in Coulomb gauge must be transverse, equation (A.12).

From (7) and (8) we can obtain the relation between the velocities $\{\dot{r}_\alpha\}$ in the gauge $\xi = 0$ and those in the gauge $\mathfrak{S} = 0$, $\{\dot{R}_\alpha, \dot{\theta}\}$. Correspondingly, we can express the momenta $\{p_\alpha\}$ in one gauge in terms of momenta $\{\Pi_\alpha\}$ and ℓ_z in the other. With these transformations we obtain from $\mathcal{H}$ in (5) the classical Hamiltonian in this gauge,

$$\mathcal{H} = \sum_{\alpha=1}^{N} \frac{1}{2m_\alpha} \Pi_\alpha^2 + \frac{\mathfrak{R}^2}{2\mathfrak{Q}^2}(\ell_z - \Lambda)^2 + \mathcal{V} \qquad \text{with} \quad \Lambda = \sum_{\beta=1}^{N} \left(X_\beta \Pi_{Y_\beta} - Y_\beta \Pi_{X_\beta} \right). \tag{12}$$

The quantity Λ defined by this equation will be henceforth referred to as the 'residual angular momentum'.

By the same token, expressing Π_α and R_α in terms of p_α and r_α and using the Poisson brackets (5), we get the Poisson brackets in this gauge. Alternatively, they can be found as Dirac brackets [16] relative to the second-class constraints $\mathfrak{S}(\{R_\alpha\}) = 0 = \mathfrak{S}(\{\Pi_\alpha/m_\alpha\})$. The result is, written in the notation of quantum commutators,

$$\left[X_\beta, \Pi_{X_\gamma} \right] = i \left(\delta_{\beta\gamma} - \frac{A_\beta A_\gamma m_\gamma}{\mathfrak{R}^2} \right) \qquad \left[Y_\beta, \Pi_{Y_\gamma} \right] = i \left(\delta_{\beta\gamma} - \frac{B_\beta B_\gamma m_\gamma}{\mathfrak{R}^2} \right)$$

$$\left[X_\beta, \Pi_{Y_\gamma} \right] = -i \frac{A_\beta B_\gamma m_\gamma}{\mathfrak{R}^2} \qquad\qquad \left[Y_\beta, \Pi_{X_\gamma} \right] = -i \frac{m_\gamma A_\gamma B_\beta}{\mathfrak{R}^2}. \tag{13}$$

All other commutators among components of R_α and Π_β vanish. The correspondence between (13) and (A.14) is apparent. Using (13) we obtain the commutators for Λ,

$$[X_\alpha, \Lambda] = -iY_\alpha - i\frac{A_\alpha \mathfrak{Q}}{\mathfrak{R}^2} \qquad\qquad [Y_\alpha, \Lambda] = iX_\alpha - i\frac{B_\alpha \mathfrak{Q}}{\mathfrak{R}^2}$$

$$\left[\Lambda, \Pi_{X_\gamma} \right] = i\Pi_{Y_\gamma} + i\frac{A_\gamma m_\gamma}{\mathfrak{R}^2}\mathfrak{Q}(\{\Pi_\alpha/m_\alpha\}) \qquad \left[\Lambda, \Pi_{Y_\gamma} \right] = -i\Pi_{X_\gamma} + i\frac{B_\gamma m_\gamma}{\mathfrak{R}^2}\mathfrak{Q}(\{\Pi_\alpha/m_\alpha\}). \tag{14}$$

Furthermore, from (13) and (14) we get

$$\left[\mathfrak{S}, \Pi_{X_\alpha} \right] = \left[\mathfrak{S}, \Pi_{Y_\alpha} \right] = 0 = [\mathfrak{S}, \Lambda] = [\mathfrak{S}(\{\Pi_\alpha/m_\alpha\}), \Lambda]$$

$$\left[\mathfrak{Q}, \Pi_{X_\alpha} \right] = im_\alpha B_\alpha \qquad \left[\mathfrak{Q}, \Pi_{Y_\alpha} \right] = -im_\alpha A_\alpha \tag{15}$$

$$[\mathfrak{Q}, \mathfrak{S}(\{\Pi_\alpha/m_\alpha\})] = 0 \quad [\mathfrak{Q}, \Lambda] = -i\mathfrak{S}.$$

We see from (13)–(15) that Π_α and Λ generate translations and rotations, respectively, of $\{R_\alpha\}$ on the surface $\mathfrak{S} = 0$. We also see that the gauge condition $\mathfrak{S} = 0$ and (11) are operator equations, which can be evaluated within commutators.

In the quantum theory a realization of the commutators (13) is obtained by defining Π_α as the projection of the gradient ∇_α on the hyperplane tangent to the surface $\mathfrak{S} = 0$ (which in this case is the surface itself, since $\mathfrak{S}$ is a linear function),

$$\Pi_{X_\alpha} = \frac{1}{i}\frac{\partial}{\partial X_\alpha} - \frac{1}{i}\frac{m_\alpha A_\alpha}{\mathfrak{R}^2} \sum_{\beta=1}^{N} \left(A_\beta \frac{\partial}{\partial X_\beta} + B_\beta \frac{\partial}{\partial Y_\beta} \right)$$

$$\Pi_{Y_\alpha} = \frac{1}{i}\frac{\partial}{\partial Y_\alpha} - \frac{1}{i}\frac{m_\alpha B_\alpha}{\mathfrak{R}^2} \sum_{\beta=1}^{N} \left(A_\beta \frac{\partial}{\partial X_\beta} + B_\beta \frac{\partial}{\partial Y_\beta} \right). \tag{16}$$

These operators, which are analogous to (A.15) in QED in Coulomb gauge, satisfy the equation $\mathfrak{S}(\{\Pi_\alpha/m_\alpha\}) = 0$. From (12) and (16) we obtain the expression for the residual angular momentum operator Λ,

$$\Lambda = \sum_{\beta=1}^{N} \left\{ \left(X_\beta - \frac{B_\beta \mathfrak{Q}}{\mathfrak{R}^2} \right) \frac{1}{i}\frac{\partial}{\partial Y_\beta} - \left(Y_\beta + \frac{A_\beta \mathfrak{Q}}{\mathfrak{R}^2} \right) \frac{1}{i}\frac{\partial}{\partial X_\beta} \right\} \tag{17}$$

which is shown in appendix B to have integer eigenvalues.

Using relations (7) and (8) between $\{r_\alpha\}$ and $\{R_\alpha, \theta\}$ and applying the chain rule we obtain, after appropriately rearranging the derivative operators,

$$
\begin{aligned}
p_{x\alpha} &\equiv \frac{1}{\mathrm{i}}\frac{\partial}{\partial x_\alpha} = \cos\theta\left(\Pi_{X\alpha} + \frac{m_\alpha A_\alpha}{\mathfrak{Q}}(L_z - \Lambda)\right) - \sin\theta\left(\Pi_{Y\alpha} + \frac{m_\alpha B_\alpha}{\mathfrak{Q}}(L_z - \Lambda)\right) \\
p_{y\alpha} &\equiv \frac{1}{\mathrm{i}}\frac{\partial}{\partial y_\alpha} = \sin\theta\left(\Pi_{X\alpha} + \frac{m_\alpha A_\alpha}{\mathfrak{Q}}(L_z - \Lambda)\right) + \cos\theta\left(\Pi_{Y\alpha} + \frac{m_\alpha B_\alpha}{\mathfrak{Q}}(L_z - \Lambda)\right)
\end{aligned}
\tag{18}
$$

with $L_z = 1/\mathrm{i}\partial/\partial\theta$. The first-class constraint $L_z\psi = \ell_z\psi$ is trivial to solve in this gauge, $\psi(\{R_\alpha\}, \theta) = \psi(\{R_\alpha\})\exp(\mathrm{i}\ell_z\theta)/\sqrt{2\pi}$. An analogue of (18) in QED is the simpler relation (A.18).

The Hamiltonian operator in this gauge is obtained from $\mathcal{H}$ in the gauge $\xi = 0$ as given by (5), through the transformation rules (8) and (18),

$$
\mathcal{H} = \sum_{\beta=1}^{N}\frac{1}{2m_\beta}\left(\frac{1}{\mathfrak{Q}}\Pi_{X_\beta}\mathfrak{Q}\Pi_{X_\beta} + \frac{1}{\mathfrak{Q}}\Pi_{Y_\beta}\mathfrak{Q}\Pi_{Y_\beta}\right) + \frac{\mathfrak{R}^2}{2\mathfrak{Q}^2}(\ell_z - \Lambda)^2 + \mathcal{V}.
\tag{19}
$$

The first term in $\mathcal{H}$ has a structure similar to that of the Laplacian in curvilinear coordinates, with $\mathfrak{Q}$ as the Jacobian and $\mathbf{\Pi}$ as derivative operators. (In the case $N = 1$ the similarity turns, in fact, into an identity, see below.) Note, however, that we did not postulate (19), rather, we derived it from expression (5) in the laboratory frame.

The inner product in Hilbert space can be found from expression (5) for $\langle\phi|\psi\rangle$ in the gauge $\xi = 0$ by the familiar Faddeev–Popov method [18], the relevant resolution of the identity being in this case,

$$
1 = \int_{-\pi}^{\pi}\mathrm{d}\alpha\,\delta(\mathfrak{S}(\{U(\alpha)r_\beta\}))\Theta(\mathfrak{Q}(\{U(\alpha)r_\beta\}))\mathfrak{Q}(\{U(\alpha)r_\beta\})
\tag{20}
$$

with $\Theta(\mathfrak{Q})$ being a step function enforcing positivity of the Faddeev–Popov determinant $\mathfrak{Q}$. As mentioned above, the condition $\mathfrak{Q} \geqslant 0$ guarantees that there is only one root $\alpha = \theta$ (with θ from (7)), and not $\theta + \pi$, to the equation $\mathfrak{S} = 0$ in (20). Inserting (20) in expression (5) for $\langle\phi|\psi\rangle$, we get

$$
\langle\phi|\psi\rangle = \int\prod_{\beta=1}^{N}\mathrm{d}^2 R_\beta\delta(\mathfrak{S})\Theta(\mathfrak{Q})\mathfrak{Q}\phi^*(\{R_\alpha\})\psi(\{R_\alpha\})
\tag{21}
$$

where we dropped a factor of 2π, the measure of the group $SO(2)$. The hermiticity of Λ and $\mathcal{V}$ with respect to the inner product (21) is immediate in view of the commutation relations. In order to check the hermiticity of the Hamiltonian (19), it is enough to show that the first term in (19) is Hermitian. The calculation is straightforward, though somewhat lengthy, so we omit the details.

It is sometimes convenient to redefine the state space by absorbing the Jacobian in the wavefunctions and eliminating it from the integration measure in the inner product. The redefined wavefunctions are $\widetilde{\psi} = \mathfrak{Q}^{1/2}\psi$, leading to the Hamiltonian

$$
\widetilde{\mathcal{H}} \equiv \mathfrak{Q}^{1/2}\mathcal{H}\mathfrak{Q}^{-1/2} = \sum_{\beta=1}^{N}\frac{1}{2m_\beta}\left(\Pi_{X_\beta}^2 + \Pi_{Y_\beta}^2\right) + \frac{\mathfrak{R}^2}{2\mathfrak{Q}^2}(\ell_z - \Lambda)^2 + \mathcal{V} - \frac{\mathfrak{R}^2}{8\mathfrak{Q}^2}
\tag{22}
$$

the last term being the quantum-mechanical potential [2, 4]. Equation (22), with classical $\mathbf{\Pi}$ and Λ, is the Hamiltonian found in this gauge in the path-integral approach. Since the transformation (7) depends non-linearly on $\{r_\alpha\}$, the associated change of integration variables in the generating functional entails a change in its discretization [19], which ultimately gives rise to the quantum potential term.

3.1. The case N = 1

The case $N = 1$ is instructive [2, 4]. By means of a time-independent rotation, we can always reduce the condition $\mathfrak{S} = 0$ to $Y = 0$. We thus fix a reference frame rotating together with the particle, so that it is on the X axis for all t, with $X \geqslant 0$. In order to specify the position of the particle, we give its coordinate X and the angle θ of the X axis relative to the laboratory x axis. We are then describing the motion in terms of polar coordinates with X as the radial coordinate.

From (16) we have $\Pi_X = -i\partial/\partial X$ and $\Pi_Y = 0 = \Lambda$. The Faddeev–Popov determinant in this case is $\mathfrak{Q} = X$, and the Hamiltonian (19) reduces to that of a particle in polar coordinates, with angular momentum ℓ_z. Similarly, the inner product (21) corresponds to polar coordinates. Due to the constraint $L_z \psi = \ell_z \psi$, the integration over the angle variable θ is trivial, so only the radial wavefunction appears in (21). If the wavefunction in Cartesian coordinates is $\psi(x, y)$, the radial wavefunction is $\psi(X, 0)$. The quantum potential term in (22) also reduces in this case to its well-known form [2, 4] for polar coordinates, $-1/(8mX^2)$.

4. Quadratic gauge condition: the instantaneous principal axes

The quantization of the system (1) in a rotating frame defined by a quadratic gauge condition follows the same lines as the linear case studied in section 3. Both the treatment and the results are technically more involved, however, so instead of considering a general quadratic gauge condition, we restrict ourselves to the particular case of the instantaneous principal axes frame. This reference frame plays a central role in the treatment of rigid body dynamics. In the case of many-body systems, their quantization in the instantaneous principal axes frame has been proposed as a method for separating the 'collective' rotations from the 'intrinsic' dynamics. We briefly discuss this issue in section 7. In this section we compute the quantum Hamiltonian and inner product by means of a gauge transformation from the gauge $\xi = 0$.

We define the quantities

$$Q(\{r_\alpha\}) = \frac{1}{2}\sum_{\alpha=1}^{N} m_\alpha(x_\alpha^2 - y_\alpha^2) \qquad S(\{r_\alpha\}) = \sum_{\alpha=1}^{N} m_\alpha x_\alpha y_\alpha \qquad R^2(\{r_\alpha\}) = \sum_{\alpha=1}^{N} m_\alpha r_\alpha^2.$$

$$(23)$$

R^2 is the trace of the inertia tensor of the system, whose traceless part is given by $\begin{pmatrix} -Q & -S \\ -S & Q \end{pmatrix}$. The instantaneous principal axes frame is then defined by the condition $S = 0$. As above, we denote vectors referred to this frame with capital letters, so that $S(\{R_\alpha\}) = 0$. The gauge transformation from the gauge $\xi = 0$ to the gauge $S = 0$ has the form (7), with the parameter,

$$\theta(t) = \frac{1}{2}\arctan\left(\frac{S(\{r_\alpha\})}{Q(\{r_\alpha\})}\right) + \frac{n}{2}\pi. \tag{24}$$

Due to the fact that the inertia tensor is second rank, the number of Gribov ambiguities doubles with respect to the linear case (7), there being now four solutions in the range $-\pi \leqslant \theta \leqslant \pi$. We fix the ambiguity by requiring $Q(\{R_\alpha\}) \geqslant 0$ and $0 \leqslant \theta \leqslant \pi$.

The Lagrangian is now (3) with ξ having the same form as in (9). Consistency with the gauge condition $S(\{R_\alpha\}) = 0$ requires the velocities and momenta to satisfy,

$$\sum_{\alpha=1}^{N} m_\alpha(X_\alpha \dot{Y}_\alpha + Y_\alpha \dot{X}_\alpha) = 0 \tag{25a}$$

$$\sum_{\alpha=1}^{N} \left(X_\alpha \Pi_{Y_\alpha} + Y_\alpha \Pi_{X_\alpha} \right) = 0. \tag{25b}$$

We obtain the conjugate momenta in terms of velocities by deriving $\mathcal{L}$ with respect to $\dot{\boldsymbol{R}}_\alpha$ under the constraint (25a),

$$\Pi_{X_\alpha} = m_\alpha \dot{X}_\alpha + \xi m_\alpha Y_\alpha \left(1 + \frac{2Q(\{\boldsymbol{R}_\alpha\})}{R^2(\{\boldsymbol{R}_\alpha\})} \right) \qquad \Pi_{Y_\alpha} = m_\alpha \dot{Y}_\alpha - \xi m_\alpha X_\alpha \left(1 - \frac{2Q(\{\boldsymbol{R}_\alpha\})}{R^2(\{\boldsymbol{R}_\alpha\})} \right). \tag{26}$$

The basic Poisson brackets in this gauge can be obtained as in section 3. Since the momenta $\boldsymbol{\Pi}_\alpha$ generate translations on the curved hypersurface $S(\{\boldsymbol{R}_\alpha\}) = 0$, which do not commute, the Poisson brackets among momenta do not vanish. Correspondingly, in the quantum theory the operators $\boldsymbol{\Pi}_\alpha$ do not commute with each other. The non-vanishing commutators among coordinates and momenta are

$$\left[X_\beta, \Pi_{X_\gamma} \right] = i \left(\delta_{\beta\gamma} - \frac{Y_\beta Y_\gamma m_\gamma}{R^2} \right) \qquad \left[Y_\beta, \Pi_{Y_\gamma} \right] = i \left(\delta_{\beta\gamma} - \frac{X_\beta X_\gamma m_\gamma}{R^2} \right)$$

$$\left[X_\beta, \Pi_{Y_\gamma} \right] = -i \frac{Y_\beta X_\gamma m_\gamma}{R^2} \qquad \left[Y_\beta, \Pi_{X_\gamma} \right] = -i \frac{X_\beta Y_\gamma m_\gamma}{R^2}$$

$$\left[\Pi_{X_\beta}, \Pi_{X_\gamma} \right] = \frac{i}{R^2} \left(m_\gamma Y_\gamma \Pi_{Y_\beta} - m_\beta Y_\beta \Pi_{Y_\gamma} \right) \tag{27}$$

$$\left[\Pi_{X_\beta}, \Pi_{Y_\gamma} \right] = \frac{i}{R^2} \left(m_\gamma X_\gamma \Pi_{Y_\beta} - m_\beta Y_\beta \Pi_{X_\gamma} \right)$$

$$\left[\Pi_{Y_\beta}, \Pi_{Y_\gamma} \right] = \frac{i}{R^2} \left(m_\gamma X_\gamma \Pi_{X_\beta} - m_\beta X_\beta \Pi_{X_\gamma} \right).$$

As in the previous section, we obtain a realization of this commutator algebra in terms of differential operators by projecting the gradient operator on the hyperplane tangent to $S = 0$,

$$\Pi_{X_\alpha} = \frac{1}{i} \frac{\partial}{\partial X_\alpha} - \frac{1}{i} \frac{m_\alpha Y_\alpha}{R^2} \sum_{\beta=1}^{N} \left(Y_\beta \frac{\partial}{\partial X_\beta} + X_\beta \frac{\partial}{\partial Y_\beta} \right)$$

$$\Pi_{Y_\alpha} = \frac{1}{i} \frac{\partial}{\partial Y_\alpha} - \frac{1}{i} \frac{m_\alpha X_\alpha}{R^2} \sum_{\beta=1}^{N} \left(Y_\beta \frac{\partial}{\partial X_\beta} + X_\beta \frac{\partial}{\partial Y_\beta} \right). \tag{28}$$

Both the classical momenta (26) and the quantum operators (28) satisfy the constraint (25b). The gauge condition $S(\{\boldsymbol{R}_\alpha\}) = 0$ and its counterpart (25b) are operator equations, which can be evaluated inside commutators as can be easily checked from (27). The Hamiltonian operator is written in terms of momentum operators (28) as

$$\mathcal{H} = \sum_{\beta=1}^{N} \frac{1}{2m_\beta} \left(\frac{R}{2Q} \Pi_{X_\beta} \frac{2Q}{R} \Pi_{X_\beta} + \frac{R}{2Q} \Pi_{Y_\beta} \frac{2Q}{R} \Pi_{Y_\beta} \right) + \frac{R^2}{8Q^2} (\ell_z - \Lambda)^2 + \mathcal{V} \tag{29}$$

with $R = \sqrt{R^2}$ and

$$\Lambda \equiv \sum_{\alpha=1}^{N} \left(X_\alpha \Pi_{Y_\alpha} - Y_\alpha \Pi_{X_\alpha} \right) = \left(1 - \frac{2Q}{R^2} \right) \sum_{\alpha=1}^{N} X_\alpha \frac{1}{i} \frac{\partial}{\partial Y_\alpha} - \left(1 + \frac{2Q}{R^2} \right) \sum_{\alpha=1}^{N} Y_\alpha \frac{1}{i} \frac{\partial}{\partial X_\alpha} \tag{30}$$

the residual angular momentum in this gauge. From (29) we find the form of the quantum potential,

$$\mathcal{V}_Q = -\frac{R^2}{8Q^2} + \frac{7 - 4N}{8R^2}. \tag{31}$$

In order to find the inner product in this gauge, we start from the resolution of the identity,

$$1 = \int_0^\pi d\alpha \, \delta(S(\{U(\alpha)r_\beta\}))\Theta(Q(\{U(\alpha)r_\beta\}))2Q(\{U(\alpha)r_\beta\}). \tag{32}$$

Note that we restricted the integration range to $0 \leqslant \alpha \leqslant \pi$. Alternatively, we can integrate from $-\pi$ to π, and set the l.h.s. of (32) equal to 2. The inner product is then obtained as

$$\langle\phi|\psi\rangle = \frac{1}{2}\int \prod_{\beta=1}^N d^2R_\beta\delta(S)\Theta(Q)2Q\phi^*(\{R_\alpha\})\psi(\{R_\alpha\})$$

$$= \frac{1}{2}\int \prod_{\beta=1}^N d^2R_\beta\delta\left(\frac{S}{R}\right)\Theta(Q)\frac{2Q}{R}\phi^*(\{R_\alpha\})\psi(\{R_\alpha\}) \tag{33}$$

where we divided by 2π, and omitted the argument $\{R_\alpha\}$ in S, Q and R for simplicity. In the second line we wrote the gauge condition as S/R, taking into account that the factor $1/R$ has no finite zeros and that its singularity at the origin is suppresed by the zeros of S and Q there. The last expression for $\langle\phi|\psi\rangle$ is convenient to check the hermiticity of $\mathcal{H}$. We again omit the details of the proof.

As a consequence of the gauge condition $S(\{R_\alpha\}) = 0$ being quadratic, the momentum operators Π_α in (28) have coefficients which are ratios of quadratic polynomials in the coordinates, whereas the operators (16) for a linear gauge have constant coefficients. Accordingly, the basic commutators (27) are rational functions of coordinates and, furthermore, momentum operators do not commute with each other. The structure of the Hamiltonian operator in this gauge, equation (29), is also much more complicated than in linear gauges, equation (19). As shown in appendix B, the residual angular momentum operator Λ, (30), does not have integer eigenvalues.

5. 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 motion of the centre of mass is dynamically trivial, we restrict our treatment to dynamical states with vanishing total momentum. We consider linear gauge conditions only.

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

$$r'_\alpha = U(\theta)r_\alpha + u \tag{34}$$

with U being an orthogonal matrix. We define the covariant derivative $D_t r_\alpha = \dot{r}_\alpha - \xi\hat{z} \wedge r_\alpha - \rho$. Under time-dependent transformations, r_α transforms as in (34) and

$$\xi' = \xi - \dot\theta \qquad \rho' = U(\theta)\rho + \dot{u} - (\xi - \dot\theta)\hat{z} \wedge u \qquad (D_t r_\alpha)' = U(\theta)D_t r_\alpha. \tag{35}$$

Substituting $\dot{r}_\alpha$ by $D_t r_\alpha$ in (1), we obtain a Lagrangian that is quasi-invariant under the transformations (34) and (35), and which has the form $\mathcal{L} + \mathcal{L}_\rho$, with $\mathcal{L}$ given by (3) and

$$\mathcal{L}_\rho = \frac{1}{2}\sum_{\alpha=1}^N m_\alpha\rho^2 - \rho \cdot \sum_{\alpha=1}^N m_\alpha\dot{r}_\alpha + \xi\hat{z} \cdot \sum_{\alpha=1}^N m_\alpha r_\alpha \wedge \rho. \tag{36}$$

If we choose the gauge conditions $\xi = 0 = \rho$ we recover the Lagrangian (1), constrained by the equations of motion for ξ and ρ in this gauge,

$$\sum_{\alpha=1}^N m_\alpha r_\alpha \wedge \dot{r}_\alpha = \ell_z \qquad \sum_{\alpha=1}^N m_\alpha\dot{r}_\alpha = 0. \tag{37}$$

These constraints are first class. In the quantum theory they restrict the state space of the theory, $L_z \psi = \ell_z \psi$, $\sum_{\alpha=1}^{N} \nabla_\alpha \psi = 0$, analogously to Gauss law (A.8) in QED.

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

$$\mathfrak{S}(\{R_\alpha\}) = 0 \qquad \mathfrak{C}(\{R_\alpha\}) \equiv \frac{1}{M} \sum_{\beta=1}^{N} m_\beta R_\beta = 0 \tag{38}$$

with $\mathfrak{S}$ defined in (6a) and $M = \sum_{\alpha=1}^{N} m_\alpha$. (38) defines a reference frame in a particular state of rotation, with origin at the centre of mass. As in section 3 we denote vectors referred to this frame by capital letters. The gauge conditions (38) are not mutually consistent unless $\mathfrak{S}$ is translation invariant,

$$\sum_{\alpha=1}^{N} m_\alpha A_\alpha = 0 = \sum_{\alpha=1}^{N} m_\alpha B_\alpha. \tag{39}$$

From the equations of motion for ρ and ξ in this gauge, we obtain $\rho = 0$ and expression (9) for ξ. The momenta conjugate to R_α are given by (10) in terms of velocities. They satisfy (11) and also $\mathfrak{C}(\{\Pi_\alpha/m_\alpha\}) = \sum_{\gamma=1}^{N} \Pi_\gamma = 0$. The classical Hamiltonian is given by (12).

The non-vanishing quantum commutators among coordinates and momenta in this gauge are

$$\left[X_\beta, \Pi_{X_\gamma}\right] = i\left(\delta_{\beta\gamma} - \frac{A_\beta A_\gamma m_\gamma}{\mathfrak{R}^2} - \frac{m_\gamma}{M}\right) \qquad \left[Y_\beta, \Pi_{Y_\gamma}\right] = i\left(\delta_{\beta\gamma} - \frac{B_\beta B_\gamma m_\gamma}{\mathfrak{R}^2} - \frac{m_\gamma}{M}\right)$$
$$\left[X_\beta, \Pi_{Y_\gamma}\right] = -i\frac{A_\beta B_\gamma m_\gamma}{\mathfrak{R}^2} \qquad \left[Y_\beta, \Pi_{X_\gamma}\right] = -i\frac{m_\gamma A_\gamma B_\beta}{\mathfrak{R}^2}. \tag{40}$$

A realization of this algebra in terms of first order differential operators with constant coefficients can be obtained as in (16),

$$\Pi_{X_\alpha} = \frac{1}{i}\frac{\partial}{\partial X_\alpha} - \frac{1}{i}\frac{m_\alpha}{M}\sum_{\beta=1}^{N}\frac{\partial}{\partial X_\beta} - \frac{1}{i}\frac{m_\alpha A_\alpha}{\mathfrak{R}^2}\sum_{\beta=1}^{N}\left(A_\beta\frac{\partial}{\partial X_\beta} + B_\beta\frac{\partial}{\partial Y_\beta}\right)$$
$$\Pi_{Y_\alpha} = \frac{1}{i}\frac{\partial}{\partial Y_\alpha} - \frac{1}{i}\frac{m_\alpha}{M}\sum_{\beta=1}^{N}\frac{\partial}{\partial Y_\beta} - \frac{1}{i}\frac{m_\alpha B_\alpha}{\mathfrak{R}^2}\sum_{\beta=1}^{N}\left(A_\beta\frac{\partial}{\partial X_\beta} + B_\beta\frac{\partial}{\partial Y_\beta}\right). \tag{41}$$

These operators satisfy the constraints $\mathfrak{S}(\{\Pi_\alpha/m_\alpha\}) = 0 = \mathfrak{C}(\{\Pi_\alpha/m_\alpha\})$. The realization of the residual angular momentum as a differential operator is the same as in section 3, equation (17), since the extra terms in (41) with respect to (16) do not contribute to $\Lambda = \sum_{\alpha=1}^{N}\left(X_\alpha\Pi_{Y_\alpha} - Y_\alpha\Pi_{X_\alpha}\right)$ due to the gauge condition $\mathfrak{C} = 0$. The Hamiltonian operator has the same form as in (19), but now with the momentum operators Π_α from (41). The inner product obtained with the Faddeev–Popov procedure is

$$\langle\phi|\psi\rangle = \int \prod_{\beta=1}^{N} d^2 R_\beta \delta(\mathfrak{S})\delta^{(2)}(\mathfrak{C})\Theta(\mathfrak{Q})\mathfrak{Q}\phi^*(\{R_\alpha\})\psi(\{R_\alpha\}). \tag{42}$$

The quantum-mechanical potential in this case is the same as in (22).

6. Quasi-rigid systems and the Eckart frame

We assume now that the potential energy $\mathcal{V}$ (with $U = 0$) has a minimum for some configuration $\{z_\alpha\}$ of the system, such that $z_\alpha \neq z_\beta$ for some $\alpha \neq \beta$, and that $\mathcal{V}_0 \equiv \mathcal{V}(\{z_\alpha\}) \leqslant \mathcal{V}(\{r_\gamma\})$

for all configurations $\{r_\gamma\}$. Due to the invariance of $\mathcal{V}$ under the Euclidean group E_2, any configuration $\{z'_\alpha\}$ related to $\{z_\alpha\}$ by a transformation of the form (34) is also a minimum. Denoting by $\mathcal{M}_\mathcal{V}$ the manifold of configuration space defined by $\mathcal{V}(\{r_\gamma\}) = \mathcal{V}_0$, 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 $\{Z_\alpha\}$ the unique (up to discrete degeneracy) minimum of $\mathcal{V}$ satisfying

$$\sum_{\alpha=1}^{N} m_\alpha Z_{\alpha x} Z_{\alpha y} = 0 \qquad \sum_{\alpha=1}^{N} m_\alpha Z_\alpha = 0. \tag{43}$$

The small oscillations of the system are therefore described by trajectories of the form

$$r_\alpha(t) = z_\alpha(t) + \delta r_\alpha(t) \qquad \text{with} \qquad z_\alpha(t) = U(t) Z_\alpha + u \tag{44}$$

for some orthogonal matrix $U(t)$ and u appropriately chosen so that $\delta r_\alpha(t)$ are small with respect to their characteristic scale for all t. We do not assume, however, that the velocities $\delta \dot{r}_\alpha$ are small. Since we restrict ourselves to states with vanishing total momentum, the translation vector u in (44) must be time independent.

It is convenient to apply the inverse of the gauge transformation defined by the second equation in (44) in order to switch to a reference frame, the 'body frame' of the rigid equilibrium configuration, so that

$$r_\alpha(t) = Z_\alpha + \delta r_\alpha(t). \tag{45}$$

This fixes the gauge only to leading order in δr_α. We fix the residual gauge freedom by imposing a gauge condition on δr_α, which amounts to correcting the definition (45) 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 δr_α the gauge conditions must be of the form (38). The choice of the coefficients A_α, B_α is arbitrary as long as (39) is satisfied. We then have

$$R_\alpha(t) = Z_\alpha + \delta R_\alpha(t) \qquad \mathfrak{S}(\{\delta R_\alpha\}) = 0 \qquad \mathfrak{C}(\{\delta R_\alpha\}) = 0. \tag{46}$$

The instantaneous principal axes frame of section 4, for example, is defined to first order in δR_α by setting $A_\alpha = Z_{\alpha y}$ and $B_\alpha = Z_{\alpha x}$ in (46). Translational invariance of $\mathfrak{S}$ is ensured by the last equation in (43). Furthermore, not all A_α and B_α can vanish in this case, since we assumed $Z_\alpha \neq Z_\beta$ for some $\alpha \neq \beta$.

The residual angular momentum in a general linear gauge (46) is given in the classical theory, to first order in δR_α, by

$$\Lambda = \hat{z} \cdot \sum_{\alpha=1}^{N} m_\alpha Z_\alpha \wedge \delta \dot{R}_\alpha + \hat{z} \cdot \sum_{\alpha=1}^{N} m_\alpha \delta R_\alpha \wedge \delta \dot{R}_\alpha - \xi \left(\mathfrak{R}^2 + 2 \sum_{\alpha=1}^{N} m_\alpha Z_\alpha \cdot \delta R_\alpha \right)$$
$$+ \xi \frac{\mathfrak{Q}(\{Z_\alpha\})}{\mathfrak{R}^2} (\mathfrak{Q}(\{Z_\alpha\}) + 2\mathfrak{Q}(\{\delta R_\alpha\})) \tag{47}$$

with $\mathfrak{R}^2 = \sum_{\beta=1}^{N} m_\beta Z_\beta^2$ and

$$\xi = \frac{1}{\sum_{\beta=1}^{N} m_\beta R_\beta^2} \left(\hat{z} \cdot \sum_{\alpha=1}^{N} m_\alpha R_\alpha \wedge \dot{R}_\alpha - \ell_z \right) = \frac{1}{\mathfrak{R}^2} \left(1 - \frac{2}{\mathfrak{R}^2} \sum_{\beta=1}^{N} m_\beta Z_\beta \cdot \delta R_\beta \right)$$
$$\times \left(\hat{z} \cdot \sum_{\alpha=1}^{N} m_\alpha Z_\alpha \wedge \delta \dot{R}_\alpha - \ell_z \right) + \frac{1}{\mathfrak{R}^2} \hat{z} \cdot \sum_{\alpha=1}^{N} m_\alpha \delta R_\alpha \wedge \delta \dot{R}_\alpha + \mathcal{O}(\delta R_\alpha^2). \tag{48}$$

The expression for Λ in the linearized principal axes gauge is obtained by substituting $A_\alpha = Z_{\alpha y}$ and $B_\alpha = Z_{\alpha x}$ in (47). In general, Λ does not vanish at the equilibrium positions $\delta R_\alpha = 0$. In order to make Λ of first order in δR_α, we impose instead the gauge condition

$$\sum_{\alpha=1}^{N} m_\alpha Z_\alpha \wedge R_\alpha = \sum_{\alpha=1}^{N} m_\alpha Z_\alpha \wedge \delta R_\alpha = 0 \qquad (49)$$

which corresponds to (46) with $A_\alpha = -Z_{\alpha y}$ and $B_\alpha = Z_{\alpha x}$. The gauge condition (49) defines the Eckart frame [12]. The general expression (47) for Λ in this gauge simplifies to

$$\Lambda = \hat{z} \cdot \sum_{\alpha=1}^{N} m_\alpha \delta R_\alpha \wedge \delta \dot{R}_\alpha. \qquad (50)$$

Fixing a gauge in which Λ is of first order in δR_α as in (50) is a necessary condition to satisfying Casimir's criterion for the decoupling of rotational and vibrational degrees of freedom in a quasi-rigid system in low orders in perturbation theory [12]. As shown above, such a condition is not fulfilled by the principal axes frame [12].

In Eckart gauge the momentum operators Π_α conjugate to δR_α are given by (41), with the values of A_α, B_α corresponding to (49), and with derivatives $\partial/\partial X_\alpha$, $\partial/\partial Y_\alpha$ substituted by $\partial/\partial \delta X_\alpha$ and $\partial/\partial \delta Y_\alpha$. The operator Λ is then of the form

$$\Lambda = \frac{1}{i} \sum_{\alpha=1}^{N} \left(\delta X_\alpha \frac{\partial}{\partial \delta Y_\alpha} - \delta Y_\alpha \frac{\partial}{\partial \delta X_\alpha} \right) - \frac{1}{i} \frac{\mathfrak{Q}(\{\delta R_\gamma\})}{\mathfrak{R}^2} \sum_{\alpha=1}^{N} \left(Z_{X\alpha} \frac{\partial}{\partial \delta Y_\alpha} - Z_{Y\alpha} \frac{\partial}{\partial \delta X_\alpha} \right). \qquad (51)$$

Its coefficients are of first order in δR_α. The Hamiltonian operator is obtained by substituting these expressions for Π_α and Λ, into (19), with $\mathfrak{Q}(\{R_\alpha\}) = \mathfrak{Q}(\{Z_\alpha\}) + \mathfrak{Q}(\{\delta R_\alpha\}) = \mathfrak{R}^2 + \sum_{\gamma=1}^{N} m_\gamma Z_\gamma \cdot \delta R_\gamma$. The inner product, finally, is given by (42).

6.1. The case $N = 2$

As a very minimal verification of the formalism, we consider a system of two particles interacting through an elastic potential that models a spring with rest length a, $\mathcal{V} = k/2(|r_1 - r_2| - a)^2$. We verify that the Hamiltonian operator in the previous section, with the corresponding inner product, leads to the correct energy spectrum and wavefunctions in a semiclassical expansion for large a. Since the residual angular momentum Λ vanishes in a translationally invariant system for $N < 3$, this simple example does not provide an illustration of the role of terms linear in ℓ_z in $\mathcal{H}$, nor of Casimir's condition. In this section we restore $\hbar$ in all expressions.

We choose the minimum $Z_{1,2}$ of the potential as, $(Z_{1,2})_x = \pm a m_{2,1}/M$, $(Z_{1,2})_y = 0$, with $M = m_1 + m_2$. These $Z_{1,2}$ satisfy (43). The gauge conditions defining the Eckart frame are then

$$\mathfrak{S}(\{\delta R_\alpha\}) = a\mu(\delta Y_1 - \delta Y_2) = 0 \qquad \mathfrak{C}(\{\delta R_\alpha\}) = \frac{m_1}{M} \delta R_1 + \frac{m_2}{M} \delta R_2 = 0 \qquad (52)$$

where μ is the reduced mass. Together, (52) implies $\delta Y_1 = 0 = \delta Y_2$. The Faddeev–Popov determinant $\mathfrak{Q}$ and $\mathfrak{R}^2$ are given by

$$\mathfrak{Q} = \mu a (a + \delta X_1 - \delta X_2) \qquad \mathfrak{R}^2 = \mu a^2. \qquad (53)$$

The momentum operators (41) are then

$$\Pi_{X_1} = \frac{\hbar}{i} \left(\frac{m_2}{M} \frac{\partial}{\partial \delta X_1} - \frac{m_1}{M} \frac{\partial}{\partial \delta X_1} \right) = -\Pi_{X_2} \qquad \Pi_{Y_1} = 0 = \Pi_{Y_2} \qquad (54)$$

consistent with the gauge conditions (52). In terms of these operators, we write the Hamiltonian (22) as

$$\widetilde{\mathcal{H}} = \frac{1}{2m_1}\Pi_{X_1}^2 + \frac{1}{2m_2}\Pi_{X_2}^2 + \frac{\mu\omega^2}{2}(\delta X_1 - \delta X_2)^2 + \frac{\hbar^2\mathfrak{R}^2}{2\mathfrak{Q}^2}\left(\ell_z^2 - \frac{1}{4}\right) \tag{55}$$

where $k = \mu\omega^2$, and the last term gathers the centrifugal and quantum potentials. Using $\Pi_{X_1} = -\Pi_{X_2}$, we rewrite $\widetilde{\mathcal{H}}$ as

$$\widetilde{\mathcal{H}} = \widetilde{\mathcal{H}}_0 + \widetilde{\mathcal{H}}_1 \qquad \widetilde{\mathcal{H}}_0 = \frac{1}{2\mu}\Pi_{X_1}^2 + \frac{\mu\omega^2}{2}(\delta X_1 - \delta X_2)^2$$

$$\widetilde{\mathcal{H}}_1 = \frac{\hbar^2\mathfrak{R}^2}{2\mathfrak{Q}^2}\left(\ell_z^2 - \frac{1}{4}\right) = \frac{\hbar\omega}{2}\epsilon^2\left(\ell_z^2 - \frac{1}{4}\right)\left(1 - 2\epsilon\sqrt{\frac{\mu\omega}{\hbar}}(\delta X_1 - \delta X_2) + \mathcal{O}(\epsilon^2)\right). \tag{56}$$

In $\widetilde{\mathcal{H}}_1$ we denoted $\epsilon = \sqrt{\hbar/(\mu\omega a^2)}$, which is our perturbation expansion parameter. Taking into account (52) and (53) and the fact that the Jacobian has been absorbed in the wavefunctions, the inner product (42) takes the form

$$\langle\widetilde{\phi}|\widetilde{\psi}\rangle = \frac{1}{\mu a}\iint_{-\infty}^{+\infty} d\delta X_1\, d\delta X_2\, \delta\left(\frac{m_1}{M}\delta X_1 + \frac{m_2}{M}\delta X_2\right)$$
$$\times \Theta(a + \delta X_1 - \delta X_2)(\widetilde{\phi}^*\widetilde{\psi})(X_1, 0, X_2, 0). \tag{57}$$

Using (56) and (57), we can compute the perturbative expansion. Since $\left[m_1\delta X_1 + m_2\delta X_2, \Pi_{X_1}\right] = 0$, the eigenfunctions of $\widetilde{\mathcal{H}}_0$ depend on $\delta X_{1,2}$ only through $\delta X_1 - \delta X_2$. The eigenvalues $E_{(0)n}$ and eigenfunctions $\phi_{(0)n}(\delta X_1 - \delta X_2)$ of $\widetilde{\mathcal{H}}_0$ are then those of a one-dimensional harmonic oscillator.

To order $\mathcal{O}(\epsilon^2)$, the perturbed energies can be read off expression (56) for $\widetilde{\mathcal{H}}_1$,

$$E_n = E_{(0)n} + E_{(1)n} \qquad E_{(1)n} = \frac{\hbar\omega}{2}\epsilon^2\left(\ell_z^2 - \frac{1}{4}\right). \tag{58}$$

Using the inner product (57), the perturbed wavefunctions are found to be, to $\mathcal{O}(\epsilon^3)$,

$$\phi_n(\delta X_1 - \delta X_2) = \phi_{(0)n} + \frac{\epsilon^3}{2}\left(\ell_z^2 - \frac{1}{4}\right)\left(\sqrt{\frac{n}{2}}\phi_{(0)n-1} - \sqrt{\frac{n+1}{2}}\phi_{(0)n+1}\right) \tag{59}$$

where on the r.h.s. we omitted the argument $(\delta X_1 - \delta X_2)$ of wavefunctions for brevity. These results, (58) and (59), agree with a conventional perturbative calculation as they should.

7. Final remarks

We considered above the classical and quantum dynamics of two-dimensional many-body systems in rotating reference frames, in a gauge-invariant approach [1, 5]. Our treatment is similar to the formulation of gauge field theories in non-covariant gauges in the Schrödinger representation [2, 4, 17], and generalizes to N-body systems the analysis of the one-particle case of [2, 4, 20].

The gauge-invariant approach allows us to deal with constrained degrees of freedom without necessarily solving the constraints. Yet, this approach also entails a reduction of configuration space by the elimination of the angular degree of freedom. The remaining, constrained dynamical variables only span the reduced configuration space. Our formalism has a direct physical and geometrical interpretation which we have tried to emphasize. In the gauges in sections 3–6, it is not difficult to obtain the metric tensor on the gauge hypersurface in terms of coordinates $(\{\boldsymbol{R}_\alpha\}, \theta)$ (and ρ if there is translation invariance). In these coordinates the

metric has as many zero eigenvalues as the dimension of the gauge group, its kernel comprising the subspace orthogonal to the gauge surface. From the restriction of this metric tensor to the gauge surface, the kinetic energy operator in the quantum theory can be constructed by applying the usual expression for the Laplacian in curvilinear coordinates.

In sections 3–5 we gave a derivation of the quantum theory in rotating frames. A detailed discussion is provided there of Gribov ambiguities and of the commutator algebra, which are essential for obtaining of the inner product and the momentum and Hamiltonian operators. These issues seem to us to have been neglected in the previous literature. Also discussed in detail is the residual angular momentum operator Λ. In linear gauges its eigenvalues are integers. In the quadratic gauge in section 4, its eigenvalues depend on the dynamical variables $\{R_\alpha\}$ though, remarkably, only through Q and R^2 (see (B.13), (B.8) and (23)), which are measures of the instantaneous shape of the system. The relation between wavefunctions in the laboratory frame and in rotating ones, which we treat rather briefly, is summarized in the expression for the inner product in the different gauges, (5), (21), (33) and (42). Such a relation is best understood by going through the successive steps of the derivation of the inner product by the Faddeev–Popov technique. For systems of identical particles, the formalism is clearly symmetric under permutations of particles if the gauge conditions are chosen so that they are symmetric in the position vectors $\{R_\alpha\}$.

In the case of quasi-rigid systems, we recovered in section 6 some of Eckart's classic results [12]. In particular, in the classical theory the residual angular momentum Λ becomes manifestly small of $\mathcal{O}(\delta R)$ in Eckart gauge. Thus, in a perturbative expansion the term $L_z\Lambda$ in $\mathcal{H}$ is of higher order than the term L_z^2. This leads to a decoupling of rotational (L_z) and vibrational ($\{\delta R_\alpha\}$) degrees of freedom in low orders in perturbation theory. (In the elementary example in section 6.1, in which $\Lambda = 0$, the decoupling is apparent through $\mathcal{O}(\epsilon^2)$ in (56).) Such decoupling would not be manifest in other gauges in which $\Lambda \sim \mathcal{O}(1)$ [12, 21], since in that case the terms L_z^2 and $L_z\Lambda$ would be of the same perturbative order. This is the case of the instantaneous principal axes frame [12, 21].

We do not agree with the point of view of [9] (see also [5, 6]) that, by quantizing a many-body system in the instantaneous principal axes frame (see equation (II.4) in [9]), it is possible to separate the collective rotation from the intrinsic dynamics. If this statement were generally valid, in the quasi-rigid case it should imply the decoupling of the total angular momentum from the vibrational degrees of freedom in perturbation theory. But, as shown in [12], this decoupling is not manifest in the principal axes frame.

Acknowledgments

Appendix A. Electrodynamics

The methods used in the preceding sections are common to all (Abelian) gauge theories and, therefore, have a direct counterpart in electrodynamics. In this appendix we briefly discuss those aspects of electrodynamics, following the treatment of [4, 2, 17]. In terms of the field-strength tensor $F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu$, the Lagrangian density of the e.m. field coupled to an external current density j^μ has the familiar expression

$$\mathcal{L} = -\tfrac{1}{4}F^{\mu\nu}F_{\mu\nu} - j^\mu A_\mu. \tag{A.1}$$

We assume that the current is conserved, $\partial^\mu j_\mu = 0$, so that the action of the system is invariant under the e.m. gauge transformations $A^{\mu\prime} = A^\mu - \partial^\mu \Lambda$, with $\Lambda = \Lambda(x)$ being an arbitrary function of the space-time coordinates. We consider only fields, currents, and gauge-parameter functions vanishing at spatial infinity. Furthermore, we assume that j^μ is such that there is an inertial frame in which $\partial^0 j^0 = 0$, and therefore $\nabla \cdot \boldsymbol{j} = 0$. We choose this reference frame to formulate the Hamiltonian formalism. The extension to the general case $\partial^0 j^0 \neq 0$, which involves time-dependent constraints, is not necessary for our purposes.

Weyl gauge. Since the time derivative of A^0 does not enter $\mathcal{L}$, it is an auxiliary field. By means of a gauge transformation, any field configuration can be brought into the form $A^0 = 0$. We denote fields in Weyl gauge by $V^\mu(x)$, with $V^0 = 0$. In this gauge the Lagrangian density reduces to

$$\mathcal{L} = \tfrac{1}{2}\dot{V}^2 - \tfrac{1}{2}(\nabla \wedge V)^2 + \boldsymbol{j} \cdot \boldsymbol{V}. \tag{A.2}$$

$\mathcal{L}$ must be supplemented by the equation of motion for V^0 derived from (A.1), which is Gauss law,

$$\nabla \cdot \dot{V} = -j^0 \tag{A.3}$$

with $\dot{V} = -\boldsymbol{E}$. In the Hamiltonian formulation, equation (A.3) is written in terms of the momenta canonically conjugate to V, $-\boldsymbol{E}$, and constitutes a primary first-class constraint. It does not give rise to further secondary constraints. The Hamiltonian density is given by

$$\mathcal{H} = \tfrac{1}{2}\boldsymbol{E}^2 + \tfrac{1}{2}(\nabla \wedge V)^2 - \boldsymbol{j} \cdot \boldsymbol{V} \qquad \nabla \cdot \boldsymbol{E} = j^0. \tag{A.4}$$

The Poisson brackets are canonical,

$$[E^j(t, \boldsymbol{x}), V^k(t, \boldsymbol{y})]_P = \delta^{jk}\delta(\boldsymbol{x} - \boldsymbol{y}). \tag{A.5}$$

All other brackets among basic dynamical variables vanish. The theory in this gauge is invariant under gauge transformations with a time-independent parameter $\Lambda(\boldsymbol{x})$. The canonical generator of this symmetry is the l.h.s. of Gauss law, $\nabla \cdot \boldsymbol{E} - j^0$ (or just $\nabla \cdot \boldsymbol{E}$). We have the Poisson brackets

$$\begin{aligned} \left[\nabla \cdot \boldsymbol{E}(t, \boldsymbol{x}) - j^0(\boldsymbol{x}), H\right]_P &= 0 \\ [\nabla \cdot \boldsymbol{E}(t, \boldsymbol{x}) - j^0(\boldsymbol{x}), V^k(t, \boldsymbol{y})]_P &= \partial^k \delta(\boldsymbol{x} - \boldsymbol{y}) \end{aligned} \tag{A.6}$$

where $H = \int \mathrm{d}^3x\, \mathcal{H}(t, \boldsymbol{x})$. The first equation in (A.6) expresses the consistency of the constraint with the dynamics, and the second shows that the constraint is the infinitesimal generator of the residual gauge symmetry.

In the quantum theory in the Schrödinger representation, the field operators are time independent, the basic commutators are obtained from (A.5) and the Hamiltonian density operator is given by

$$\mathcal{H}(\boldsymbol{x}) = -\frac{1}{2}\frac{\delta^2}{\delta V^k(\boldsymbol{x})\delta V^k(\boldsymbol{x})} + \frac{1}{2}(\nabla \wedge V(\boldsymbol{x}))^2 - \boldsymbol{j}(\boldsymbol{x}) \cdot \boldsymbol{V}(\boldsymbol{x}). \tag{A.7}$$

Gauss law is imposed as a constraint on the state space of the system,

$$\frac{1}{\mathrm{i}}\nabla \cdot \frac{\delta}{\delta V(\boldsymbol{x})}\Psi[V] = j^0(\boldsymbol{x})\Psi[V] \tag{A.8}$$

where $\Psi[V]$ is the wave functional.

Coulomb gauge. Any field V^μ in Weyl gauge can be transformed into Coulomb gauge, $\nabla \cdot \boldsymbol{A} = 0$, and conversely,

$$\begin{aligned} A^\mu(t, \boldsymbol{x}) &= V^\mu(t, \boldsymbol{x}) + \partial^\mu \Lambda(t, \boldsymbol{x}) \\ \Lambda(t, \boldsymbol{x}) &= \frac{1}{\nabla^2}(\nabla \cdot V(t, \boldsymbol{x})) \equiv -\frac{1}{4\pi}\int \mathrm{d}^3x'\frac{\nabla' \cdot V(t, \boldsymbol{x}')}{|\boldsymbol{x}' - \boldsymbol{x}|} \end{aligned} \tag{A.9a}$$

$$V^\mu(t, \boldsymbol{x}) = A^\mu(t, \boldsymbol{x}) - \partial^\mu \lambda(t, \boldsymbol{x}) \qquad \lambda(t, \boldsymbol{x}) = \int_{t_0}^{t} \mathrm{d}t' A^0(t', \boldsymbol{x}). \qquad \text{(A.9}b\text{)}$$

A^0 in (A.1) is an auxiliary field which is determined by its Lagrangian equation,

$$A^0 = -\frac{1}{\boldsymbol{\nabla}^2} j^0. \qquad \text{(A.10)}$$

Once the gauge has been fixed, we can substitute this expression back into the Lagrangian to obtain

$$\mathcal{L} = \frac{1}{2}\dot{\boldsymbol{A}}^2 - \frac{1}{2}(\boldsymbol{\nabla} \wedge \boldsymbol{A})^2 + \frac{1}{2}j^0\frac{1}{\boldsymbol{\nabla}^2}j^0 + \boldsymbol{j} \cdot \boldsymbol{A} \qquad \boldsymbol{\nabla} \cdot \boldsymbol{A} = 0. \qquad \text{(A.11)}$$

The electric field is

$$\boldsymbol{E} = \boldsymbol{E}_T + \boldsymbol{E}_L \qquad \boldsymbol{E}_L = -\boldsymbol{\nabla}A^0 = \boldsymbol{\nabla}\frac{1}{\boldsymbol{\nabla}^2}\boldsymbol{\nabla} \cdot \boldsymbol{E} \qquad \boldsymbol{E}_T = -\dot{\boldsymbol{A}}. \qquad \text{(A.12)}$$

The momentum conjugate to $\boldsymbol{A}$ is $\boldsymbol{\Pi} = -\boldsymbol{E}_T$. Substituting (A.9$b$) and (A.12) into (A.4), we get the classical Hamiltonian density in this gauge,

$$\mathcal{H} = \frac{1}{2}\boldsymbol{\Pi}^2 + \frac{1}{2}(\boldsymbol{\nabla} \wedge \boldsymbol{A})^2 - \frac{1}{2}j^0\frac{1}{\boldsymbol{\nabla}^2}j^0 - \boldsymbol{j} \cdot \boldsymbol{A} \qquad \boldsymbol{\nabla} \cdot \boldsymbol{A} = 0 = \boldsymbol{\nabla} \cdot \boldsymbol{\Pi}. \qquad \text{(A.13)}$$

Furthermore, from the inverse transformation (A.9a) and (A.12), and the Poisson brackets (A.6), we can compute the brackets among coordinates and momenta in this gauge. The corresponding equal-time quantum commutators are

$$\left[A^j(t, \boldsymbol{x}), E_T^k(t, \boldsymbol{x}')\right] = \mathrm{i}\left(-\delta^{jk} + \nabla^j\nabla'^k\frac{1}{\boldsymbol{\nabla}^2}\right)\delta(\boldsymbol{x} - \boldsymbol{x}'). \qquad \text{(A.14)}$$

The gauge condition $\boldsymbol{\nabla} \cdot \boldsymbol{A} = 0$ and the derived relation $\boldsymbol{\nabla} \cdot \boldsymbol{\Pi} = 0$ constitute second-class constraints, valid as operator equations. Their associated Dirac brackets are given by (A.14).

A realization of the commutator algebra (A.14) in the Schrödinger representation can be found as in sections 3 and 4,

$$\Pi^j(\boldsymbol{x}) = \frac{1}{\mathrm{i}}\frac{\delta}{\delta A^j(\boldsymbol{x})} - \frac{1}{\mathrm{i}}\nabla^j\nabla^k\frac{1}{\boldsymbol{\nabla}^2}\frac{\delta}{\delta A^k(\boldsymbol{x})} \qquad \text{(A.15)}$$

where the repeated index k is summed from 1 to 3. We can express the momentum operators in Weyl gauge in terms of the operators (A.15) by means of the chain rule,

$$\frac{\delta}{\delta V^m(\boldsymbol{x})} = \int \mathrm{d}^3\boldsymbol{y}\,\frac{\delta A^k(\boldsymbol{y})}{\delta V^m(\boldsymbol{x})}\frac{\delta}{\delta A^k(\boldsymbol{y})}. \qquad \text{(A.16)}$$

From (A.9a) we see that

$$\frac{\delta A^k(\boldsymbol{x}')}{\delta V^m(\boldsymbol{x})} = \delta^{km}\delta(\boldsymbol{x} - \boldsymbol{x}') - \frac{1}{4\pi}\nabla'^k\nabla^m\left(\frac{1}{|\boldsymbol{x}' - \boldsymbol{x}|}\right). \qquad \text{(A.17)}$$

Replacing (A.17) into (A.16), we get

$$\frac{\delta}{\delta V^m(\boldsymbol{x})} = \mathrm{i}\Pi^m(\boldsymbol{x}) \qquad \text{(A.18)}$$

and therefore, from the Hamiltonian density operator (A.7) in Weyl gauge, we obtain the operator in Coulomb gauge which has the same form as the classical density (A.13) with $\boldsymbol{\Pi}$ from (A.15). The Faddeev–Popov Jacobian in this case is field independent, as can be seen from (A.17), which is why it does not appear in the Hamiltonian.

Appendix B. Eigenvalues and eigenfunctions of Λ

In this appendix we discuss the eigenvalues and eigenfunctions of the residual angular momentum $\Lambda = \sum_{\beta=1}^{N} \left(X_\beta \Pi_{Y_\beta} - Y_\beta \Pi_{X_\beta} \right)$. Since the definition of $\boldsymbol{\Pi}_\alpha$ depends on the gauge conditions, the form of Λ as a differential operator is different in the cases of linear and quadratic gauge conditions.

Appendix B.1. Linear gauges

In the linear gauges in sections 3, 5 and 6, Λ is given by (17). In order to find its eigenvalues and eigenfunctions we apply the method of characteristic lines [22] (which can also be applied, of course, to the standard angular momentum operator in Cartesian coordinates). It is therefore necessary to obtain first the classical orbits generated by Λ.

Classical orbits. The orbits generated by the classical Λ on the gauge surface in configuration space are described by the equations

$$\frac{dX_\gamma}{d\alpha} = [\Lambda, X_\gamma]_P \qquad \frac{dY_\gamma}{d\alpha} = [\Lambda, Y_\gamma]_P \qquad \mathfrak{S}(\{\boldsymbol{R}_\gamma\}) = 0. \qquad (B.1)$$

With the Poisson brackets given in (14) (as quantum commutators), we obtain the solution to (B.1) as

$$X_\gamma(\alpha) = \exp\left([\Lambda, \bullet]_P\right) X_\gamma = \frac{B_\gamma \mathfrak{Q}}{\mathfrak{R}^2} + \cos\alpha\left(X_\gamma - \frac{B_\gamma \mathfrak{Q}}{\mathfrak{R}^2}\right) + \sin\alpha\left(Y_\gamma + \frac{A_\gamma \mathfrak{Q}}{\mathfrak{R}^2}\right)$$

$$Y_\gamma(\alpha) = \exp\left([\Lambda, \bullet]_P\right) Y_\gamma = -\frac{A_\gamma \mathfrak{Q}}{\mathfrak{R}^2} + \cos\alpha\left(Y_\gamma + \frac{A_\gamma \mathfrak{Q}}{\mathfrak{R}^2}\right) - \sin\alpha\left(X_\gamma - \frac{B_\gamma \mathfrak{Q}}{\mathfrak{R}^2}\right). \qquad (B.2)$$

If $\mathfrak{S}(\{\boldsymbol{R}_\gamma(0)\}) = 0$, then $\mathfrak{S}(\{\boldsymbol{R}_\gamma(\alpha)\}) = 0$ for all α. In this case $\mathfrak{Q}$ is constant along the orbits. The centre of mass also vanishes for all α if it vanishes for $\alpha = 0$, as long as $\mathfrak{S}$ is translationally invariant, as explained in section 5.

Kernel. We consider first functions C satisfying $\Lambda C = 0$. From (B.2), we see that the quantities

$$\rho_\gamma^2 = \left(X_\gamma - \frac{B_\gamma \mathfrak{Q}}{\mathfrak{R}^2}\right)^2 + \left(Y_\gamma + \frac{A_\gamma \mathfrak{Q}}{\mathfrak{R}^2}\right)^2 \qquad (B.3)$$

are constant on the classical orbits. Thus, any $f = f(\{\rho_\beta\})$ satisfies $\Lambda f = 0$. Furthermore, from (15) we have $\Lambda \mathfrak{Q} = i\mathfrak{S}$, so that for any function $f = f(\mathfrak{Q})$ we get $\Lambda f(\mathfrak{Q}) = f'(\mathfrak{Q})\mathfrak{S}$, which vanishes on the gauge surface. We therefore have $\Lambda C = 0$ if $C = C(\{\rho_\beta\}, \mathfrak{Q})$ and $\mathfrak{S} = 0$.

Eigenvalues and eigenfunctions. Next, we consider the eigenvalue equation $i\Lambda\Psi = i\lambda\Psi$, with $\lambda \neq 0$. The characteristic lines of this equation are defined by the differential system

$$\frac{dX_1}{-\left(Y_1 + \frac{A_1 \mathfrak{Q}}{\mathfrak{R}^2}\right)} = \cdots = \frac{dX_N}{-\left(Y_N + \frac{A_N \mathfrak{Q}}{\mathfrak{R}^2}\right)} = \frac{dY_1}{X_1 - \frac{B_1 \mathfrak{Q}}{\mathfrak{R}^2}} = \cdots = \frac{dY_N}{X_N - \frac{B_N \mathfrak{Q}}{\mathfrak{R}^2}} = \frac{d\Psi}{i\lambda\Psi}$$

$$\mathfrak{S}(\{\boldsymbol{R}_\gamma\}) = 0. \qquad (B.4)$$

Writing $\Psi = \exp(i\lambda\alpha)$, the solutions of (B.4) are given by the classical orbits $\{X_\gamma(-\alpha), Y_\gamma(-\alpha)\}$ from (B.2). A solution α to the eigenvalue equation is obtained by inverting a relation of the form

$$G(X_1(0), \ldots, X_N(0), Y_1(0), \ldots, Y_n(0)) = 0.$$

A possible choice is $G = Y_\gamma(0) + \frac{A_\gamma \mathfrak{Q}}{\mathfrak{R}^2}$. Setting $Y_\gamma(\alpha) = Y_\gamma$ and $X_\gamma(\alpha) = X_\gamma$, we are led to

$$\tan \alpha_\gamma = \frac{\mathfrak{R}^2 Y_\gamma + \mathfrak{Q} A_\gamma}{\mathfrak{R}^2 X_\gamma - \mathfrak{Q} B_\gamma}.$$

From here we obtain the family of eigenfuntions,

$$\Psi = C \exp\left(i \sum_{\gamma=1}^{N} \lambda_\gamma \alpha_\gamma\right) \qquad \text{with} \quad \sum_{\gamma=1}^{N} \lambda_\gamma = \lambda. \tag{B.5}$$

The proportionality 'constant' C in (B.5) can be any function belonging to the kernel of Λ, as described above. For Ψ to be single valued λ_γ, and therefore λ, must be integers.

Appendix B.2. Instantaneous principal axes gauge

In the quadratic gauge in section 4, Λ has the form (30). We proceed as in the previous case, starting from the classical orbits generated by Λ. The notation is the same as in section 4.

Classical orbits. In this gauge we have the following equations for the classical orbits on the gauge surface,

$$\frac{dX_\gamma}{d\alpha} = [\Lambda, X_\gamma]_P = \left(1 + \frac{2Q}{R^2}\right) Y_\gamma \qquad \frac{dY_\gamma}{d\alpha} = [\Lambda, Y_\gamma]_P = -\left(1 - \frac{2Q}{R^2}\right) X_\gamma$$

$$S(\{\mathbf{R}_\gamma\}) = 0. \tag{B.6}$$

Their solution is,

$$X_\gamma(\alpha) = \exp([\Lambda, \bullet]_P) X_\gamma = \cos(\Omega\alpha) X_\gamma + \left(\frac{R^2 + 2Q}{R^2 - 2Q}\right)^{1/2} \sin(\Omega\alpha) Y_\gamma$$

$$\tag{B.7}$$

$$Y_\gamma(\alpha) = \exp([\Lambda, \bullet]_P) Y_\gamma = -\left(\frac{R^2 - 2Q}{R^2 + 2Q}\right)^{1/2} \sin(\Omega\alpha) X_\gamma + \cos(\Omega\alpha) Y_\gamma$$

with

$$\Omega = \left(1 - \frac{4Q^2}{R^4}\right)^{1/2}. \tag{B.8}$$

The condition $S = 0$ is preserved along these orbits and, if it is satisfied, Q and R^2 are constant on them. Note that we require $Q \geqslant 0$ due to the Gribov ambiguity (see section 4) and, therefore, by definition $0 \leqslant 2Q \leqslant R^2$.

Kernel. The quantities

$$\rho_\gamma^2 = \left(1 - \frac{2Q}{R^2}\right) X_\gamma^2 + \left(1 + \frac{2Q}{R^2}\right) Y_\gamma^2 \tag{B.9}$$

are constant along the orbits (B.7). Thus, if $S = 0$, any function $C = C(\{\rho_\gamma^2\}, Q, R^2)$ satisfies $\Lambda C = 0$.

Eigenvalues and eigenfunctions. The characteristic lines of the equation $i\Lambda\Psi = i\lambda\Psi$, $\lambda \neq 0$, in this gauge are the solutions to the system,

$$\frac{dX_1}{-Y_1\left(1 + \frac{2Q}{R^2}\right)} = \cdots = \frac{dX_N}{-Y_N\left(1 + \frac{2Q}{R^2}\right)} = \frac{dY_1}{X_1\left(1 - \frac{2Q}{R^2}\right)} = \cdots = \frac{dY_N}{X_N\left(1 - \frac{2Q}{R^2}\right)} = \frac{d\Psi}{i\lambda\Psi}$$

$$\tag{B.10}$$

together with the gauge condition $S(\{\boldsymbol{R}_\gamma\}) = 0$. As in the previous section, we set $\Psi = \exp(\mathrm{i}\lambda\alpha)$. With this, the solution to (B.10) is given by $\{X_\gamma(-\alpha), Y_\gamma(-\alpha)\}$, see (B.7). Inverting the relation $Y_\gamma(0) = 0$, we get

$$\alpha_\gamma = \frac{1}{\Omega}\arctan\left(\left(\frac{R^2 + 2Q}{R^2 - 2Q}\right)^{1/2}\frac{Y_\gamma}{X_\gamma}\right). \tag{B.11}$$

We then have

$$\Psi = C\exp\left(\mathrm{i}\sum_{\gamma=1}^{N}\lambda_\gamma\alpha_\gamma\right) \qquad \lambda = \sum_{\gamma=1}^{N}\lambda_\gamma. \tag{B.12}$$

For Ψ to be singled valued, we need

$$\lambda_\gamma = n_\gamma\Omega \qquad \lambda = n\Omega \qquad n = \sum_{\gamma=1}^{N}n_\gamma \tag{B.13}$$

with n_γ integers. We see that the eigenvalues λ are not integers in general, and that they depend through Ω on $Q(\{\boldsymbol{R}_\alpha\})$ and $R^2(\{\boldsymbol{R}_\alpha\})$, which in turn are functions of the dynamical variables $\{\boldsymbol{R}_\alpha\}$.

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