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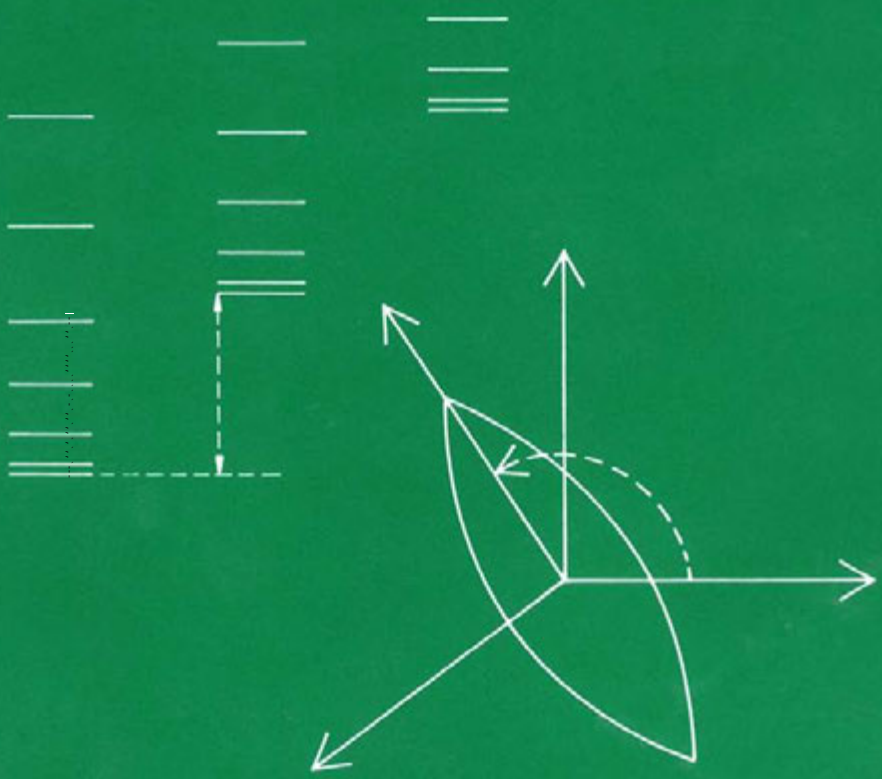
THE TREATMENT OF COLLECTIVE COORDINATES IN MANY-BODY SYSTEMS

An Application of the BRST Invariance

D R Bes and J Kurchan



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D R Bes and J Kurchan
CNEA, Buenos Aires, Argentina

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1 Introduction

"Why did I decide to add to the infinite
Series one more symbol? Why, to the vain
Skein which unwinds in eternity
Did I add another cause, effect, and woe?" J.L. Borges, The Golem [1]

The central object of these notes is the description of physical systems using variables which are subject to transformations, such as for example the coordinates measured with respect to a moving frame.

To the extent that the parameters determining the motion of the frame are just that (i.e., parameters with a time dependence which is externally determined), the resulting classical or quantal treatments do not bring in any essentially new feature. However, a different approach can be followed: these parameters may also be treated as genuine coordinates on an equal footing with the original ones. Since they affect the description of all the other variables they are traditionally called *collective coordinates*, while the remaining ones are called *intrinsic*. For instance, in the case of a rigid top, the quantal transformation from the laboratory to the rotating frame can be expressed in terms of Wigner's matrices $D^I_{MK}(\phi_v)$, depending on the Euler parameters ϕ_v. These parameters are treated as variables in the quantal treatment of the motion of the top, and the corresponding wavefunctions are given in terms of the same matrices D^I_{MK}.

This procedure may be generalized to cases in which the intrinsic variables of the system cannot be frozen (as in the case of the rigid top) and thus disregarded. Nuclei with large quadrupole moments behave approximately like quantum rotors. Superfluid systems display "rotational" bands associated with the number of pairs of particles. A similar situation arises when an extended classical solution of a field equation such as a soliton breaks the translational or rotational invariance. Such systems admit an (independent-particle) approximation that violates a symmetry of the hamiltonian (i.e., the approximate wavefunctions do not belong to an irreducible representation of the corresponding symmetry group). However, the exact wavefunctions do not break this symmetry (i.e., they can be labelled by the quantum numbers associated with the irreducible the representations). In such cases, the symmetry can be restored "through a motion in the broken symmetry group". At the level of small oscillations (or plane waves) the broken symmetries manifest themselves through the appearance of zero frequency modes (or massless fields) which make impossible the naive application of perturbative procedures. However, the zero modes do not yield a satisfactory description of the motion associated with the breaking of symmetries, if this breaking is only approximate (as for finite systems).

There are also other types of motion of many-body systems and extended objects which involve a great number of degrees of freedom and which can be associated with a certain group of transformations that are not necessarily

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symmetries (e.g. dilatations, quadrupole deformations, etc).

The most straightforward treatment that singles out these specially relevant degrees of freedom is to isolate them from the remaining variables. We may thus describe the system in a way that displays clearly the role played by the collective degrees of freedom (this, of course, does not mean that in general they will uncouple from the other variables). However, this procedure becomes unfeasible for realistic systems, since these cases must be treated within some approximation involving independent fermion and/or phonon fields, and in such representations it is very difficult to isolate the collective variables.

A second (less straightforward) approach is to use an overcomplete system of collective plus intrinsic variables. For example, in unified models in nuclear physics one has intrinsic coordinates describing the nucleons "in a rotating frame" plus collective variables describing the motion of the frame [2].

More precisely, throughout these notes we understand by collective coordinates as those describing a group of transformations on the system (in fact the main results of this work can be adapted to the more general case in which the set of transformations do not form a true Lie group). In general, we do not know how relevant these particular coordinates may be: this depends on the system under consideration. The choice of the transformation group is dictated by the intuition that we have a priori on the dynamics of the system. The case of strongly broken symmetries is specially clear since we know that these degrees of freedom dominate the low energy behaviour of physical systems.

The overcompleteness of variables however poses a problem already at a classical level, which becomes worse at the quantum level: it is not clear for example what is to be understood by "rotating frame", if the coordinates describing such a frame are quantum variables. The observation that clarifies this problem of overcompleteness is the following: *a classical system that is described in terms of variables subject to time-dependent (canonical) transformations and such that the parameters defining the transformations are treated as (collective) dynamical variables on an equal footing with the original variables possesses a local (i.e. time-dependent) gauge symmetry.* This gauge symmetry consists of the group of all time-dependent transformations which simultaneously moves the frame of reference and the particle system so as to reproduce the same physical situation. Choosing a particular transformation of the frame is, in this language, choosing a gauge.

Now, the classical as well as the quantum mechanical treatment of systems with gauge invariance has been extensively studied [3,4]. Following the previous observation and using the Faddeev-Popov [5] path-integral treatment of gauge systems, Gervais, Jevicki and Sakita and Hosoya and Kikkawa [6] formulated a functional version of the method of collective coordinates. This method was later adapted in ref. [7] for the hamiltonian treatment of the many-fermion problem. Several applications were made involving collective rotations of fermion systems in two and three dimensions [8]. However, the procedure as it stood was cumbersome to apply, specially in non-abelian cases. In order to simplify the

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calculations a different form of the method was implemented [9]. It was still based on the Faddeev-Popov path-integral but a gauge condition was imposed in a way that bears analogy with the Lorentz gauge in electromagnetism.

In recent years a simple and elegant approach for the treatment of gauge systems has called the attention of many field theoreticians. Instead of reducing the number of degrees of freedom in the overcomplete description, additional fermionic variables (ghosts) are introduced. This apparent complication simplifies the problem, because in gauge systems there is a supersymmetry involving variables and ghosts, which was discovered by Becchi, Rouet, Stora and Tyutin [10,11,12,13].

Recently we have showed how this method can be applied for the classical and quantal treatment of systems with collective coordinates [14]. The resulting formalism is purely algebraic and thus, in particular, it does not rely on functional methods (although path-integrals can readily be constructed a posteriori). We have applied this method to derive variational as well as perturbative approximations for rotating systems in two and three dimensions [15,16].

The outlay of these notes is as follows: the classical and quantal treatments of systems described from moving frame of references are discussed in sections 2 and 3, respectively. The central part of these notes is given in section 4, which contains the treatment following the (supersymmetric) invariance with respect to a BRST transformation. A parallel formulation in terms of path integrals (in fact the original formulation in [6]) is given in section 5. Broken symmetries are discussed in section 6. Sections 7 and 8 contain illustrative applications on abelian and non-abelian systems, respectively. The last section discusses a procedure to obtain (perturbatively) a purely collective dynamics. These notes admit different readings: the shortest path in order to operate with the formalism follows through sections 3, 4 and 6, and through the examples in sections 7 and 8. However, the notes are self-contained and thus they include the formalization and the proof of the BRST procedure. These aspects are emphasized in sections 2-5.

In these notes we intend to cover three main objectives. The first one is to present a formalism which both justifies and allows for the correction of the independent mean-field approximation in many-body problems displaying a breakdown of symmetries. Our second aim is to convey to the many-body physicists part of the beauty displayed in recent treatments of gauge systems. Finally, we illustrate these developments through simple mechanical examples.

Some items in these notes have not been published elsewhere, to the best of our knowledge. Such is the case, in particular, of the discussion concerning the structure and metric of the space of wavefunctions associated with the BRST treatment of collective coordinates.

Discussions with V. Alessandrini and F. Schaposnik have greatly stimulated this work. The support of colleagues and friends from TANDAR, C.N.E.A. is gratefully acknowledged.

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2 The classical treatment of systems described by means of collective coordinates

The present section is devoted to the study of classical systems which are described from moving frames of reference. The parameters determining the motion of these frames are treated as dynamical variables on an equal footing with the original variables.

In subsection 2.1 we show the analogy between "gauging" a charged field to obtain electromagnetism and describing the motion of a particle in two dimensions from a rotating frame. The lagrangian and hamiltonian treatments of this mechanical system are discussed in subsection 2.2, stressing again the analogy with the electromagnetic case. In subsection 2.3 we consider the general case of a classical system whose dynamical variables are subject to an arbitrary (not necessarily symmetry) group of transformations. In appendix 2.A we discuss the particular problem of a general N-particle system which is described from a frame of reference that performs rotations in three dimensions. We thus exemplify some complications due to the non-abelian nature of the group of transformations. Finally, in appendix 2.B we derive some useful properties of Lie groups.

Our treatment makes use of the classical formalism for constrained systems developed by Dirac [17], as described in the presentation of Sudarshan and Mukunda [18].

2.1 The gauge nature of problems described from moving frames

Mechanical systems that are described from a moving frame of reference are indeed mechanical analogues of gauge field theories, with the simplification that the time is the single variable. As an example, we recall the derivation of the properties of the electromagnetic field using gauge methods [3] and, simultaneously, we translate this derivation to the case of a particle moving in a two-dimensional plane[1]. The expressions corresponding to the mechanical case are given below within square brackets.

We consider a complex scalar field $\Psi(x)$, where x denotes both space and time coordinates [$z(t) = q_1(t) + iq_2(t)$, where t is the time] whose classical lagrangian density [lagrangian] in the absence of electromagnetic coupling [in the laboratory frame] has the form

$$\mathcal{L}(\Psi(x), \partial_\mu \Psi(x)) = \frac{1}{2}\partial_\mu \Psi^* \partial^\mu \Psi - V(\Psi^*, \Psi) \tag{2.1}$$

$$L(z(t), d_t z(t)) = \frac{1}{2}|d_t z|^2 - V(z^*, z) \tag{2.2}$$

[1]Similar considerations can be found in [19] for the three dimensional case.

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The gauge principle states that the electromagnetic coupling [the coupling between the intrinsic and rotational degrees of freedom] arises from an extension of "global invariance" to "local invariance". The term with derivatives in the lagrangian (2.1) [(2.2)] is obviously invariant under a constant phase change of Ψ [z]

$$\left.\begin{array}{lll} \Psi & \longrightarrow & U\Psi \\ z & \longrightarrow & Uz \end{array}\right\} U = exp[-i\alpha] \tag{2.3}$$

where α is an arbitrary real constant. This transformation is called a global (i.e. coordinate-independent) transformation and the theory is said to have global invariance under the group U(1). If also the potential has circular symmetry

$$V(\Psi^*, \Psi) = V(|\Psi|^2) \tag{2.4}$$

$$V(z^*, z) = V(|z|^2) \tag{2.5}$$

by Noether's theorem there is a conserved current

$$J_\mu = \Psi^* \overleftrightarrow{\partial_\mu} \Psi \tag{2.6}$$

$$J = -\frac{i}{2}(z^* \frac{dz}{dt} - z\frac{dz^*}{dt}) = q_1\dot{q}_2 - \dot{q}_1 q_2 \tag{2.7}$$

Now we consider local gauge transformations

$$\Psi \longrightarrow U(x)\Psi \quad U(x) = exp[-i\,\alpha(x)] \tag{2.8}$$

$$z \longrightarrow U(t)\,z \quad U(t) = exp[-i\,\alpha(t)] \tag{2.9}$$

where α is an arbitrary real function. That is, the transformations at different points of space-time [time] are independent of one another. Although $\partial_\mu\Psi$ [$d_t z$] transforms in the same manner as Ψ [z] under a global transformation, it acquires an extra term under a local transformation

$$\partial_\mu\Psi \longrightarrow U\partial_\mu\Psi + (\partial_\mu U)\Psi \tag{2.10}$$

$$d_t z \longrightarrow U d_t z + z d_t U \tag{2.11}$$

Therefore, the lagrangian is not invariant under a local transformation. In order to make the theory locally gauge invariant, we replace $\partial_\mu\Psi$ [$d_t z$] by a suitable generalization that transforms in the same manner as Ψ [z]. We define a vector [scalar] field $A_\mu(x)$ [$\omega(t)$] called a "gauge field", which transforms under the local transformation according to the rule

$$A_\mu(x) \longrightarrow A_\mu(x) + \frac{1}{e}\partial_\mu\alpha \tag{2.12}$$

$$\omega(t) \longrightarrow \omega(t) + d_t\alpha \tag{2.13}$$

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Then, the "covariant derivative" ["invariant derivative"] defined by

$$D_\mu \Psi \equiv (\partial_\mu + ieA_\mu)\Psi \tag{2.14}$$

$$D_t z \equiv (d_t + i\omega)z \tag{2.15}$$

transforms in the same manner as Ψ $[z]$

$$D_\mu \Psi \longrightarrow U D_\mu \Psi \tag{2.16}$$

$$D_t z \longrightarrow (d_t + i\omega + i d_t \alpha) exp[-i\alpha] z = U D_t z \tag{2.17}$$

By replacing $\partial_\mu \Psi$ $[d_t z]$ by $D_\mu \Psi$ $[D_t z]$ in (2.1) [(2.2)], we obtain a new lagrangian density $\mathcal{L}(\Psi, D_\mu \Psi)$ [lagrangian $L(z, D_t z)$] which is obviously invariant under local gauge transformations. However, it contains the gauge field A_μ $[\omega]$ as an external field.

In Maxwell's theory one adds a term involving $\partial_\nu A_\mu$ quadratically. The only gauge-invariant Lorentz-scalar of this type is proportional to $F_{\mu\nu}F^{\mu\nu}$, where

$$F_{\mu\nu}(x) \equiv \partial_\mu A_\nu - \partial_\nu A_\mu \tag{2.18}$$

is called the field strength tensor. The lagrangian density for a closed dynamical system invariant under local gauge transformations is

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu}F^{\mu\nu} + \mathcal{L}(\Psi, D_\mu \Psi) \tag{2.19}$$

The factor $-\frac{1}{4}$ in the first term is purely conventional. The global U(1) symmetry, which is now enlarged with a local symmetry, is said to have been "gauged". The classical equations of motion following from (2.19) are just Maxwell's equations. Thus we have "derived" electromagnetism. The charge is a given real number that fixes the scale of A_μ relative to Ψ.

In the case of a two dimensional motion, the new lagrangian is

$$L = \frac{1}{2}|D_t z|^2 - V(|z|^2) = \frac{1}{2}[(\dot{q}_1 - \omega q_2)^2 + (\dot{q}_2 + \omega q_1)^2] - V(|z|^2) \tag{2.20}$$

The substitution of the invariant derivative in the lagrangian now yields the lagrangian in a rotating frame.

The lagrangian (2.20) may also be obtained through the replacement of q_i by[2] q_i' in the lagrangian (2.2), where

$$\begin{aligned} q_1' &= q_1 \cos\phi - q_2 \sin\phi \\ q_2' &= q_1 \sin\phi + q_2 \cos\phi \end{aligned} \tag{2.21}$$

Therefore, we identify the gauge field ω with the angular velocity $\dot{\phi}(t)$. If the time is our single variable, there is no quadratic term to be added, since

[2]From now on the prime and umprimed quantities refer to the laboratory and to the moving frame, respectively.

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$F_{00} = 0$ by definition (eq.(2.18)). The inclusion of a charge would have no physical consequence other than interpreting ω as $\dot{\phi}/e$.

The lagrangian (2.20) is not merely invariant with respect to global (time-independent) transformation but it is also invariant with respect to local (time-dependent) ones. This is what is called gauge invariance. We notice that there appears an extra degree of freedom, the collective degree of freedom ϕ, in the lagrangian (2.20).

Since this example may be easily generalized, we conclude that *mechanical systems which are described from moving frames (and in which the parameters describing the motion of the frame are treated as genuine coordinates) are a particular type of gauge systems.* Consequently, in the quantization of such problems we encounter many difficulties that are also present in the treatment of gauge theories. We intend to apply to the former the solutions that have been found for these last ones.

2.2 A particle moving in a two-dimensional plane

The lagrangian formalism

The Euler-Lagrange equations of motion

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0 \tag{2.22}$$

can also be written as

$$\frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j}\ddot{q}_j = \frac{\partial L}{\partial q_i} - \frac{\partial^2 L}{\partial \dot{q}_i \partial q_j}\dot{q}_j \tag{2.23}$$

Therefore, the accelerations at a given time are uniquely determined by the positions and velocities at that time if the determinant of the matrix $\partial^2 L/\partial \dot{q}_i \partial \dot{q}_j$ does not vanish. This is, for instance, the case for the lagrangian (2.2) in the laboratory frame

$$det\left(\frac{\partial^2 L}{\partial \dot{q}'_i \partial \dot{q}'_j}\right) = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} = 1 \tag{2.24}$$

However, we want to consider the lagrangian (2.20) corresponding to the description from a moving frame and to treat the *three* coordinates q_i ($q_3 \equiv \phi$) on an equal footing. In this case,

$$det\left(\frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j}\right) = \begin{vmatrix} 1 & 0 & -q_2 \\ 0 & 1 & q_1 \\ -q_2 & q_1 & q_1^2 + q_2^2 \end{vmatrix} = 0 \tag{2.25}$$

Such a lagrangian is called singular. We want to show now that only two of the three equations of motion (2.23) are independent of each other. It may be straightforwardly verified that the vector $\vec{\eta}$ in the three dimensional space

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$$\eta_1 = q_2 \quad ; \quad \eta_2 = -q_1 \quad ; \quad \eta_3 = 1 \tag{2.26}$$

satisfies the equation

$$\frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j} \eta_j = 0 \tag{2.27}$$

Therefore, if we multiply (2.23) to the left by the vector $\vec{\eta}$, we can check that

$$\begin{aligned} \eta_i \left(-\frac{\partial^2 L}{\partial \dot{q}_i \partial q_j} \dot{q}_j + \frac{\partial L}{\partial q_i}\right) &= \frac{\partial V}{\partial q_1} q_2 - \frac{\partial V}{\partial q_2} q_1 + \frac{\partial V}{\partial q_3} \\ &= \frac{\partial V}{\partial q_1} \frac{\partial q_1}{\partial \phi}(q_i', \phi) + \frac{\partial V}{\partial q_2} \frac{\partial q_2}{\partial \phi}(q_i', \phi) + \frac{\partial V}{\partial \phi} \\ &= \frac{\partial V}{\partial \phi}|_{q_1' \cdot q_2' = const.} = 0 \end{aligned} \tag{2.28}$$

where we have used the inverse of the transformation equations (2.21). This result expresses the obvious fact that the lagrangian in the laboratory frame does not depend on the coordinates of the moving frame. Therefore eq.(2.28), which is derived from the equations of motion, carries no dynamical information and is valid independently of the original form of V (in fact, it does not even require that the potential should be rotationally invariant). In this simple example we find that there is 'something missing', since we are not able to solve the equations of motion for the three variables. The solutions of the equations of motion of a singular lagrangian contain arbitrary functions of time. In our case, this is due to the fact that a lagrangian describing the system from a rotating frame lacks the information concerning the rotation of the frame itself (in electromagnetism, Maxwell's equations lack the information on the choice of the gauge).

As mentioned in subsection 2.1, the lagrangian (2.20) has a local time invariance which is independent of the original symmetries. It is invariant under the infinitesimal transformation

$$\begin{aligned} \delta q_1 &= \delta\alpha(t) q_2 \\ \delta q_2 &= -\delta\alpha(t) q_1 \\ \delta\phi &\equiv \delta q_3 = \delta\alpha(t) \end{aligned} \tag{2.29}$$

This invariance holds independently of the original form of the lagrangian in the laboratory frame. While the third eq.(2.29) changes the motion of the moving frame, the first two equations transform the coordinates q_1 and q_2 to the new frame. A gauge transformation maps a given trajectory into an equivalent one in which the same physical motion is described from another frame. Two trajectories belong to the same "class" if they are obtained from each other

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through a gauge transformation. All members of the same class represent the same physical trajectory. To choose a gauge means to select one member of each class. This is accomplished by imposing a supplementary relation between the coordinates and velocities.

$$G(q_i, \dot{q}_i, t) = 0 \tag{2.30}$$

G is called the gauge-fixing function and is arbitrary to a large extent. For instance, with the selection $G = \phi$ we are left with the original laboratory gauge. Another option is to choose $G = q_2$ which amounts to solve the problem in cylindrical variables, q_1 being the radial and ϕ the angular coordinate. Some other possibilities are discussed in following sections. It is precisely this freedom in the choice of G which makes a description using collective coordinates more flexible than the original one.

The hamiltonian formalism

The departing point of the hamiltonian formalism is to define the canonical momenta as functions of the coordinates and velocities. Our aim is to work in a phase-space $\mathcal{F}_2$ which includes ϕ, I as variables ($\phi \equiv q_3$; $I \equiv p_3$).

As usual, the conjugate momenta are defined by

$$p_i \equiv \frac{\partial L}{\partial \dot{q}_i} \quad i = 1, 2, 3 \tag{2.31}$$

The vanishing of the determinant (2.25) is just the condition for the non-invertibility of the velocities as functions of the coordinates and momenta. The momenta are not all independent from each other: there exist relations between them which follow from (2.31) and which are called constraints. For instance, for the lagrangian (2.20), eq.(2.31) yields the three equations

$$p_1 = \dot{q}_1 - q_2\dot{\phi} \tag{2.32}$$

$$p_2 = \dot{q}_2 + q_1\dot{\phi} \tag{2.33}$$

$$I = J \tag{2.34}$$

where J is defined as in (2.7),

$$J = q_1'\dot{q}_2' - q_2'\dot{q}_1' = q_1p_2 - q_2p_1 \tag{2.35}$$

The two eqs. (2.32) and (2.33) can be considered to be definitions of momenta, while (2.34) is a constraint.

Since not all the velocities can be expressed in terms of the momenta, we choose the set of variables $(q_1, q_2, p_1, p_2, \phi, \dot{\phi})$ and we define the hamiltonian

$$H = \sum_{i=1}^{2} p_i\dot{q}_i + J\dot{\phi} - L$$

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$$= \frac{1}{2}\sum_{i=1}^{2} p_i^2 + V \tag{2.36}$$

It is remarkable that the dependence on $\dot{q}_3$ disappears from the second line: this is a property of the Legendre transformation. We obtain the equation of motion following the usual procedure of varying both expressions for H with respect to the six variables and equating the coefficients of the independent variations [21]

$$\begin{aligned} \dot{p}_i &\simeq -\frac{\partial H}{\partial q_i} + \dot{\phi}\frac{\partial}{\partial q_i}(J-I) \\ \dot{q}_i &\simeq \frac{\partial H}{\partial p_i} - \dot{\phi}\frac{\partial}{\partial p_i}(J-I) \end{aligned} \tag{2.37}$$

where the symbol $\simeq$ denotes weak equality: equality when restricted to the constrained surface in $\mathcal{F}_2$ defined by (2.34). These equations are trivial for $\dot{q}_3 \equiv \dot{\phi}$. They imply that the time derivative of any phase space function M is[3]

$$\dot{M} \simeq \{M, H\} - \dot{\phi}\{M, (J-I)\} \tag{2.38}$$

where the Poisson brackets are those of $\mathcal{F}_2$. Notice that the constraint is preserved by the equations of motion. There is a dependence on the yet unspecified velocity $\dot{\phi}$, which is to be expected from the previous discussion using the lagrangian approach. Accordingly, we must choose a gauge fixing function $G(q_i, p_i)$. From eqs. (2.30) and (2.38)

$$0 = \dot{G} \simeq \{G, H\} - \dot{\phi}\{G, (J-I)\} \tag{2.39}$$

Solving $\dot{\phi}$ and introducing this value in eq. (2.34), we obtain the final expression for the equations of motion

$$\dot{M} \simeq \{M, H\} - \{M, (J-I)\}\frac{1}{\{G, (J-I)\}}\{G, H\} = \{M, H\}_D \tag{2.40}$$

The Dirac brackets

$$\begin{aligned} \{A, B\}_D \equiv \{A, B\} \quad & -\{A, (J-I)\}\tfrac{1}{\{G,(J-I)\}}\{G, B\} \\ & +\{B, (J-I)\}\tfrac{1}{\{G,(J-I)\}}\{G, A\} \end{aligned} \tag{2.41}$$

are a generalisation of the Poisson brackets and share most of their properties. From (2.40) we clearly see that if the constraint (2.34) and the gauge condition (2.30) are satisfied at $t = 0$, they will be satisfied at any subsequent time.

[3] We recall the definition of the Poisson bracket $\{A, B\} = \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i}$

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In phase-space $\mathcal{F}_2$, the finite transformation corresponding to the infinitesimal transformation (2.29) may be written

$$\begin{aligned} T(\alpha(t)) &= exp[-\alpha\{(J-I),\ \}] \\ &= 1 - \alpha\{(J-I),\ \} + \frac{1}{2}\alpha^2\{(J-I),\{(J-I),\ \}\} + \ldots \end{aligned} \tag{2.42}$$

Thus $(J-I)$ is the generator of the gauge transformation. The Poisson bracket between this generator and any physical magnitude vanishes, reflecting the fundamental invariance of gauge systems: while I changes the rotation of the frame of reference, J changes the coordinates in an appropriate way to leave the description invariant. In particular, the transformation (2.42) leaves invariant the phase-space lagrangian.

As in configuration space, the transformation (2.42) maps a given trajectory in phase space into another trajectory representing the same physical trajectory, but described from another gauge (i.e., from a different rotating system). This group of transformations is the gauge group. It leaves invariant the constraining hypersurface, which is mapped into itself.

Up to now we have seen that the original dynamics of the problem can be reproduced in a six-dimensional phase-space $\mathcal{F}_2$ with the constraint (2.34). We cast now these results in a form which is also used in the quantal treatments of sections 3 -5.

We impose the constraint by introducing a Lagrange multiplier Ω, which is also treated as a dynamical variable. The hamiltonian and phase-space lagrangian can be written in the new phase-space $\mathcal{F}_3$

$$\begin{aligned} H &= \frac{1}{2}\sum_{i=1}^{2} p_i^2 + V - \Omega(J-I) \\ L &= \sum_{i=1}^{3} p_i \dot{q}_i + P\dot{\Omega} - H \end{aligned} \tag{2.43}$$

where we have introduced the canonical momentum P conjugate to Ω. The term $P\dot{\Omega}$ added in the lagrangian is zero if we impose the new constraint

$$P = 0 \tag{2.44}$$

Hamilton's equation for P thus yields

$$0 = \dot{P} = -\frac{\partial H}{\partial \Omega} = J - I \tag{2.45}$$

Therefore, the old constraint (2.34) appears now as a consequence of the equations of motion and hence it is called a secondary constraint, as opposed to eq.(2.44) which is a primary constraint (it is not a consequence of the dynamics).

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In the present eight-dimensional phase-space $\mathcal{F}_3$ the gauge group of transformations is generated by

$$T(\beta(t)) = exp[-\dot{\beta}\{P,\ \} + \beta\{(J-I),\ \}] \tag{2.46}$$

which leaves invariant the lagrangian (2.43) in the moving frame when restricted to the surface defined by eq. (2.44).

To conclude this section we show that the hamiltonian H together with the primary and secondary constraints are a "caricature" of the electromagnetic problem. The electromagnetic field has the four-fold coordinates $A_\mu(x,t)$ where $\mu = i,t$ and $i = 1,2,3$ are the spatial indices. The lagrangian density is (c.f. eq.(2.19))

$$\mathcal{L} = -\frac{1}{4}F_{ij}F^{ij} - \frac{1}{2}F_{oi}F^{oi} \tag{2.47}$$

The momenta are defined in the usual way

$$E_\mu(x) = \frac{\partial \mathcal{L}}{\partial(\partial_o A_\mu)} = \dot{A}_\mu + \partial_\mu A^o \tag{2.48}$$

They represent the electric field components for $\mu = i$. For $\mu = 0$

$$E_o = \dot{A}_o + \partial_o A^o = 0 \tag{2.49}$$

which is a primary constraint. The hamiltonian density equals

$$\begin{aligned} \mathcal{H} &= \dot{A}_\mu E^\mu - \mathcal{L} = \frac{1}{2}E_i E^i + \frac{1}{4}F_{ij}F^{ij} - (\partial_i A^o)E^i \\ &\rightarrow \frac{1}{2}E_i E^i + \frac{1}{4}F_{ij}F^{ij} + A^o(\partial_i E^i) \end{aligned} \tag{2.50}$$

where we have added a divergency. From the equations of motion for E_0 we obtain

$$\dot{E}_o = \frac{\partial H}{\partial A_o} = \partial_i E^i(x) \tag{2.51}$$

Therefore the Gauss law appears as a secondary constraint. Table 1 shows the relation between the electromagnetic and the mechanical case. In electromagnetism, as in classical mechanics employing moving frames, we must impose additional gauge fixing conditions.

2.3 A general canonical transformation

In the present subsection we generalise the previous treatment of collective coordinates for two-dimensional rotations to the case of general canonical transformations[4].

[4]Although we sometimes continue to use the vocabulary associated with rotations, we are not restricted to this type of transformations.

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	Electromagnetism	Mechanical case
Coordinates	$A_\mu(x,t)$	ϕ, Ω, q_1, q_2
Momenta	$E_\mu(x,t)$	I, P, p_1, p_2
Primary constraint	$E_o(x) = 0$	$P = 0$
Secondary constraint	$\partial_i E^i = 0$	$J - I = 0$

Table 1: The analogy between the electromagnetic and the mechanical case.

The laboratory variables in the original phase space $\mathcal{F}_1$ are denoted by q_i', p_i' $(i = 1, ..., n)$. There are k generators which form a Lie algebra [5]

$$\{J_v, J_w\} = c_{vws} J_s \tag{2.52}$$

They generate the transformations

$$\tilde{T}(\phi_s) = exp\,[\phi_v \{J_v, \ \}] \tag{2.53}$$

where the ϕ_v are parameters[6]. Given a phase-space function $M'(q_i', p_i')$ of the original variables we reexpress it in terms of the transformed variables q_i, p_i as follows

$$M'(q_i', p_i') = T^{-1} M'(q_i, p_i) = M(q_i, p_i) \tag{2.54}$$

where $M'(q_i', p_i')$ and $M'(q_i, p_i)$ have the same functional dependence while $M'(q_i', p_i')$ and $M(q_i, p_i)$ take the same values. In particular, we can write a relation like (2.54) for the generators J_v themselves, and thus obtain a set of transformed generators which satisfy the same Poisson bracket algebra (2.52).

Since the transformation is an artifact introduced by us, the laboratory version of physical functions should be independent of the transformation parameters ϕ_v. This fact implies that not all the functions M are physical. In order to be so, they must satisfy the condition

$$\begin{aligned} 0 &= \tilde{T}^{-1} \frac{\partial}{\partial \phi_v} M'(q_i, p_i, \phi_w) = \tilde{T}^{-1} (\frac{\partial \tilde{T}}{\partial \phi_v}) M + \frac{\partial M}{\partial \phi_v} \\ &= \zeta_{wv}(\phi_s) \{J_w, M\} + \frac{\partial M}{\partial \phi_v} = D_v M \end{aligned} \tag{2.55}$$

[5]For compact Lie groups the structure constants can be taken to be antisymmetric in the three indices v, w, s. We will assume this to be the case throughout these notes

[6]It may also be possible to parametrize the transformation in a different way, as with the Euler angles in the case of three-dimensional rotations.

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The matrix $\varsigma(\phi_\sigma)$ is a function of the parameters ϕ_σ and depends on the particular group of transformations (see appendix 2.B). In eq. (2.55) we have introduced the "invariant" derivative

$$D_\nu \equiv \varsigma_{\omega\nu}\{J_\omega, \ \} + \frac{\partial}{\partial \phi_\nu} \tag{2.56}$$

We now raise the ϕ_ν to the rank of true dynamical variables and introduce their associated momenta which satisfy

$$\{\phi_\nu, P'_\omega\} = \{\phi_\nu, P_\omega\} = \delta_{\nu\omega} \tag{2.57}$$

The P' and P complete the canonical set in the laboratory and in the transformed variables, respectively. We call this new phase-space $\mathcal{F}_2$. The definition of the transformation (2.53) must be slightly changed in order to insure that it continues to be canonical in the enlarged phase-space $\mathcal{F}_2$. Thus we now define, for instance in the canonical parametrization

$$T(\phi_\sigma) = exp\,[\{\phi_\nu J_\nu, \ \}] \tag{2.58}$$

The transformation T coincides with the previous $\tilde{T}$ when applied to functions that do not contain the momenta P'_ν. However, we note that whereas the transformation $\tilde{T}$ in $\mathcal{F}_1$ is time-dependent (the time-dependency arising from the parameters ϕ_ν) the transformation T in $\mathcal{F}_2$ is time-independent (the ϕ_ν now being variables in $\mathcal{F}_2$). The transformation T can be verified to act on the collective momenta as follows

$$P'_\nu = T^{-1} P_\nu = -F_\nu \qquad F_\nu \equiv \varsigma_{\omega\nu} J_\omega - P_\nu \tag{2.59}$$

Therefore, the conditions for a function to be physical read

$$\begin{aligned} \{M'(q'_i, p'_i, \phi_\omega), P'_\nu\} &= 0 \\ \{M(q_i, p_i, \phi_\omega), F_\nu\} &= 0 \end{aligned} \tag{2.60}$$

in the laboratory and transformed frame, respectively.

We may also use an alternative form of these conditions. Introducing the matrix $\eta(\phi_\sigma)$ that is inverse to ς, we obtain from the last of eqs. (2.60)

$$\begin{aligned} \{M, f_\nu\} &= 0 \\ f_\nu &\equiv \eta_{\omega\nu} F_\omega = J_\nu - I_\nu \end{aligned} \tag{2.61}$$

where the collective generators are defined as

$$I_\nu \equiv \eta_{\omega\nu} P_\omega \tag{2.62}$$

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In the laboratory frame the constraints f_v take a similar form

$$f'_v = -\eta_{wv} P'_w \tag{2.63}$$

The following commutation relations hold for the general case

$$\begin{aligned} \{J_v, J_w\} &= c_{vws} J_s \qquad \{I_v, I_w\} = -c_{vws} I_s \\ \{f_v, f_w\} &= c_{vws} f_s \qquad \{F_v, F_w\} = 0 \end{aligned} \tag{2.64}$$

These Poisson brackets are defined within the enlarged phase-space $\mathcal{F}_2$. The difference in sign for the collective angular momentum is well known since the pioneering work on rotation of molecules.

Since the collective coordinates ϕ_v, P'_v separate in the laboratory system (and in fact they are irrelevant for physical functions), we may impose for physical trajectories the conditions (slightly more severe than (2.55))

$$P'_v = 0 \tag{2.65}$$

which in terms of the transformed variables read

$$F_v = 0 \quad \text{or} \quad f_v = 0 \tag{2.66}$$

The Poisson brackets between two of these constraints and between the hamiltonian and each of them vanish on the hypersurface in $\mathcal{F}_2$ constrained by these equations. Thus, they are preserved at all times by the dynamics of the system.

In the original phase-space the lagrangian can be written

$$L' = p'_i \dot{q}'_i - H' = p'_i \dot{q}'_i + P'_v \dot{\phi}_v - H' - P'_v \dot{\phi}_v \tag{2.67}$$

The first three terms in the r.h.s. are the ones that one would expect from a lagrangian in $\mathcal{F}_2$. Since T is a time-independent canonical transformation in $\mathcal{F}_2$, we have (up to total time-derivatives)

$$p'_i \dot{q}'_i + P'_v \dot{\phi}_v - H' \rightarrow p_i \dot{q}_i + P_v \dot{\phi}_v - H \tag{2.68}$$

while from (2.59)

$$P'_v \dot{\phi}_v \longrightarrow -F_v \dot{\phi}_v \tag{2.69}$$

so that the phase-space lagrangian becomes

$$\begin{aligned} L &= p_i \dot{q}_i + P_v \dot{\phi}_v + F_v \dot{\phi}_v - H \\ &= p_i \dot{q}_i + \varsigma_{wv} J_w \dot{\phi}_v - H \\ &= p_i \dot{q}_i - (H - \omega_v J_v) \end{aligned} \tag{2.70}$$

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where we have defined

$$\omega_v \equiv \zeta_{vw}\dot{\phi}_w \tag{2.71}$$

which is a generalisation of the angular frequencies.

Following the same procedure as in (2.37) (i.e., varying H independently with respect to $p_i, q_i, \phi_v, \dot{\phi}_v$), we obtain

$$\dot{q}_i \simeq \frac{\partial H}{\partial p_i} - \dot{\phi}_v \hat{\zeta}_{wv} \frac{\partial J_w}{\partial p_i} = \frac{\partial H}{\partial p_i} - \dot{\phi}_v \frac{\partial F_v}{\partial p_i} \tag{2.72}$$

$$\dot{p}_i \simeq -\frac{\partial H}{\partial q_i} - \dot{\phi}_v \hat{\zeta}_{wv} \frac{\partial J_w}{\partial q_i} = -\frac{\partial H}{\partial q_i} + \dot{\phi}_v \frac{\partial F_v}{\partial q_i} \tag{2.73}$$

where again $\simeq$ denotes weak equality. Similar equations hold for ϕ_v, namely

$$\dot{\phi}_v \simeq -\dot{\phi}_w \frac{\partial F_w}{\partial P_v} \tag{2.74}$$

which is trivial ($\dot{\phi}_v = \dot{\phi}_w \delta_{vw}$). From the requirement that the constraints are preserved at all times we obtain

$$\dot{P}_w \simeq -\frac{\partial H}{\partial \phi_w} + \dot{\phi}_v \frac{\partial F_v}{\partial \phi_w} \tag{2.75}$$

so that we can write for any function in the $2n + 2k$ phase-space $\mathcal{F}_2$

$$\dot{M} \simeq \{M, H\} - \dot{\phi}_v \{M, F_v\} = 0 \tag{2.76}$$

Note that if M is independent of ϕ_v, P_v, this equation reduces to the familiar expression (cf. eq. (2.70))

$$\dot{M} \simeq \{M, (H - \omega_v J_v)\} \tag{2.77}$$

Eq.(2.76) is a generalisation of eq.(2.37). It is as far as we can go without fixing a gauge.

Let us consider now k gauge-fixing functions G_v

$$G_v(q_i, p_i, \phi_s) = 0 \tag{2.78}$$

If these gauge conditions are to hold at all times

$$\dot{G}_v \simeq \{G_v, H\} - \dot{\phi}_w \{G_v, F_w\} = 0 \tag{2.79}$$

Provided that

$$det[\{G_v, F_w\}] \neq 0 \tag{2.80}$$

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we may solve (2.79) for $\dot{\phi}_v$ and insert these derivatives in (2.76). We thus obtain the time evolution of an arbitrary function in terms of Dirac brackets

$$\begin{aligned} \dot{M} &\simeq \{M,H\} - \{M,F_w\}\ |\{G_\alpha,F_\beta\}|^{-1}_{wv}\ \{G_v,H\} \\ &\simeq \{M,H\} - \{M,f_w\}\ |\{G_\alpha,f_\beta\}|^{-1}_{wv}\ \{G_v,H\} \\ &\simeq \{M,H\}_D \end{aligned} \tag{2.81}$$

with

$$\begin{aligned} \{A,B\}_D \equiv\ & \{A,B\} - \{A,f_w\}\ |\{G_\alpha,f_\beta\}|^{-1}_{wv}\ \{G_v,B\} \\ & +\{B,f_w\}\ |\{G_\alpha,f_\beta\}|^{-1}_{wv}\ \{G_v,A\} \end{aligned} \tag{2.82}$$

We can also verify that the phase-space lagrangian (2.70) is left invariant by the group of gauge transformations

$$T(\alpha(t)) = exp[-\alpha_v(t)\{f_v,\ \}] \tag{2.83}$$

These results can be summarised by saying that within the extended phase-space $\mathcal{F}_2$, physical trajectories are restricted to a hypersurface defined by the constraining equations (2.66). On this hypersurface each trajectory is copied an infinite number of times. By choosing a gauge, we select a copy of each class of equivalent trajectories.

Finally, we can include the constraints as in (2.44).

$$\tilde{H} = H - \Omega_v f_v \tag{2.84}$$

with the primary constraints

$$P_v = 0 \tag{2.85}$$

where

$$\{\Omega_v, P_w\} = \delta_{vw} \tag{2.86}$$

In this new phase-space $\mathcal{F}_3$, eqs.(2.68) appear as secondary constraints

$$0 = \dot{P}_v = -\frac{\partial \tilde{H}}{\partial \Omega_v} = f_v \tag{2.87}$$

One can check that in $\mathcal{F}_3$ the gauge group is generated by the transformation [12]

$$T(\beta(t)) = exp[(-\dot{\beta}_s + \beta_v \Omega_w c_{svw})\{P_s,\ \} + \beta_v\{f_v,\ \}] \tag{2.88}$$

which leaves the phase-space version of the lagrangian invariant when restricted to the hypersurface (2.85).

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appendix 2.A The three-dimensional rotation of a N-particl system

If the N-particle system constitutes a rigid rotor, a suitable description can be obtained from a rotating frame associated with the principal axis of the tensor of inertia. In this case, the useful coordinates are the collective coordinates determining the orientation of the moving frame. In this appendix we study the generalisation of this description to the case of a system which is not completely rigid, and thus the internal degrees of freedom have to be considered as well as the collective ones. The overcomplete set of variables must be treated in a self-consistent way.

We start with the lagrangian in the laboratory frame

$$L' = \sum_i \frac{m_i}{2} |\dot{\vec{r}}_i'|^2 - V(\vec{r}_i') \tag{2.89}$$

where $i = 1, 2...N$ and $\vec{r}_i$ is the position vector of the i-th particle. The expression for the lagrangian in the rotating frame may be found in textbooks

$$L = \sum_i \frac{m_i}{2} |\dot{\vec{r}}_i + \vec{\omega} \wedge \vec{r}_i|^2 - V(\vec{r}_i, \phi_v) \tag{2.90}$$

The angles ϕ_v parametrise the motion of the rotating frame. The relation between the components ω_v of the angular frequencies and the time derivative of the angles ϕ_v is written

$$\omega_v = \varsigma_{vw}(\phi_s)\dot{\phi}_w \tag{2.91}$$

where the matrix $\varsigma(\phi_s)$ depends on the chosen parametrisation. As in the previous subsection we calculate the 3N+3 momenta associated with the coordinates $\vec{r}_i, \phi_v$ (which complete the new phase-space $\mathcal{F}_2$)

$$\vec{p}_i = m_i(\dot{\vec{r}}_i + \vec{\omega} \wedge \vec{r}_i) \tag{2.92}$$

$$\begin{aligned} P_v &= \sum_i m_i(\dot{\vec{r}}_i + \vec{\omega} \wedge \vec{r}_i)(\frac{\partial \vec{\omega}}{\partial \dot{\phi}_v} \wedge \vec{r}_i) \\ &= \sum_i m_i \frac{\partial \vec{\omega}}{\partial \dot{\phi}_v} \left[\vec{r}_i \wedge (\dot{\vec{r}}_i + \vec{\omega} \wedge \vec{r}_i)\right] = \frac{\partial \vec{\omega}}{\partial \dot{\phi}_v} \vec{J} \end{aligned} \tag{2.93}$$

where the generator $\vec{J}$ is defined

$$\vec{J} = \sum_i \vec{r}_i \wedge \vec{p}_i \tag{2.94}$$

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We find again that the 3N+3 momenta are not independent of each other. They satisfy three constraint equations which play the same role as eq.(2.34)

$$F_v = \varsigma_{wv} J_w - P_v = 0 \tag{2.95}$$

A new set of constraints is obtained if we multiply F by η, (the inverse of ς).

$$f_v \equiv \eta_{wv} F_w = J_v - I_v = 0 \tag{2.96}$$

where

$$I_v \equiv \eta_{wv} P_w \tag{2.97}$$

are to be interpreted as the collective components of the angular momentum in the intrinsic frame. While the F_v commute between themselves, the J_v, I_v and f_v are generators of SU(2) algebrae (see appendix 2.B).

$$\begin{aligned} \{J_v, J_w\} &= \epsilon_{vws} J_s \qquad \{I_v, I_w\} = -\epsilon_{vws} I_s \\ \{f_v, f_w\} &= \epsilon_{vws} f_s \qquad \{F_v, F_w\} = 0 \end{aligned} \tag{2.98}$$

Here ϵ_{vws} is the Levi-Civita tensor.

Two useful parametrizations for this group are: i)the canonical parametrization

$$T(\phi_s) = exp[\phi_v \tilde{J}_v] \tag{2.99}$$

and ii)the Euler parametrization

$$T(\phi_s) = exp[\psi \tilde{J}_3]\, exp[\theta \tilde{J}_2]\, exp[\varphi \tilde{J}_3] \tag{2.100}$$

For the canonical parametrization we have

$$\eta_{vw} = \delta_{vw} \frac{\phi}{2} cot\frac{\phi}{2} + \frac{\phi_v \phi_w}{\phi^2} \left(1 - \frac{\phi}{2} cot\frac{\phi}{2}\right) - \epsilon_{vws} \frac{\phi_s}{2} \tag{2.101}$$

$$\varsigma_{vw} = \delta_{vw} \frac{sin\phi}{\phi} + \frac{\phi_v \phi_w}{\phi^2} \left(1 - \frac{\sin\phi}{\phi}\right) - \epsilon_{vws} \phi_s \frac{(1 - cos\phi)}{\phi^2} \tag{2.102}$$

with

$$\phi = \sqrt{\phi_v^2}$$

Similar relations for the Euler parametrization [20] are read off from (cf. eq. (2.97))

$$\begin{aligned} I_1 &= cos\psi\ P_\theta + sin\psi\ cosec\theta\ P_\varphi - cot\theta\ sin\psi\ P_\psi \\ I_2 &= -sin\psi\ P_\theta + cos\psi\ cosec\theta\ P_\varphi - cot\theta\ cos\psi\ P_\psi \\ I_3 &= P_\psi \end{aligned} \tag{2.103}$$

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Similarly to the previous cases, we have three unspecified velocities which should be fixed by means of the three gauge-fixing conditions

$$G_v(\vec{r}_i, \vec{p}_i, \phi_s) = 0 \tag{2.104}$$

A possible choice associating the moving frame with the principal axis is to equate G_v to the non-diagonal components of the quadrupole tensor

$$G_v = Q_{v+1.v+2} = \sum_i m_i (r_{v+1})_i (r_{v+2})_i \tag{2.105}$$

appendix 2.B Some useful properties of Lie groups

In this appendix we derive some results that are used throughout the present notes.

Let $J_v \quad (v = 1, ..., k)$ be k phase-space functions satisfying the Lie algebra (2.52) with Poisson brackets. We have the identities:

$$\begin{aligned} \{J_v, J_w\} &= -\{J_w, J_v\} \\ \sum_{(vws)\ cyclic} \{\{J_v, J_w\}, J_s\} &= 0 \end{aligned} \tag{2.106}$$

which imply

$$\begin{aligned} c_{vws} &= -c_{wvs} \\ \sum_{(vws)\ cyclic} c_{vwt} c_{tsu} &= 0 \end{aligned} \tag{2.107}$$

We shall further assume for simplicity that the c_{ijk} are totally antisymmetric[7].

We define

$$\tilde{J}_v \equiv \{J_v, \ \} \tag{2.108}$$

and from (2.107) we find that:

$$[\tilde{J}_v, \tilde{J}_w] = c_{vws} \tilde{J}_s \tag{2.109}$$

where $[\ ,\ ]$ denotes the commutator. With this algebra we can generate a group of canonical transformations parametrised by ϕ_v. For example, in the canonical parametrisation

$$T(\phi_s) = exp[\phi_v \tilde{J}_v] \tag{2.110}$$

From the group composition law

[7] This can always be assumed for compact groups.

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$$
\begin{aligned}
T(\phi_v^{(c)}) &= T(\phi_v^{(b)})T(\phi_v^{(a)}) \\
\phi_v^{(c)} &= g_v(\phi_s^{(b)}, \phi_s^{(a)})
\end{aligned}
\tag{2.111}
$$

We define the matrix $\eta_{vw}(\phi_s^{(b)})$ and its inverse $\varsigma_{vw}(\phi_s^{(b)})$

$$
\begin{aligned}
\eta_{vw} &= \frac{\partial g_v}{\partial \phi_w^{(a)}}|_{\phi_s^{(a)}=0} \\
\varsigma_{vs}\eta_{sw} &= \delta_{vw}
\end{aligned}
\tag{2.112}
$$

Let us consider that the $\phi_v^{(a)}$ are small increments $\delta\phi^a_{(v)}$. To first order

$$
\begin{aligned}
\delta\phi_v^{(c)} &= \phi_v^{(b)} + \delta\phi_v^{(b)} = \phi_v^{(b)} + \eta_{vw}\delta\phi_w^{(a)} \\
\delta\phi_v^{(a)} &= \varsigma_{vw}\delta\phi_w^{(b)}
\end{aligned}
\tag{2.113}
$$

After replacement in (2.111) we obtain

$$
T(\phi_v + \delta\phi_v) = T(\phi_v)T(\varsigma_{vw}\delta\phi_w) \tag{2.114}
$$

where we have dropped the supraindex b labelling *all* the parameters that appear in (2.114). We also obtain to first order

$$
\begin{aligned}
T^{-1}[T(\phi_v + \delta\phi_v) - T(\phi_v)] &= T^{-1}\frac{\partial T}{\partial \phi_v}\delta\phi_v \\
T(\varsigma_{wv}\delta\phi_v) - 1 &= \varsigma_{wv}\tilde{J}_w\delta\phi_v
\end{aligned}
\tag{2.115}
$$

Therefore, if we subtract T and multiply to the left by T^{-1} in both members of eq. (2.114) we obtain[8]

$$
T^{-1}\frac{\partial T}{\partial \phi_v} = \varsigma_{wv}\tilde{J}_w \tag{2.116}
$$

Furthermore, we obtain from $T.T^{-1} = 1$

$$
\frac{\partial T}{\partial \phi_v}T^{-1} + T\frac{\partial T^{-1}}{\partial \phi_v} = \frac{\partial T^{-1}}{\partial \phi_v}T + T^{-1}\frac{\partial T}{\partial \phi_v} = 0 \tag{2.117}
$$

[8]The formula (2.116) has been derived assuming a canonical parametrization but it is easy shown to be valid with any other (good) parametrization.

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Let us now derive differential relations for the η, ς. From eq. (2.116) we obtain

$$\begin{aligned} \frac{\partial T}{\partial \phi_v} &= T\varsigma_{wv}\tilde{J}_w \\ \frac{\partial^2 T}{\partial \phi_v \partial \phi_w} &= T\varsigma_{sw.v}\tilde{J}_s + \varsigma_{sw}\tilde{J}_s\frac{\partial T}{\partial \phi_v} \\ &= T(\varsigma_{sw.v}\tilde{J}_s + \varsigma_{sw}\tilde{J}_s\varsigma_{tv}\tilde{J}_t) \end{aligned} \tag{2.118}$$

where the comma denotes derivation. Similarly,

$$\frac{\partial^2 T}{\partial \phi_w \partial \phi_v} = T(\varsigma_{sv.w}\tilde{J}_s + \varsigma_{sv}\tilde{J}_s\varsigma_{tw}\tilde{J}_t) \tag{2.119}$$

Subtracting and multiplying by T^{-1} to the left yields

$$(\varsigma_{uw.v} - \varsigma_{uv.w})\,\tilde{J}_u + \varsigma_{sw}\varsigma_{tv}[\tilde{J}_s, \tilde{J}_t] = 0 \tag{2.120}$$

where we have swapped the indices in the second term of (2.119). Using the structure constants and swapping indices again

$$\varsigma_{uw.v} - \varsigma_{uv.w} + \varsigma_{sw}\varsigma_{tv}c_{stu} = 0 \tag{2.121}$$

These relations imply other relations between the inverse η

$$\eta_{ws}\eta_{vt.w} - \eta_{wt}\eta_{vs.w} = -c_{tsu}\eta_{vu} \tag{2.122}$$

The commutation relations

Using the previous formulae we can derive the Poisson brackets (2.64) as follows

$$\{I_v, I_w\} = \{\eta_{sv}P_s\ ,\ \eta_{tw}P_t\}$$

$$= \{\eta_{sv}, P_t\}\,\eta_{tw}\ P_s - \{\eta_{tw}, P_s\}\,\eta_{sv}\ P_t$$

$$= \eta_{sv.t}\ \eta_{tw}P_s - \eta_{tw.v}\ \eta_{sv}P_t$$

$$= (\eta_{sv.t}\ \eta_{tw} - \eta_{sw.t}\ \eta_{tv})P_s$$

$$= -c_{vws}\eta_{ts}calP_t = -c_{vws}I_s$$

where eq. (2.122) has been used. From this relation we immediately find that:

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$$\{f_v, f_w\} = \{(J_v - I_v), (J_w - I_w)\} = c_{vws}(J_s - I_s) = c_{vws} f_s$$

We may also calculate

$$\{F_v, F_w\} = \{(\varsigma_{uv} J_u - P_v), (\varsigma_{tw} J_t - P_w)\}$$

$$= -\varsigma_{sv,w}\, J_s + \varsigma_{tw,v}\, J_w + \varsigma_{sv}\, \varsigma_{tw}\, \{J_s, J_t\}$$

$$= \varsigma_{sv}\, \varsigma_{tw}\, c_{stu} J_u - \varsigma_{sv,w}\, J_s + \varsigma_{tw,v}\, J_t$$

$$= (\varsigma_{uw,v} - \varsigma_{uv,w} - \varsigma_{tv}\, \varsigma_{sw}\, c_{stu})\, J_s = 0$$

where we have applied eq. (2.121).

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3 The Hilbert spaces associated with collective coordinates

3.1 The constraints

In the present section we translate the classical results of section 2 to the quantal language. We start with the Hilbert space $\mathcal{H}_1$ of wavefunctions $\Psi'(q_i')$ $(i = 1, ..., n)$ and we consider a general group of unitary transformations $T(\phi_v)$. Its generators $\hat{J}_v$ $(v = 1, ..., k)$ satisfy a closed algebra.

$$[\hat{J}_v, \hat{J}_w] = ic_{vws}\hat{J}_s \tag{3.1}$$

where $[\ ,\ ]$ denotes the commutation operation (c.f. eq. (2.52)). Most developments in this and the following sections can be straightforwardly extended to the case in which the transformations $T(\phi_v)$ do not constitute a Lie group (see comment in section 4), although in the present work we restrict ourselves to such a case.

The transformation operator reads, in the canonical parametrization[9]

$$\hat{T} = exp[-i\phi_v\hat{J}_v] \tag{3.2}$$

It relates the wavefunctions Ψ' and operators $\hat{O}'$ in the laboratory frame to those in the moving frame

$$\begin{aligned} |\Psi'> &= \hat{T}|\Psi> \\ \hat{O}' &= \hat{T}\hat{O}\hat{T}^\dagger \end{aligned} \tag{3.3}$$

In particular, one obtains the transformed versions of the $\hat{J}_v$ themselves.

We wish to treat the k parameters ϕ_v as genuine coordinates. Therefore, we define the overcomplete Hilbert space $\mathcal{H}_2$ whose wave functions depend both on q_i and ϕ_v. We also introduce the operators $\hat{\phi}_v$ and their canonical momenta $\hat{P}_v$. We assume that $-\infty < \phi_v < \infty$ and thus that P_v has continuous eigenvalues[10]

$$\begin{aligned} [\hat{\phi}_v, \hat{P}_w] &= i\delta_{vw} \\ \hat{P}_v &= -i\frac{\partial}{\partial\phi_v} \end{aligned} \tag{3.4}$$

In $\mathcal{H}_2$, the laboratory version of physical states $|ph'>$ is independent of the ϕ_v (c.f. eq.(2.55)). (In fact they are the wavefunctions belonging to $\mathcal{H}_1$ times a unit state in the collective space).

[9] Any other parametrization of the transformation (such as the Euler parametrization of the three dimensional rotations) can be used as well.

[10] However, for example in the case of rotations, we will be free to work in the subspace of integer values of P_v since the rotational one-turn operator $exp[2\pi i\hat{P}_v]$ is, in practical cases a conserved magnitude, and thus we may choose periodic wavefunctions in ϕ_v.

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$$0 = i\hat{T}^\dagger \frac{\partial}{\partial \phi_v} |ph'> = \hat{F}_v |ph>$$

$$\hat{F}_v \equiv i\hat{T}^\dagger \left(\frac{\partial \hat{T}}{\partial \phi_v}\right) + i\frac{\partial}{\partial \phi_v} = -\hat{T}^\dagger \hat{P}_v \hat{T} = \varsigma_{wv}(\phi_s)\hat{J}_w - \hat{P}_v \tag{3.5}$$

The alternative set of constraints is obtained through the multiplication of F by η (the inverse matrix of ς).

$$\hat{f}_v |ph> = 0$$

$$\hat{f}_v \equiv \eta_{wv} F_w = \hat{J}_v - \hat{I}_v \tag{3.6}$$

where

$$\hat{I}_v \equiv \eta_{wv} \hat{P}_w \tag{3.7}$$

Thus $\hat{I}_v$ is the collective version of $\hat{J}_v$. In addition to (3.1), the following commutation relations are satisfied [11].

$$[\hat{P}_v, \hat{P}_w] = 0 \quad [\hat{I}_v, \hat{I}_w] = -ic_{vws}\hat{I}_s$$

$$[\hat{F}_v, \hat{F}_w] = 0 \quad [\hat{f}_v, \hat{f}_w] = ic_{vws}\hat{f}_s, \tag{3.8}$$

The constraint operators are generators of the gauge group of transformations. Physical states carry the zero-representation of such group. Of course, this does not imply that they are left invariant by the transformations generated by the $\hat{J}_v$ or by the collective transformations generated by the operators $\hat{I}_v$ separately.

In practical cases it is easier to work with the constraints f_v. However, since the constraints F_v are in involution (i.e., they commute among themselves) they are useful for demonstration purposes (cf., for instance, subsection 4.2). For any physical operator acting on $\mathcal{H}_2$ (i.e., an operator that maps physical states into physical states) it can be seen that

$$[\hat{O}_{ph}, \hat{F}_v] \simeq 0 \tag{3.9}$$

$$[\hat{O}_{ph}, \hat{f}_v] \simeq 0 \tag{3.10}$$

The symbol $\simeq$ means that the l.h.s. vanishes if applied to physical states.

As in the classical treatment, we can impose the constraints (3.6) by further enlarging the Hilbert space as follows: we add k new variables Ω_v, their associated momenta P_v and the corresponding operators $\hat{\Omega}_v$ and $\hat{P}_v$ The constraints (3.6) are dynamically satisfied by the new hamiltonian $\hat{\tilde{H}}$

$$\hat{\tilde{H}} \simeq \hat{H} - \Omega_v \hat{f}_v \tag{3.11}$$

[11] The minus sign in the commutation relations for the I_v is obtained through a quantal transcription of the procedure followed in appendix 2.B

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with new primary constraints

$$\hat{P}_v|ph>=-i\frac{\partial}{\partial\Omega_v}|ph>=0 \tag{3.12}$$

where the functions in the enlarged Hilbert space $\mathcal{H}_3$ depend on q_i, ϕ_v and Ω_v. The new hamiltonian preserves the original dynamics for physical states (i.e., for those states that satisfy the constraint (3.6)). Physical operators in $\mathcal{H}_3$ also satisfy

$$[\hat{O}_{ph}, \hat{P}_v] \simeq 0 \tag{3.13}$$

The Hilbert spaces $\mathcal{H}_1$, $\mathcal{H}_2$ and $\mathcal{H}_3$ are seen to be the quantal counterpart of the phase spaces $\mathcal{F}_1$, $\mathcal{F}_2$ and $\mathcal{F}_3$ (cf. subsection 2.3). The constraints (3.5), (3.6) and (3.12), are also the quantal versions of the constraints (2.66) and (2.85). They tell us that only a subspace of the enlarged Hilbert spaces $\mathcal{H}_2$ and $\mathcal{H}_3$ is relevant, the one annihilated by them. In appendix 3.B and section 4 we show two different formalisms that enable us to operate in these spaces. For this purpose we must impose the quantal versions of the gauge conditions (2.78).

Finally, it is useful to rewrite these results in the laboratory frame using the transformation (3.3). The laboratory version of the constraints (2.66) and (2.85) read:

$$\begin{aligned}
\hat{F}^v_v|ph'>&=-\hat{p}'_v|ph'>=i\frac{\partial}{\partial\phi_v}|ph'>=0\\
\hat{f}'_v|ph'>&=-\eta_{wv}\hat{p}'_w|ph'>=i\eta_{wv}\frac{\partial}{\partial\phi_w}|ph'>=0\\
\hat{P}_v|ph'>&=-i\frac{\partial}{\partial\Omega_v}|ph'>=0
\end{aligned} \tag{3.14}$$

whose meaning is clear: in the laboratory frame the physical wave functions of $\mathcal{H}_3$ are independent of the variables ϕ_v, Ω_v.

Eqs. (3.10) and (3.13) take the form:

$$[\hat{O}'_{ph}, \hat{F}'_v] \simeq [\hat{O}'_{ph}, \hat{f}'_v] \simeq i\frac{\partial}{\partial\phi_v}\hat{O}'_{ph} \simeq 0 \tag{3.15}$$

$$[\hat{O}'_{ph}, \hat{P}'_v] \simeq -i\frac{\partial}{\partial\Omega_v}\hat{O}'_{ph} \simeq 0 \tag{3.16}$$

3.2 The inner products

The inner product associated with the original variables q'_i in the Hilbert space $\mathcal{H}_1$ is given ab initio and we are not free to alter it. However, when we extend the space $\mathcal{H}_1$ to construct $\mathcal{H}_2$ and $\mathcal{H}_3$, we are introducing artificial dependencies of wavefunctions on the parameters ϕ_v, Ω_v. The definition of the inner products in $\mathcal{H}_2$ and $\mathcal{H}_3$ is to a large extent arbitrary, and we only need to require that

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for physical functions (those which satisfy the constraints) the overlaps coincide with the original ones in $\mathcal{H}_1$.

The measure is most easily constructed in the laboratory frame, in which it takes the product form. Given the overlap of two functions Ψ'_1, Ψ'_2 in the original space $\mathcal{H}_1$

$$\int \Psi_1^{*'} \Psi'_2 \, d\mu(q_i) \tag{3.17}$$

we extend it to functions in $\mathcal{H}_2$ in the product form

$$\int \Psi_1^{*'} \Psi'_2 \, d\mu(q_i) \, d\mu_\phi \tag{3.18}$$

In order to define the measure $d\mu_\phi$ we also require: i) that the operators $\hat{\phi}_v$ be hermitean (and thus that the transformation (3.2) is unitary) and ii) that the constraint operators be hermitean. This can be enforced either for the constraints $\hat{F}_v$ (eq.(3.5)) or for the $\hat{f}_v$ (eq.((3.6))). Thus the measure $d\mu_\phi$ associated with the collective coordinates ϕ_v depends on the choice of the set of constraints.

For the constraints $\hat{F}_v$ we define the measure as the simple product [12]

$$d\mu_\phi^{(F)} = \Pi_v d\phi_v \tag{3.19}$$

With this definition the operators $\hat{\phi}_v$, $\hat{P}_v$ and $\hat{F}_v$ are hermitean.

In the case of the constraints $\hat{f}_v$, we define the measure following the usual prescription for the rotational case [13]

$$d\mu_\phi^{(f)} = |\varsigma| \, \Pi_v d\phi_v \tag{3.20}$$

where $|\varsigma|$ denotes the determinant $det[\varsigma_{vw}]$. We show in appendix 3.A that the $\hat{f}_v$ (or, equivalently, the $\hat{I}_v$) are hermitean with respect to this measure.

At this point we notice that physical wavefunctions in $\mathcal{H}_2$ (which are independent of ϕ_v) have infinite norm. This is characteristic of gauge invariant systems. The problem can be cured within $\mathcal{H}_2$ by redefining the overlaps suitably. We outline this procedure in appendix 3.B. It will take us close to the treatment in the "Coulomb gauge" of section 5. However in these notes we emphasize the procedure discussed in section 4, where we proceed by further enlarging the Hilbert space.

We now go on to define the overlap associated with the coordinates Ω_v. Since the operators $\hat{P}_v$ commute among themselves (as well as with the constraint

[12] In these inner product, the integrals extend from $-\infty$ to ∞ (cf. the footnote on p.25).

[13] In the Euler parametrization of the rotational case

$$|\varsigma| = sin\beta$$

is the familiar factor appearing in the measure associated with the Wigner functions D^I_{MK} [20]

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operators $\hat{F}_v$ and $\hat{f}_v$) we discuss first the case of a single coordinate Ω. We construct the operators

$$\begin{aligned} \Gamma_\Omega &= \frac{1}{\sqrt{2}}(\hat{\Omega} + i\hat{P}) = \frac{1}{\sqrt{2}}(\Omega + \frac{\partial}{\partial\Omega}) \\ \Gamma_\Omega^\dagger &= \frac{1}{\sqrt{2}}(\hat{\Omega} - i\hat{P}) = \frac{1}{\sqrt{2}}(\Omega - \frac{\partial}{\partial\Omega}) \end{aligned} \tag{3.21}$$

$$[\Gamma_\Omega, \Gamma_\Omega^\dagger] = 1 \tag{3.22}$$

We could construct a basis for the Hilbert space of the form

$$\begin{aligned} \psi_n^{(h.o.)} &= \frac{1}{\sqrt{n!}}(\Gamma_\Omega^\dagger)^n \psi_o^{(h.o.)} \\ \Gamma_\Omega \psi_o^{(h.o.)} &= 0 \\ < \psi_n^{(h.o.)} | \psi_m^{(h.o.)} > &= \delta_{nm} \end{aligned} \tag{3.23}$$

This basis corresponds to the usual inner product in configuration space

$$< g|h >= \int_{\Omega=-\infty}^{\Omega=\infty} g^*(\Omega) h(\Omega) d\Omega \tag{3.24}$$

According to ref. [23] it is possible to use such a (positively defined) metric in connection with these coordinates.

However, using the freedom that we have in the definition of operations in the unphysical space, we may introduce an indefinite metric already at this level. It turns out that this definition is very convenient both from the theoretical point of view (an equivalence is proved straightforwardly without problems of regularization) and from the practical point of view (the actual calculations are indeed simpler). We discuss this in further detail in the next section.

The rationale is that the "error" spuriously produced by enlarging the Hilbert space with the collective coordinate ϕ may be "cancelled" by the introduction of the Lagrange multiplier Ω[14].

$$\begin{aligned} |n_\Omega > &= \frac{1}{\sqrt{n!}}(\Gamma_\Omega)^n |0_\Omega > \\ \Gamma_\Omega^\dagger |0_\Omega > &= 0 \\ < n_\Omega | m_\Omega > &= (-1)^n \delta_{nm} \end{aligned} \tag{3.25}$$

Hence $\mathcal{H}_3$ has indefinite norm and is not a "Hilbert" but a "pseudo-Hilbert" space. Let us first explicitly construct this basis in the coordinate representation. The second of eqs. (3.25) implies

$$|0_\Omega >= exp|\Omega^2/2| \tag{3.26}$$

[14]This is the case in electromagnetism where an indefinite metric for the photon associated with the Lagrange multiplier is used [22].

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and thus

$$|n_\Omega >= \frac{1}{\sqrt{n!}}(\Omega + \frac{\partial}{\partial \Omega})^n |0_\Omega >= (-i)^n \psi_n^{(h.o.)}(i\Omega) \tag{3.27}$$

The inner product associated with (3.25) can be written, in coordinate representation,

$$\begin{aligned} < g|h > &= -i \int_{\Omega=-i\infty}^{\Omega=i\infty} [g(-\Omega)]^* h(\Omega) d\Omega \\ &= \int_{\tau=-\infty}^{\tau=\infty} [g(-i\tau)]^* h(i\tau) d\tau \end{aligned} \tag{3.28}$$

where $\Omega = i\tau$ and the conjugation applies both to the constants defining the function g and to the argument. In (3.28) Ω should be regarded as imaginary and τ as real, since the integration path is taken to be the imaginary axis in Ω. It is straightforward to show that this inner product satisfies the requirement that $\hat{\Omega}$ and $\hat{P}$ should be hermitean. This measure is implicitly used in refs. [9,15,16].

Finally, we obtain for the inner product of wavefunctions in $\mathcal{H}_3$ (laboratory frame)

$$\begin{aligned} < \Psi_1' | \Psi_2' >_{\mathcal{H}_3}^{(F)} &= (-i)^k \int_{\Omega_v=-i\infty \; \phi_v=-\infty}^{\Omega_v=i\infty \; \phi_v=\infty} \Pi_v \, d\Omega_v \, d\phi_v \, d\mu(q_i') \\ & \quad [\Psi_1'(-\Omega_w, \phi_w, q_i')]^* \Psi_1'(\Omega_w, \phi_w, q_i') \end{aligned} \tag{3.29}$$

$$\begin{aligned} < \Psi_1' | \Psi_2' >_{\mathcal{H}_3}^{(f)} &= (-i)^k \int_{\Omega_v=-i\infty \; \phi_v=-\infty}^{\Omega_v=i\infty \; \phi_v=\infty} |\varsigma| \, \Pi_v \, d\Omega_v \, d\phi_v \, d\mu(q_i') \\ & \quad [\Psi_1'(-\Omega_w, \phi_w, q_i')]^* \Psi_1'(\Omega_w, \phi_w, q_i') \end{aligned} \tag{3.30}$$

With the overlaps $< \; | \; >_{\mathcal{H}_3}^{(F)}$ and $< \; | \; >_{\mathcal{H}_3}^{(f)}$ the constraints $\hat{F}_v$ and $\hat{f}_v$ are hermitean, respectively.

The problem of infinities in the overlaps of physical wavefunctions is solved in the next section through a further enlargement of the space.

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appendix 3.A The hermiticity properties of operators using the measure associated with the constraints f_v

To prove the hermiticity of f_v we must show that

$$\int h^{*\prime}(\eta_{wv}\frac{\partial}{\partial\phi_w})g'\ d\mu_\phi^{(f)} = -(\int g^{*\prime}(\eta_{wv}\frac{\partial}{\partial\phi_w})h'\ d\mu_\phi^{(f)})^* \tag{3.31}$$

for every g', h' in the lab frame (cf. the second of eqs. (3.14)). Assuming that surface terms vanish, eq.(3.31) requires

$$\frac{\partial}{\partial\phi_w}(|\varsigma|\ \eta_{wv}) = 0 \tag{3.32}$$

Eq. (3.32) is equivalent to

$$\begin{aligned} 0 &= \eta_{wv,w} + \eta_{wv}\frac{\partial ln|\varsigma|}{\partial\phi_w} \\ &= \eta_{wv,w} + \eta_{wv}\frac{\partial ln|\varsigma|}{\partial\varsigma_{rs}}\varsigma_{rs,w} \end{aligned} \tag{3.33}$$

Using the expression for the derivative of a logarithm of a determinant

$$\begin{aligned} 0 &= \eta_{wv,w} + \eta_{wv}\eta_{sr}\varsigma_{rs,w} \\ &= \eta_{wv,w} - \eta_{wv}\varsigma_{rs}\eta_{sr,w} \end{aligned} \tag{3.34}$$

Applying eq. (2.122) we obtain

$$\begin{aligned} 0 &= \eta_{wv,w} - \eta_{sv,w}\eta_{wr}\varsigma_{rs} + c_{rvw}\eta_{sw}\varsigma_{rs} \\ &= \eta_{wv,w} - \eta_{sv,s} + c_{rvr} \end{aligned} \tag{3.35}$$

which is an identity since we have assumed that the c_{vws} are completely antisymmetric.

appendix 3.B An internal product for the Hilbert space $\mathcal{H}_2$

In order to construct an inner product that is suitable for the treatment in $\mathcal{H}_2$ (without further extensions) we have to modify (3.18) so that it remains finite and agrees for physical states with the internal product in $\mathcal{H}_1$. Such an extension is straightforward in the laboratory frame

$$< \Psi_1'|\Psi_2' >= \int \Pi_i\Pi_v d\mu(q_i')d\phi_v\Psi_1^*(q_i')\Psi_2(q_i')\delta(\phi_v) \tag{3.36}$$

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