Gauge fields in the separation of rotations and internal motions in the *n*-body problem

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The problem of separating rotations from internal motions in systems such as macroscopic flexible bodies, atoms, molecules, nuclei, and solar systems is an old one, with many applications in physics, chemistry, and engineering. A new element, however, which has not been appreciated until fairly recently, is the existence of certain gauge fields on the reduced configuration space for such systems. These (non-Abelian) gauge fields arise in the ''falling cat'' problem, in which changes in shape induce changes in external orientation; but they also have a dynamical significance, and enter as gauge potentials in the Lagrangian or Hamiltonian describing the internal or reduced dynamics. Physically these gauge fields represent Coriolis effects. This review concentrates on the case of nonrelativistic, *n*-body systems not subject to external torques, and develops the gauge theory of rotations and internal motions in detail. Both classical and quantum treatments are given. The gauge theory is developed from the standpoint of classical, coordinate-based tensor analysis; more abstract mathematical notation is generally not used, although the basic geometrical ideas of fiber-bundle theory are developed as needed. Certain old results, such as the Wilson-Howard-Watson Hamiltonian of molecular physics, are examined from a gauge-theoretical standpoint; and several new results are presented, including field equations of the Kaluza-Klein type satisfied by the gauge fields, and geometrical interpretations of the Eckart frame.
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I. INTRODUCTION

Systems of n particles such as isolated atoms, molecules, nuclei, and solar systems possess $3n$ degrees of freedom, of which three can be eliminated on the basis of translational invariance, and two more on the basis of rotational invariance. Although the rotation group is three-dimensional, it allows only the elimination of two degrees of freedom, due to its non-Abelian character. An exception to these rules is the special case of vanishing total angular momentum when $n \geqslant 3$, in which case rotational invariance allows the elimination of three degrees of freedom. Another exception is the case $n=2$, which is the elementary case of central force motion. These rules hold in both classical and quantum mechanics. After the allowed number of degrees of freedom have been eliminated, we are left with a reduced system representing the intrinsic or internal dynamics of the original system; in addition, it is possible to specify methods for reconstructing the original dynamics from the reduced dynamics.

For example, a three-body system such as the earth-moon-sun system or the helium atom possesses nine de-

grees of freedom, of which five can be eliminated in the case of nonvanishing angular momentum ($\mathbf{L} \neq 0$), leaving a reduced system of four degrees of freedom. The remaining four degrees of freedom are heterogeneous: three describe the evolution of the "shape" of the three-body system, i.e., the shape of the triangle formed by the three bodies, and the fourth describes the evolution of the angular momentum vector in a body frame, much as in rigid-body theory. But if $\mathbf{L}=0$, then the angular momentum degree of freedom drops out, and we are left with only three shape degrees of freedom. The situation for other numbers of particles ($n \geqslant 3$) is similar.

In this review we shall be concerned with nonrelativistic systems of the kinetic-plus-potential type. Our central problem will be to carry out the explicit elimination of those degrees of freedom which can be eliminated on the basis of translational and rotational invariance, and to reveal the structure possessed by the reduced system. This problem is an old one, with a history that dates back at least to the eighteenth century, but a relatively new element, due to Guichardet (1984), Tachibana and Iwai (1986), Iwai (1987a, 1987b, 1987c), and Shapere and Wilczek (1989a, 1989b), is the realization that certain gauge fields play an important role in the reduction process and in the description of the reduced dynamics. Physically, the gauge fields in question represent Coriolis forces, and the associated gauge conventions and gauge transformations are connected with the definition and redefinition of body frames. The notion that the internal dynamics of n-body systems is a gauge theory is a new one in the applied literature of physics, chemistry, and engineering, and it has wide-ranging implications for the understanding of such systems.

The history of this problem goes back at least to Lagrange and Jacobi, who found a coordinate transformation, "the elimination of the nodes," which eliminates the ignorable degrees of freedom in n-body gravitational systems. This work is described by Whittaker (1960), who gives references to the early literature. A more modern treatment of the elimination of the nodes has been presented by Deprit (1983), who uses a sequence of canonical transformations.

After the invention of quantum mechanics, n-body problems in atomic, molecular, and nuclear physics, especially the problem of molecular vibrations and rotations, gave new impetus to the study of the elimination of ignorable degrees of freedom in systems with rotational invariance. Molecules are n-body systems with several special features, including the adiabatic separation of rotational and vibrational time scales, the fact that n may not be small, and the fact that the interactions between the atoms are not truly described by potential energies because the atoms are composite particles (that is, molecular theory is part of the Born-Oppenheimer approximation scheme). These and other special demands of the problem of molecular vibrations, such as the requirement due to Casimir (1931) that the Coriolis coupling terms in the Hamiltonian be as small as possible, led Eckart (1935) to formulate the "Eckart frame," which is a particular convention for the assignment of body frames as a field over the shape space of a molecule. A vast amount of literature on molecular theory has since that time been constructed around Eckart's conventions; these conventions have been reviewed and reappraised by Louck and Galbraith (1976), Biedenharn and Louck (1981), and Ezra (1982).

When the amplitude of vibrations is large, or when the very concept of vibrations is not appropriate (as in problems in celestial mechanics or atomic physics), other techniques are called for. The large literature on the separation of rotations and internal motions in three-body atomic and molecular problems falls into this area. Many of the papers on the three-body problem differ from one another in the conventions adopted for body frame, assigned as a field over shape space. In addition, there are different choices made for coordinates on shape space. Papers in this area include those of Breit (1930), Smith (1960, 1962), Bhatia and Temkin (1964), Dragt (1965), Zickendraht (1965), Meyer and Günthard (1968), De Celles and Darling (1969), Pickett (1972), Mead and Truhlar (1979), Johnson (1980, 1983a, 1983b), Tennyson and Sutcliffe (1982), Sutcliffe and Tennyson (1986, 1991), and Pack and Parker (1987). There are many others we could mention.

Of course, the role of symmetry and ignorable coordinates in classical mechanics is a subject found in all textbooks. A notable example is the book by Sudarshan and Mukunda (1974), which deals with the differential geometry of group manifolds and phase space in coordinate language. Beginning in the 1970s, certain mathematicians, including Smale, Marsden, and Weinstein, began to apply geometric methods to the problem of reducing classical Hamiltonian systems with continuous symmetries, of which the n-body problem with rotational symmetry is a special case. This work is laid out in detail and anterior references are given in the book by Abraham and Marsden (1978). The theory of "reduction" as worked out by these authors is a geometrical one, in which the differential geometry of group manifolds is coupled with that of Hamiltonian phase space (symplectic manifolds), and the natural geometrical structures involved in constructing the reduced phase space and the reduced Hamiltonian are identified. For example, it turns out that the reduced phase space is a certain quotient space of a certain subspace of the original phase space.

The reduction theory of Abraham and Marsden is general, and makes few assumptions other than the existence of a continuous symmetry group which leaves the Hamiltonian invariant and which acts on phase space by means of canonical transformations. On the other hand, in the case of the n-body systems that are of interest in this review, the symmetry groups (translations and rotations) act on configuration space. This action can be lifted into phase space, but it is more natural and physically immediate to think of these groups as acting primarily on configuration space. This fact alone imposes on configuration space the structure of a principal fiber bundle (for $n \geqslant 3$), which in turn is endowed with a connection by the kinetic energy, regarded as a

metric on configuration space. Thus, as classical Hamiltonian systems with symmetry go, there are several special features of the n-body system with translational and rotational invariance, including the bundle structure of configuration space and the existence of a gauge potential on the reduced configuration space (or "shape space"). Not all of these features of n-body dynamics were explicitly acknowledged in the early work on reduction theory, although it seems that by the early 1980s certain mathematicians such as Kummer (1981) had recognized the importance of gauge fields in the n-body problem.

On the other hand, it is possible to "discover" these gauge fields and the associated bundle structure from simple kinematical arguments based in configuration space, without starting with the more general and more abstract phase-space theory and specializing it. Furthermore, these gauge fields have a simple physical interpretation, which can be understood in terms of elementary notions of conservation of angular momentum and the rotations generated by deformable bodies with changing shapes. This was the approach taken by Guichardet (1984), who dealt with the kinematics of deformable bodies such as molecules and falling cats. The same discovery was made independently by Shapere and Wilczek (1989a, 1989b), evidently as a by-product of their more substantial work on the gauge theory of the locomotion of objects such as microorganisms in a viscosity-dominated medium (Shapere and Wilczek, 1987, 1989c, 1989d).

What is particularly remarkable about these developments is the manner in which the entire structure of nontrivial connections on non-Abelian fiber bundles emerges from elementary mechanical considerations. This is much as in the various examples of "Berry's phase" (Berry, 1984; Shapere and Wilczek, 1989a; Zwanziger, Koenig, and Pines, 1990; Mead, 1992), in which fiber bundles with connections are found in various applications. Nevertheless, the gauge theory of n-body systems with rotational symmetry is an especially rich example.

The investigations begun by Guichardet were taken up and extended to cover dynamical considerations, in both classical and quantum mechanics, by Tachibana and Iwai (1986) and Iwai (1987a, 1987b, 1987c). It is this tradition that we follow in this review, mainly because of its mathematical simplicity, and we shall not have much to say about the more general phase-space theory of Abraham and Marsden. Nevertheless, the latter theory is essential for more sophisticated applications and for a deeper understanding of n-body systems.

A similar story could be told about quantum systems with symmetry. Of course, the application of group theory in quantum mechanics is a standard subject, in which a symmetry group allows one to block-diagonalize a Hamiltonian. But the standard theory makes little or no distinction between symmetry groups that can be viewed as acting on configuration space, and those that cannot, nor does it acknowledge the gauge fields that arise on the reduced configuration space in n-body systems. In fact, there is a close parallel between classical and quantum n-body systems in this regard, so that those who are interested only in quantum applications are advised to study the corresponding classical systems as well. This is the philosophy adopted in this review, which deals with both classical and quantum applications.

In recent years, the gauge theory of classical dynamical systems with rotational symmetry has continued to attract the attention of mathematicians, who have been especially interested in problems of control, bifurcations, stability, and phases. An informal overview of this work has been given by Enos (1992), while a deeper presentation, including a discussion of many new problems, is contained in the book by Marsden (1992). Montgomery (1991, 1993) has dealt especially with issues of control. A newer basic reference, covering the theory of reduction from a more up-to-date standpoint than Abraham and Marsden (1978) is Marsden and Ratiu (1994). A conference has recently been held on the falling cat and related problems, and one can get a sense of the current status of mathematical investigations in this area by examining the proceedings (Enos, 1993).

The falling cat is an attractive problem to keep in mind in our later discussion of the gauge theory of systems with rotational symmetry. This problem is the following. Everyone knows that if a cat is released upside down with zero angular momentum, it nevertheless manages to land on its feet. Since the cat cannot generate external torques by scratching the air, how does it manage to turn itself over? Obviously the answer must depend on the fact that the cat is a flexible body, since for a rigid body we would have $\mathbf{L}=\mathsf{M}\boldsymbol{\omega}$ ($\mathbf{L}$ is the angular momentum, M is the moment of inertia tensor, and $\boldsymbol{\omega}$ is the angular velocity), so that $\mathbf{L}=0$ would imply $\boldsymbol{\omega}=0$. In fact, the cat, which begins with its feet pointing up and ends with them on the ground, manages to bring about a 180° rotation of its orientation relative to an inertial frame by twisting and contorting its body. Although the shape of the cat, i.e., the positions of the different parts of its body relative to one another, is approximately the same at the initial and final times, nevertheless at intermediate times the cat has deformed its shape in various ways. One can view this process geometrically by saying that the cat has traced out a cycle or closed loop in its "shape space."

There is a long literature on the falling cat and related problems. Only recently has the role of gauge fields been appreciated in such problems, but the earlier literature does deal with the basic physics and specific applications. An elementary discussion of the physics of somersaulting and twisting, with photographs of actual cats and diagrams of human bodies, has been given by Frohlich (1980); at a more sophisticated level, Kane and Scher (1969) developed specific mechanical models to represent falling cats and compared their predictions with observations of real cats, taken in part from photographs which are reproduced in their article. These authors also surveyed some earlier literature, in which cruder models had been studied. At a similar level,

Frohlich (1979) studied the physics of springboard divers, trampolinists, gymnasts, and astronauts, and made an effort to provide realistic models for them. More recently, Montgomery (1993) has returned to the model of Kane and Scher (1969) and provided a detailed analysis of it from a gauge-theoretical standpoint.

The purpose of this review is to fill the gap between the modern, more mathematical literature on gauge theories and geometric methods in general and the older, more applied literature on the n-body problem in physical applications. The more mathematical literature has the shortcoming that it does not take into account the many practical considerations that arise in physical applications, nor does it give due regard to the language, tradition, and points of view which have developed over the years in such applications. For example, it seems that no one has heretofore given a proper geometrical interpretation of the Eckart frame, which is commonly used in studies of small-amplitude vibrations of flexible systems. On the other hand, the applied literature has the drawback that it does not make use of natural and proper mathematical tools for understanding and for performing calculations in the n-body problem, which are essentially those of differential geometry and topology. To a certain extent, one can get by without these mathematical tools, especially in specialized contexts, such as that of the three-body problem or the problem of small-amplitude vibrations. But modern applications are moving into more complicated areas, in which the need for the new methods is more critical. For example, it is now becoming feasible to perform computer calculations on the quantum four-body problem, for which it is necessary to think with some clarity in terms of higher-dimensional, abstract spaces. Even for simpler problems, current practice often has the appearance of black magic to those outside the field, since the fundamental structure and organization of the subject are not made clear in the traditional treatments in textbooks and review articles.

A second and related purpose concerns the interplay between analytical and geometrical methods in physical problems such as the n-body problem. The traditional methods of mathematical physics (differential equations, group theory, etc.) have been analytical, but in recent times geometrical methods have been assuming a greater importance. The power and depth of geometrical methods were first appreciated in such fields as relativity theory and particle physics, but more recently they have been discovered to be relevant in other areas as well. (This is the significance of the phenomenon of ''Berry's phase,'' which has already had quite an impact on atomic and molecular physics in contexts quite distinct from those covered in this review.) At their simplest level, geometrical methods do not necessarily involve any specifically geometrical picture, but rather invoke the analytical methods of tensor analysis to describe essentially geometrical realities. For example, in the n-body problem, the fact that a choice of a body frame is an arbitrary convention upon which no physical results can depend leads to a systematic investigation of how various quantities transform under a redefinition of body frame (a gauge transformation, in the language of this review), and to a systematic search for methods of constructing gauge-invariant and therefore physically meaningful quantities. In spite of the venerable history of the n-body problem, this perspective and program of investigation are entirely new, at least in the applied literature.

At a deeper level, specifically geometrical notions become important. The following are some of the geometrical constructions pertaining to the n-body problem which are discussed in this review: the foliation of configuration space into fibers or orbits under the action of rotations (essentially a geometrical interpretation of orientational and internal coordinates); the notion of horizontal and vertical subspaces and their role in the block diagonalization of the kinetic energy; the gauge potential, parallel transport, holonomy, and their role in the generation of rotations by changes in shape; the geometrical representation of a convention for a body frame in terms of a section of the fiber bundle; the clear distinction between changes in shape coordinates and changes in body frame; the description of the Eckart frame in terms of a section that is a Euclidean vector subspace of configuration space; the introduction of covariant derivatives and their use in both the classical equations of motion and the commutation relations for quantum operators; and the nontriviality of the connection, and its implication for the impossibility of transforming away the Coriolis couplings in the Hamiltonian. All these notions are almost entirely new in the applied literature on the n-body problem.

The mathematical background required for this review is basic differential geometry, at the level of Weinberg (1972) or track 1 of Misner, Thorne, and Wheeler (1973). We use the notation of classical tensor analysis in a coordinate-based approach as much as possible, although the discussion gradually becomes more geometrical as we proceed. We assume no background in fiber-bundle theory or gauge theories, and we develop the necessary tools as needed. Those who are familiar with gauge theories, either in field-theoretic applications or in a purely mathematical context, will be able to skip certain parts of this article but will probably find the specific application at hand to be interesting and revealing. Those who are not familiar with gauge theories will find the examples worked out in this article to be useful, since it illustrates most of the features which occur in any application, and since many of the mathematics books on fiber bundles and gauge theories are short on concrete examples. This article is based on a series of lectures given at the University of Chicago in 1994; it is pedagogical, and is mainly intended for applications in engineering and atomic, molecular, and nuclear physics.

The outline of this article is as follows. We begin in Sec. II with some planar mechanical models, which illustrate the gauge potential and concepts such as shape space in the context of an SO(2) (Abelian) gauge theory. In Sec. III, we move on to the gauge kinematics of the n-body problem in three dimensions, first from a

coordinate-based point of view, as is traditional in the applied literature, and then from the standpoint of fiber-bundle theory. In this section we develop several basic concepts, such as the curvature form or Coriolis tensor, and the notions of holonomy and of gauge invariance and covariance. We illustrate these concepts with explicit calculations for the three-body problem. In Sec. IV, we transform the classical n-body Lagrangian and Hamiltonian to shape and orientational coordinates and discuss how the gauge potential enters into the results. We also discuss the classical equations of motion. In the process of carrrying out these calculations, we introduce the metric tensor on shape space and notions of covariant derivatives. We also transform the quantum Hamiltonian in Sec. IV, deriving in effect the Wilson-Watson-Howard Hamiltonian in a general gauge and system of shape coordinates. The reduced Hamiltonian incorporates the gauge potential, and is written in manifestly gauge-invariant (or covariant) form, unlike the usual expressions for this Hamiltonian. In Sec. V we present various miscellaneous results, including a set of field equations or identities satisfied by the various fields over shape space. There are several different classes of such field equations; one class consists of equations of the Kaluza-Klein type. We also discuss the Eckart conventions from a geometrical point of view. It is in Sec. V that most of our new results are reported. Finally, we present some conclusions in Sec. VI, as well as indications for future lines of investigation. We conclude with a series of appendices.

II. MODELS OF DEFORMABLE BODIES

In this section we present some simple models of deformable bodies to explain the physics of shape and orientational changes in such bodies. These models also provide an introduction to the gauge theory of deformable bodies, including the gauge potential, gauge transformations, the concept of shape space, and other notions.

Later, in Sec. III, we shall be interested in n bodies moving without constraints in three-dimensional space, but the models we deal with in this section are simpler in several respects. First, these models are two dimensional, in which the motion is confined to the x-y plane. Second, in these models one point of the deformable body will be fixed in an inertial frame, as if it were attached to a mass M much larger than any other mass in the system. We do this to freeze out the translational degrees of freedom, in order to concentrate on the more interesting rotational degrees of freedom. Finally, we shall constrain our masses in various ways by means of rigid rods.

In these two-dimensional models the rotations considered belong to the Abelian group SO(2). Abelian gauge theories are simpler in several respects than non-Abelian ones, such as the SO(3) gauge theory belonging to deformable bodies moving in three-dimensional space. For example, in an Abelian gauge theory, the integrals of the gauge potential along closed contours, which in the present examples represent changes in orientation, can be transformed via Stokes' theorem into surface integrals. This cannot be done in the case of non-Abelian gauge theories.

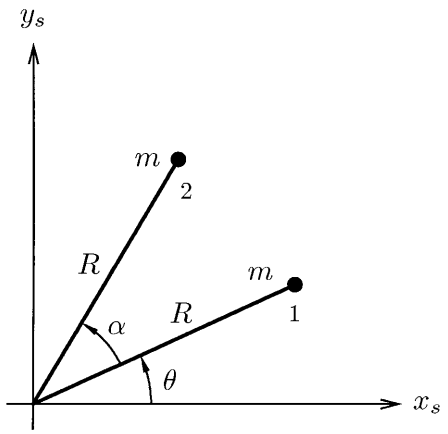

FIG. 1. A simple model of a flexible body consisting of two identical massless rods with equal masses m attached to their free ends, which are connected in a joint or hinge at their other ends. The hinge is pinned to the origin of an inertial frame.

A. Example: System of two rods

Our first example is an object consisting of two massless, rigid rods connected at one end in a joint or hinge, as illustrated in Fig. 1. The rods are of equal length R and have equal masses m attached to their free ends. The joint is pinned to the origin of an inertial frame, and the whole system is constrained to move in the x-y plane. The subscripts s on the x- and y-axis labels in the figure are a reminder that the frame is a "space" or inertial frame. We imagine that muscles or motors or other agents act at the joint to change the shape of the V-shaped assembly of rods by opening or closing the angle α; our only requirement is that these agents generate no external torques, so that the total angular momentum of the system is conserved (for example, frictional forces could be involved). This system is perhaps the simplest flexible body one can think of and serves as a simple model for a part of the cat's body.

The configuration of the two masses in Fig. 1 is specified by two angles, of which α, the opening angle of the V-shaped assembly, can be regarded as a *shape* coordinate, and θ, the angle between the space x axis and rod 1, can be regarded as an *orientational* coordinate. We regard two configurations as having the same shape if a rigid proper rotation of the whole system will take one into another; here we consider only rotations in the plane. Note that rigid rotations change θ while leaving the shape coordinate α fixed. Furthermore, we consider the two masses to be distinguishable, so that shape α is distinct from shape $2\pi-\alpha$ (they cannot be mapped into one another by a rotation in the plane). This means that α takes on all values between 0 and 2π, and shape space itself is a circle on which α is a coordinate.

The angular momentum of the system (z component only, since we are working in a plane) is

$$L_{sz}=m(x_{s1}\dot{y}_{s1}-y_{s1}\dot{x}_{s1})+m(x_{s2}\dot{y}_{s2}-y_{s2}\dot{x}_{s2}), \quad (2.1)$$

where (x_{s1},y_{s1}) and (x_{s2},y_{s2}) are the rectangular coordinates of the two masses and where we attach s subscripts to various quantities to emphasize that they are measured with respect to the space or inertial frame. (See Appendix A for a summary of conventions.) Thinking of the falling cat, we set $L_{sz}=0$ and multiply through by dt, to obtain the vanishing of a certain differential form,

$$x_{s1}dy_{s1}-y_{s1}dx_{s1}+x_{s2}dy_{s2}-y_{s2}dx_{s2}=0, \quad (2.2)$$

which implies constraints connecting the positions of the two masses and their infinitesimal increments under conditions of zero angular momentum.

It is convenient to transform Eq. (2.2) from the rectangular coordinates of the two masses to the shape and orientational coordinates α and θ. The transformation equations are

$$x_{s1}=R\cos\theta,\ \ x_{s2}=R\cos(\theta+\alpha),$$
$$y_{s1}=R\sin\theta,\ \ y_{s2}=R\sin(\theta+\alpha), \quad (2.3)$$

which, when substituted into Eq. (2.2), yield

$$d\theta=-\tfrac{1}{2}\,d\alpha. \quad (2.4)$$

This equation shows how a change in shape, represented by $d\alpha$ and carried out under conditions of vanishing angular momentum, results in a change in orientation, represented by $d\theta$. The physics is very simple, for as the angle α in Fig. 1 opens or closes while $L_{sz}=0$, the bisector of this angle remains constant, so half of the increment in α is taken up by rod 1, rotating clockwise, and half by rod 2, rotating counterclockwise.

But this model is too simple to explain how the cat can change its orientation by carrying its shape through a cycle, for if the V-shaped assembly of rods opens and closes, returning to its original shape, then the constancy of the bisector implies that θ will be the same at the end of the cycle as it was at the beginning. (Here we assume that the hinge does not turn through a complete rotation, i.e., that the closed path in shape space has a net winding number of zero around the circle.) The reason θ is the same after such a cycle of shape changes is that the right-hand side of Eq. (2.4) is a closed (locally exact) differential form, so that Eq. (2.4) can be integrated to give $\theta=-\frac{1}{2}\alpha+\text{const}$. Since θ is a function of α, if α goes through a closed cycle, then so does θ, and there is no net change in orientation. To generate changes in orientation from cycles in shape space, it is necessary to invoke a more complicated model.

Before leaving this model, however, we use it to make another point. It is convenient to regard the angle θ as the angle of a rotation which maps the space axes into a set of body axes. These body axes are labeled x_b, y_b in Fig. 2, with the body x axis lying along rod 1. But obviously there is nothing special about rod 1; we could just as well have defined a different set of body axes, such as

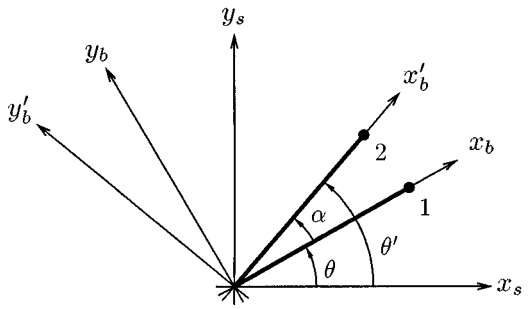

FIG. 2. The orientational angle θ, which can be thought of as the angle of the rotation connecting the space axes with a set of body axes. Alternative choices of body axes, indicated by a prime, are thought of as alternative gauge conventions.

the primed axes x_b', y_b' in the figure, which have the body x axis lying along rod 2. In this case the rotation connecting space with body axes is specified by a different angle θ', which is related to θ by

$$\theta'=\theta+\alpha. \quad (2.5)$$

We shall henceforth regard a convention for attaching a body frame to a flexible body as a *gauge convention*, and we shall regard a change in conventions as a *gauge transformation*. Thus Eq. (2.5) specifies a gauge transformation in this simple model. Since physical results cannot depend on an arbitrary convention, all physical results must be gauge invariant, although intermediate quantities useful in calculations need not be. Therefore we begin a program of examining the various quantities of our theory, to see how they transform under gauge transformations. For example, in our simple model, we see that the shape coordinate α is gauge invariant, since it does not depend on a convention for body frames. But the orientational coordinate θ is gauge dependent, as illustrated by Eq. (2.5).

B. Example: System of three rods

Next we examine a model in which shape space is two dimensional, which will allow us to see how cycles in shape give rise to changes in orientation. To this end, we add another massless rod to our system, as illustrated in Fig. 3. The three rods in the figure are all of equal length R and have equal masses m attached as shown. The system is still pinned to the origin of an inertial frame at one joint, but there is now a second joint where rod 2 connects with rod 3. The orientational coordinate is θ as before, but there are now two shape coordinates, α and β. The two-dimensional shape space can now be thought of as the square in the α-β plane, $0\leqslant\alpha,\ \beta<2\pi$, as shown in Fig. 4; more properly, since 2π increments in either α or β yield the same shape, the opposite sides of the square are identified, and shape space is a two-torus.

As before we study the angular momentum,

$$L_{sz}=m\sum_{i=1}^{3}(x_{si}\dot{y}_{si}-y_{si}\dot{x}_{si}), \quad (2.6)$$

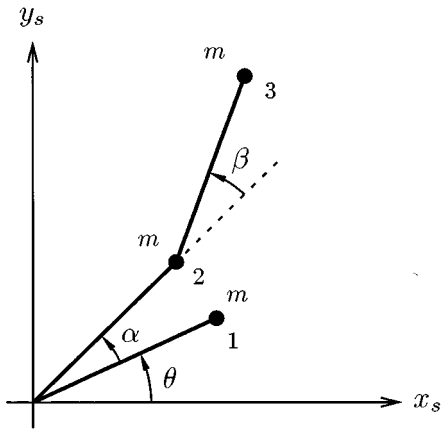

FIG. 3. A system of three rods yielding a two-dimensional shape space and illustrating how net changes of orientation result from cycles of deformation, i.e., closed loops in shape space.

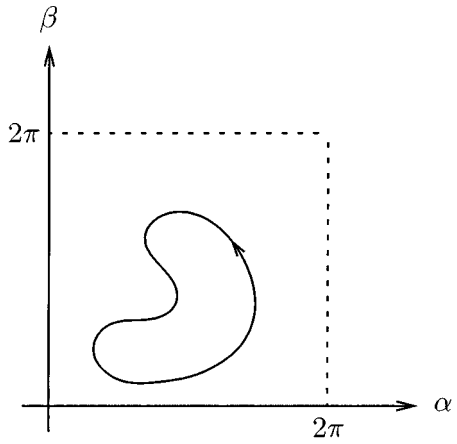

FIG. 5. Net change in orientation if the path in shape space is closed and contractible. The net change can be transformed via Stokes' theorem into an integral of the Coriolis tensor over the enclosed area.

and we transform the condition $L_{sz}=0$ from rectangular to shape and orientational coordinates. For the third mass we have

$$x_{s3}=R\cos(\theta+\alpha)+R\cos(\theta+\alpha+\beta),$$
$$y_{s3}=R\sin(\theta+\alpha)+R\sin(\theta+\alpha+\beta), \tag{2.7}$$

which is to be appended to Eqs. (2.3). Now the condition $L_{sz}=0$ is equivalent to the vanishing of a certain differential form,

$$(4+2\cos\beta)d\theta+(3+2\cos\beta)d\alpha+(1+\cos\beta)d\beta=0, \tag{2.8}$$

which we can solve for $d\theta$ to find

$$d\theta=-(A_\alpha d\alpha+A_\beta d\beta), \tag{2.9}$$

where

$$A_\alpha=\frac{3+2\cos\beta}{4+2\cos\beta}, \quad A_\beta=\frac{1+\cos\beta}{4+2\cos\beta}. \tag{2.10}$$

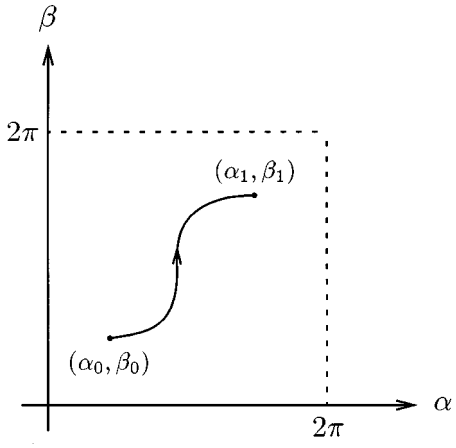

FIG. 4. Shape space for the three-rod system. Shape space can be thought of as a 2π square in the α-β plane, or as a two-torus on which α, β are coordinates. A sequence of shape deformations is represented by a path in shape space.

We regard (A_α,A_β) as two components of a vector potential, or *gauge potential*, considered as a field over shape space. The physical meaning of the gauge potential is given by Eq. (2.9): it specifies the linear mapping from infinitesimal changes in shape $(d\alpha,d\beta)$ to infinitesimal changes in orientation $(d\theta)$ under conditions of vanishing angular momentum. It is an accident of the example we are using that the components (A_α,A_β) depend on only the one shape coordinate β; more generally, the components of the gauge potential will depend on all the shape coordinates.

The effects of finite changes in shape can be obtained by integrating Eq. (2.9). Suppose that the shape of the three-rod system is carried from an initial shape (α_0,β_0) to some final shape (α_1,β_1) along a path or history in shape space specified by functions $(\alpha(t),\beta(t))$, as illustrated in Fig. 4. Then the net change in orientation is given by

$$\Delta\theta=-\int(A_\alpha d\alpha+A_\beta d\beta), \tag{2.11}$$

where the integral is carried along the path in question. Notice that the resulting angle $\Delta\theta$ is independent of the rate of traversal of the path, i.e., of its time parametrization. Thus one says that $\Delta\theta$ is "geometrical"; it is an example of a "geometrical phase" (Berry, 1984; Shapere and Wilczek, 1989a; Mead, 1992; Zwanziger, Koenig, and Pines, 1990). Note in addition that $\Delta\theta$ is independent of the nature of the forces that bring about the deformation of the flexible body, so long as they generate no external torques.

If the path is closed, as illustrated in Fig. 5, then the net change $\Delta\theta$ in orientation can be transformed by Stokes' theorem into an integral over the enclosed area:

$$\Delta\theta=-\oint(A_\alpha d\alpha+A_\beta d\beta)=-\int_{\text{area}}B\,d\alpha\,d\beta, \tag{2.12}$$

where B is the two-dimensional curl of the gauge potential (A_α,A_β),

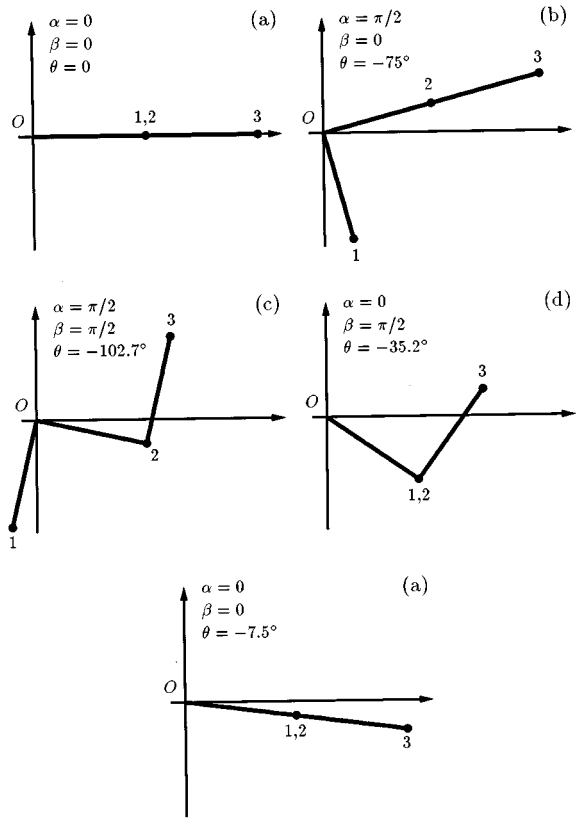

FIG. 6. The shape and orientation of the three-rod system on being taken around the square circuit in shape space shown in Fig. 7, moving from left to right and top to bottom. The labels a, b, c, and d correspond to the four corners of the square. In the final picture, the system has returned to the original shape, but the orientation has rotated by $-7.5°$.

$$B=\frac{\partial A_\beta}{\partial\alpha}-\frac{\partial A_\alpha}{\partial\beta}=\frac{\sin\beta}{2(2+\cos\beta)^2}. \tag{2.13}$$

The quantity B is the *field tensor* or *curvature form* for the example under consideration. These are generic terms, applicable to any gauge theory; but we shall also call B the *Coriolis tensor*, since, as we shall see, it is responsible for Coriolis forces in the reduced description of the n-body problem. In the present example, the Coriolis tensor B has only one component, but in other examples it is a multicomponent object.

In order to apply Stokes' theorem to a cycle in shape space as we have done, the closed path must be the boundary of some two-dimensional region, as is the path illustrated in Fig. 5. On a torus, a curve is a boundary if and only if it is contractable to a point, so for this example, Stokes' theorem can be used whenever the closed curve is contractable. But not all closed curves are contractable; for example, the path that consists of a 2π rotation in β while α is held fixed does not surround a region on the torus, nor can it be contracted to a point. Such topologically nontrivial paths are important in certain applications and lead to some interesting mathematics. In this section, however, we shall restrict attention to curves that are contractable.

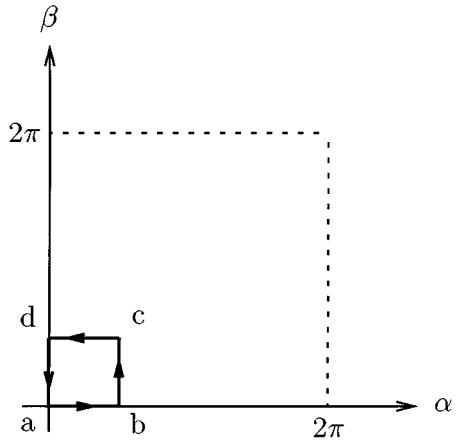

FIG. 7. A square circuit in shape space for the three-rod system whose shape and orientation are illustrated in Fig. 6.

To make the gauge potential and curvature form more vivid, we now consider a concrete example. We work with the three-rod system shown in Fig. 3, which we imagine is initially in the configuration given by $\alpha=\beta=0$, as illustrated in the first (upper left) picture in Fig. 6. In this configuration, the link $O1$ (O is the origin) lies on top of link $O2$, which as before is attached to link 23. We take this configuration through the sequence of shape changes, $(\alpha,\beta)=(0,0)\rightarrow(\pi/2,0)\rightarrow(\pi/2,\pi/2)\rightarrow(0,\pi/2)\rightarrow(0,0)$, which brings the system back to the original shape. The path in shape space is the small square of side $\pi/2$ illustrated in Fig. 7. The four corners of the square are labeled a, b, c, and d, which correspond to the labels of the five pictures in Fig. 6; these pictures illustrate the shape and orientation of the system as the shape is carried around the path in shape space. We assume as always that the changes in shape are effected by agents that conserve angular momentum.

In the first leg, $a\rightarrow b$, the angle α opens to $\pi/2$, but the angle β is fixed at 0, so the arm $O23$ remains straight. Because the moment of inertia of the arm $O23$ is five times that of the arm $O1$, the opening angle of $\pi/2$ is split in a 5:1 ratio by the two arms. As a result, at point b in shape space the angle θ is $-75°$. Equivalently, according to Eq. (2.11) we have

$$\Delta\theta=-\int_0^{\pi/2}A_\alpha d\alpha=-\frac{5\pi}{12}=-75°, \tag{2.14}$$

since $\cos\beta=1$. On the second leg, $b\rightarrow c$, the angle β opens to $\pi/2$, while α is held fixed at $\pi/2$. To conserve angular momentum, the arm $O1$ rotates backwards by the amount

$$\Delta\theta=-\int_0^{\pi/2}A_\beta d\beta=-\frac{\pi}{4}+\frac{\pi}{6\sqrt{3}}=-27.7°. \tag{2.15}$$

On the third leg, $c\rightarrow d$, the angle α closes again, causing arm $O1$ to rotate forward by

$$\Delta\theta=-\int_{\pi/2}^{0}A_\alpha d\alpha=\frac{3\pi}{8}=67.5°, \tag{2.16}$$

since $\cos\beta=0$ on this leg. Finally, in the last leg, $d\to a$, arm $O23$ straightens out again and arm $O1$ rotates forward by

$$\Delta\theta=-\int_{\pi/2}^{0}A_\beta d\beta=27.7^\circ. \tag{2.17}$$

Adding these up, we find a total rotation $\Delta\theta$ of -7.5°, which is clear in the final picture of Fig. 6. Equivalently, we can compute this angle from the curvature form,

$$\Delta\theta=-\int_0^{\pi/2}d\alpha\int_0^{\pi/2}d\beta\frac{\sin\beta}{2(2+\cos\beta)^2}=-7.5^\circ. \tag{2.18}$$

Next we consider the effect of gauge transformations in the three-rod system. Again, the orientational coordinate θ is the angle of the rotation mapping the space frame to a body frame; thus the body x_b axis lies along rod 1 in Fig. 3, and the body y_b axis is perpendicular to it (body axes are not shown in the figure). A new body frame (x_b',y_b') can be specified in many ways; in general, the angle ψ specifying the rotation that takes the old (unprimed) body frame into the new (primed) body frame is allowed to be a function of the shape coordinates, $\psi=\psi(\alpha,\beta)$. For example, if we place the x_b' axis, say, parallel to the third rod, or bisecting the angle β, we shall see the necessity of allowing ψ to depend on both α and β. Thus the orientational coordinate transforms according to

$$\theta'=\theta+\psi(\alpha,\beta), \tag{2.19}$$

which is a generalization of Eq. (2.5). The fact that ψ is allowed to be a function of shape coordinates is what qualifies the gauge transformations as "local" and gives the theory most of its interesting structure.

To find the transformation law for the gauge potential (A_α,A_β) itself under a gauge transformation, we combine Eqs. (2.19) and (2.9) to obtain

$$A_\alpha'=A_\alpha-\frac{\partial\psi}{\partial\alpha},\quad A_\beta'=A_\beta-\frac{\partial\psi}{\partial\beta}. \tag{2.20}$$

Thus the old and new gauge potentials differ by the shape-space gradient of the angle ψ. But the Coriolis tensor B is gauge invariant,

$$B'=B, \tag{2.21}$$

since the curl of the gradient vanishes.

When a flexible body changes it orientation by deforming its shape, we naturally want to know by how much the orientation has rotated. But the answer is not gauge invariant unless the curve in shape space representing the history of deformations is closed. For if the curve is open, as in Fig. 4, then from Eqs. (2.11) and (2.20) we find the transformation law,

$$\Delta\theta'=\Delta\theta+\psi_1-\psi_0, \tag{2.22}$$

where ψ_0 and ψ_1 are the values of ψ at the end points of the curve. Thus $\Delta\theta$ is gauge dependent for an open curve. But if the end points should coincide, so that $\psi_0=\psi_1$, then we have $\Delta\theta'=\Delta\theta$, and $\Delta\theta$ is gauge invariant. For closed curves that bound a region, the same conclusion follows by integrating the invariant Coriolis tensor $B=B'$ over the enclosed area, as in Eq. (2.12).

Thus it makes no sense to ask, "How much has the system rotated?" when the system is carried along an open path in shape space, because the answer depends on our convention for body frames. This question only makes sense for closed paths. The trouble with open paths is that the body frames that are attached to the system at the (different) initial and final shapes can be redefined independently of one another under a gauge transformation, and therefore the rotation of one frame relative to the other (which, as seen from the space frame at the two times, is what the angle $\Delta\theta$ represents) must be gauge dependent. On the other hand, for closed paths the initial and final points in shape space coincide, so although there is still the possibility of redefining the body frames under a gauge transformation, this redefinition will cancel out in the computation of the overall rotation of the system. This theme will recur several times throughout this review.

III. GAUGE KINEMATICS OF THE n-BODY PROBLEM

In this section we develop the gauge kinematics of deformable bodies in three dimensions. We treat the body in question as an assemblage of n point masses, upon which neither net external forces nor external torques act. (This applies to the falling cat, if viewed in a frame which itself is falling under gravity.) We restrict ourselves to kinematical considerations in this section because these are sufficient for the introduction of the gauge potential and the explanation of its physical and geometrical meaning. Dynamical considerations will be taken up in Sec. IV.

We begin by eliminating the translational degrees of freedom from our problem. This step involves the introduction of Jacobi coordinates and a discussion of democracy transformations (also known as kinematic rotations), both standard topics. Next we define shape coordinates and shape space and discuss the cases $n=3$ and $n=4$ in particular. Next we discuss orientational coordinates and introduce the notion of a convention for a body frame as a gauge convention. We also present some examples of specific gauges and discuss gauge transformations. Up to this point, the discussion is mostly analytical and mostly traditional, with a geometrical flavor. In the following step, however, we present the geometrical picture of configuration space as a fiber bundle, in which the fibers are the orbits under the action of ordinary rotations, shape space is the quotient space, and gauge conventions are sections of the bundle. We also discuss practical methods for specifying a gauge, as well as such notions as the triviality of the bundle (which implies the possibility of avoiding singularities) and the singularities that result when the bundle is nontrivial. Next we discuss the gauge potential and give its meaning in terms of the rotations generated by changes in shape under conditions of vanishing angular momentum. The rotation itself is represented in terms of a path-ordered product. Next we discuss the issues of

gauge invariance and covariance, we explore how various quantities of the theory transform under gauge transformations, and we specify rules for constructing gauge-invariant quantities. Finally, we introduce the Coriolis tensor, we describe its geometrical meaning in terms of transport around small loops in shape space, and we demonstrate its gauge covariance. The latter fact is important in the demonstration of the impossibility of transforming away the Coriolis terms in the Hamiltonian.

A. The translational degrees of freedom

The translational degrees of freedom are something of a hindrance in developing the gauge theory of deformable bodies, and it would be easier to explain the latter if they were gotten rid of, say, by pinning one of the masses to an inertial frame. This was the approach taken in Sec. II, and it was also used in a recent paper on the n-body problem (Littlejohn, 1994). This approach is realistic for systems such as helium, taken in the approximation of infinite nuclear mass. But in many other systems the translational degrees of freedom cannot be ignored, so we must deal with them properly. After we have done this, we will move on to the rotational degrees of freedom and the associated gauge theory.

We consider n particles of masses m_α and positions $\mathbf{r}_{s\alpha}$, with $\alpha=1,\ldots,n$, moving in three-dimensional space. The symbols $\mathbf{r}_{s\alpha}$ represent the components of the position vectors relative to a space or inertial frame, as indicated by the s subscript (see Appendix A for conventions). The system has $3n$ degrees of freedom, and configuration space is the $3n$-dimensional space $\mathbb{R}^{3n}$. The total kinetic energy of the system is

$$K^{\mathrm{tot}}=\frac{1}{2}\sum_{\alpha=1}^{n} m_\alpha|\dot{\mathbf{r}}_{s\alpha}|^2=\frac{1}{2}\sum_{\alpha,\beta=1}^{n} K_{\alpha\beta}(\dot{\mathbf{r}}_{s\alpha}\cdot\dot{\mathbf{r}}_{s\beta}), \tag{3.1}$$

where $K_{\alpha\beta}$ is the $n\times n$ mass tensor, defined by

$$K_{\alpha\beta}=m_\alpha\delta_{\alpha\beta} \tag{3.2}$$

(no sum on α; see Appendix A).

To separate out the translation degrees of freedom, we introduce a linear transformation of the configuration-space coordinates, $(\mathbf{r}_{s1},\ldots,\mathbf{r}_{sn})\rightarrow(\mathbf{s}_{s1},\ldots,\mathbf{s}_{s,n-1},\mathbf{R}_s)$,

$$\mathbf{s}_{s\alpha}=\sum_{\beta=1}^{n} T_{\alpha\beta}\mathbf{r}_{s\beta},\quad \alpha=1,\ldots,n-1, \tag{3.3}$$

$$\mathbf{R}_s=\frac{1}{M}\sum_{\alpha=1}^{n} m_\alpha\mathbf{r}_{s\alpha}, \tag{3.4}$$

where $M=\Sigma_{\alpha=1}^{n}m_\alpha$ is the total mass, where $\mathbf{R}_s$ is the center-of-mass position, and where T (with components $T_{\alpha\beta}$; see Appendix A) is the transformation matrix whose first $n-1$ rows are indicated in Eq. (3.3), and whose nth row specifies the center of mass,

$$T_{n\alpha}=\frac{m_\alpha}{M}. \tag{3.5}$$

Furthermore, we require the vectors $\mathbf{s}_{s\alpha}$ to be translationally invariant, i.e., invariant under $\mathbf{r}_{s\alpha}\rightarrow\mathbf{r}_{s\alpha}+\mathbf{k}_s$ for any fixed vector $\mathbf{k}_s$, so that

$$\sum_{\beta=1}^{n} T_{\alpha\beta}=0,\quad \alpha=1,\ldots,n-1. \tag{3.6}$$

These conditions guarantee the separation of the translational degrees of freedom, and imply a condition on the inverse matrix,

$$(\mathsf{T}^{-1})_{\alpha n}=1. \tag{3.7}$$

When we write the coordinates in the form $(\mathbf{r}_{s1},\ldots,\mathbf{r}_{s2})$ or $(\mathbf{s}_{s1},\ldots,\mathbf{s}_{s,n-1},\mathbf{R}_s)$, etc., we do not mean to imply that they must be arranged in a single row or column. Indeed, for some purposes it is desirable to arrange the coordinates in a $n\times 3$ matrix, as many authors have done. Obviously, the change is trivial.

Relations (3.5) and (3.6) block-diagonalize the mass tensor in the new coordinates, so that the total kinetic energy has the form

$$K^{\mathrm{tot}}=\frac{1}{2}\sum_{\alpha,\beta=1}^{n-1}\tilde{K}_{\alpha\beta}(\dot{\mathbf{s}}_{s\alpha}\cdot\dot{\mathbf{s}}_{s\beta})+\frac{M}{2}|\dot{\mathbf{R}}_s|^2, \tag{3.8}$$

where $\tilde{K}_{\alpha\beta}$ is the upper $(n-1)\times(n-1)$ block of the transformed mass tensor K, corresponding to coordinates $(\mathbf{s}_{s1},\ldots,\mathbf{s}_{s,n-1})$. To compute $\tilde{K}_{\alpha\beta}$ in practice, it is easiest to transform the inverse of the mass tensor, which is needed anyway in a Hamiltonian formulation, and then to invert it if necessary. The off-diagonal elements of $\tilde{K}_{\alpha\beta}$ (or its inverse) are the "mass polarization" terms.

In some applications it is desirable to use vectors $\mathbf{s}_{s\alpha}$ with a direct physical meaning, such as the interparticle separations. In such cases, the kinetic energy will contain mass polarization terms. For our purposes, however, it is better to work with coordinates that diagonalize the kinetic energy, such as Jacobi coordinates. The usual way to define Jacobi coordinates is to organize the particles into a hierarchy of clusters, in which each cluster consists of one or more particles and where each Jacobi vector joins the centers of mass of two clusters, thereby creating a larger cluster. Thus there is a discrete set of choices of Jacobi vectors, based on different clusterings. As is well known in scattering theory (e.g., Schatz and Kuppermann, 1976; Pack, 1994), different choices of Jacobi coordinates are appropriate for different entrance or exit channels in a scattering process, in which the locally bound subsystems in the asymptotic state define the clusters. It can be shown that in Jacobi coordinates, so defined, the tensor $\tilde{K}_{\alpha\beta}$ is diagonal with the reduced masses of the clusters joined by the corresponding Jacobi vectors appearing on the diagonal. This fact is proven by Aquilanti and Cavalli (1986). A further advantage of Jacobi coordinates is that it is easy to write down the inverse transformation matrix T^{-1} by inspection of a diagram of the Jacobi vectors, since the center of mass of the new cluster created by a given Jacobi vector $\mathbf{s}_{s\alpha}$ lies on that vector itself. Jacobi

coordinates are discussed more fully by Delves (1960), Smirnov and Shitikova (1977), and Aquilanti and Cavalli (1986).

In this paper we shall use one system of Jacobi coordinates through all our examples of the three-body problem. This system is defined by

$$\begin{pmatrix} \mathbf{s}_{s1} \\ \mathbf{s}_{s2} \\ \mathbf{R}_s \end{pmatrix} = \begin{pmatrix} +1 & 0 & -1 \\ -\dfrac{m_1}{m_1+m_3} & 1 & -\dfrac{m_3}{m_1+m_3} \\ \dfrac{m_1}{M} & \dfrac{m_2}{M} & \dfrac{m_3}{M} \end{pmatrix} \begin{pmatrix} \mathbf{r}_{s1} \\ \mathbf{r}_{s2} \\ \mathbf{r}_{s3} \end{pmatrix}. \tag{3.9}$$

These vectors are illustrated in Fig. 8. In these coordinates, $\tilde{K}_{\alpha\beta}=\mu_\alpha\delta_{\alpha\beta}$, where the reduced masses μ_α are given by

$$\frac{1}{\mu_1}=\frac{1}{m_1}+\frac{1}{m_3}, \quad \frac{1}{\mu_2}=\frac{1}{m_1+m_3}+\frac{1}{m_2}. \tag{3.10}$$

The inverse of the T matrix defined by Eq. (3.9) is given by

$$\begin{pmatrix} \mathbf{r}_{s1} \\ \mathbf{r}_{s2} \\ \mathbf{r}_{s3} \end{pmatrix} = \begin{pmatrix} \dfrac{m_3}{m_1+m_3} & -\dfrac{m_2}{M} & 1 \\ 0 & \dfrac{m_1+m_3}{M} & 1 \\ -\dfrac{m_1}{m_1+m_3} & -\dfrac{m_2}{M} & 1 \end{pmatrix} \begin{pmatrix} \mathbf{s}_{s1} \\ \mathbf{s}_{s2} \\ \mathbf{R}_s \end{pmatrix}. \tag{3.11}$$

For most of the remainder of this paper, we shall use "mass-weighted" Jacobi coordinates $\{\boldsymbol{\rho}_{s\alpha}\}$, defined by

$$\boldsymbol{\rho}_{s\alpha}=\sqrt{\mu_\alpha}\,\mathbf{s}_{s\alpha}, \quad \alpha=1,\ldots,n-1, \tag{3.12}$$

which cause the tensor $\tilde{K}_{\alpha\beta}$ to become the identity matrix. [We note that many authors prefer to divide Eq. (3.12) by the square root of some reference mass, to retain the dimensions of distance for the mass-weighted Jacobi vectors.] Mass-weighted coordinates are convenient because the masses, which are the only parameters in the kinetic energy, drop out of all subsequent analysis of the kinetic energy. (On the other hand, they cause mass dependencies to pop up in the potential energy.) For example, in mass-weighted coordinates, the gauge potential $\mathbf{A}_\mu$, which will be of interest to us below, is parameter free and depends only on the number of particles n. It is a universal field, for example, for all three-body problems. Mass-weighted coordinates also simplify the expression of certain conditions of physical significance; for example, in mass-weighted coordinates for the three-body problem, the condition ensuring that the moment of inertia tensor is degenerate in the plane of the triangle formed by the three bodies is that the vectors $\boldsymbol{\rho}_{s1}$ and $\boldsymbol{\rho}_{s2}$ have equal magnitudes and be perpendicular.

A drawback of mass-weighted Jacobi vectors is that they are not easy to visualize (and in any case, they depend on the choice of the clustering of particles). A better set of vectors for visualization purposes is the positions of the particles relative to the center of mass, which we denote by $\mathbf{c}_{s\alpha}$,

$$\mathbf{c}_{s\alpha}=\mathbf{r}_{s\alpha}-\mathbf{R}_s. \tag{3.13}$$

On the other hand, the $n-1$ vectors $\{\boldsymbol{\rho}_{s\alpha}\}$ are independent, whereas the n vectors $\{\mathbf{c}_{s\alpha}\}$ are constrained by

$$\sum_{\alpha=1}^{n} m_\alpha \mathbf{c}_{s\alpha}=0. \tag{3.14}$$

The two sets of vectors are related by

$$\mathbf{c}_{s\alpha}=\sum_{\beta=1}^{n-1}(\mathsf{T}^{-1})_{\alpha\beta}\frac{\boldsymbol{\rho}_{s\beta}}{\sqrt{\mu_\beta}}, \tag{3.15}$$

where the last column of T^{-1} is not used.

For large or variable n, the vectors $\{\boldsymbol{\rho}_{s\alpha}\}$ are not convenient for explicit calculations, since explicit expressions for $T_{\alpha\beta}$ are not simple nor do they treat the particles democratically. For this reason, standard treatments of molecular vibrations (e.g., Wilson, Decius, and Cross, 1955) bypass the vectors $\{\boldsymbol{\rho}_{s\alpha}\}$ and work instead with $\{\mathbf{c}_{s\alpha}\}$. In the following we present expressions for the kinetic energy and angular momentum in terms of both sets of vectors, and later we shall do the same for future quantities of interest.

Under the coordinate transformation $(\mathbf{r}_{s1},\ldots,\mathbf{r}_{sn})\to(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1},\mathbf{R}_s)$ the kinetic energy and angular momentum of the center of mass, K^{CM} and $\mathbf{L}_s^{\mathrm{CM}}$, respectively, separate from the total kinetic energy and angular momentum,

$$K^{\mathrm{tot}}=K^{\mathrm{CM}}+K, \quad \mathbf{L}_s^{\mathrm{tot}}=\mathbf{L}_s^{\mathrm{CM}}+\mathbf{L}_s, \tag{3.16}$$

where $\mathbf{L}_s^{\mathrm{tot}}=\Sigma_{\alpha=1}^{n} m_\alpha \mathbf{r}_{s\alpha}\times\dot{\mathbf{r}}_{s\alpha}$ and where

$$K^{\mathrm{CM}}=\frac{M}{2}|\dot{\mathbf{R}}_s|^2, \quad \mathbf{L}_s^{\mathrm{CM}}=M\mathbf{R}_s\times\dot{\mathbf{R}}_s. \tag{3.17}$$

What remains is the kinetic energy K and angular momentum $\mathbf{L}_s$ about the center of mass, both of which can be written in terms of either $\{\boldsymbol{\rho}_{s\alpha}\}$ or $\{\mathbf{c}_{s\alpha}\}$:

$$K=\frac{1}{2}\sum_{\alpha=1}^{n-1}|\dot{\boldsymbol{\rho}}_{s\alpha}|^2=\frac{1}{2}\sum_{\alpha=1}^{n} m_\alpha|\dot{\mathbf{c}}_{s\alpha}|^2, \tag{3.18}$$

$$\mathbf{L}_s=\sum_{\alpha=1}^{n-1}\boldsymbol{\rho}_{s\alpha}\times\dot{\boldsymbol{\rho}}_{s\alpha}=\sum_{\alpha=1}^{n} m_\alpha\mathbf{c}_{s\alpha}\times\dot{\mathbf{c}}_{s\alpha}. \tag{3.19}$$

We shall henceforth ignore the kinetic energy and angular momentum of the center of mass and refer to K and $\mathbf{L}_s$ as simply "the kinetic energy" and "the angular momentum," respectively.

The original configuration space, upon which $(\mathbf{r}_{s1},\ldots,\mathbf{r}_{sn})$ are coordinates, is the space $\mathbb{R}^{3n}$. But after the separation of the translational degrees of freedom, we are left with a "translation-reduced configuration space," upon which $(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1})$ are coordinates. This is the space $\mathbb{R}^{3n-3}$. In the following we shall generally refer to the translation-reduced configuration space

$\mathbb{R}^{3n-3}$ as simply "configuration space," contrasting it if necessary with the "original configuration space," $\mathbb{R}^{3n}$.

The kinetic energy (3.18) specifies a Euclidean metric on the (translation-reduced) configuration space in the Jacobi coordinates $\{\boldsymbol{\rho}_{s\alpha}\}$. Linear transformations of the $3n-3$ components of the Jacobi vectors that preserve the Euclidean form of this metric belong to the group $O(3n-3)$, which is the grand symmetry group of the kinetic energy. This group is not usually the symmetry group of the potential energy, unless the potential energy should vanish, and therefore it is not usually the symmetry group of the Hamiltonian as a whole. Nevertheless, there is considerable interest in organizing states according to the irreducible representations of $O(3n-3)$, i.e., effectively using free-particle solutions as a basis for treating the whole Hamiltonian. The subject of hyperspherical coordinates is connected with this point of view (Smith, 1960, 1962; Macek, 1968; Smirnov and Shitikova, 1977; Johnson, 1980, 1983a, 1983b; Fano, 1981; Aquilanti, Cavalli, and Grossi, 1986; Pack and Parker, 1987).

The symmetry group of the whole Hamiltonian (kinetic plus potential) is the ordinary rotation group $O(3)$, which we shall usually break up into SO(3) and parity. The action of rotations and parity on configuration space is given by

$$\boldsymbol{\rho}'_{s\alpha}=\mathsf{Q}\boldsymbol{\rho}_{s\alpha}, \tag{3.20}$$

$$\boldsymbol{\rho}'_{s\alpha}=P\boldsymbol{\rho}_{s\alpha}=-\boldsymbol{\rho}_{s\alpha}, \tag{3.21}$$

where $\mathsf{Q}\in\mathrm{SO}(3)$ and where P is the parity operator. The rotation group SO(3) or $O(3)$ is a subgroup of the grand symmetry group of the kinetic energy, $O(3n-3)$.

Another group of importance is a continuous group that interpolates between all the discrete choices of Jacobi coordinates. Any two choices of mass-weighted Jacobi vectors, say, $\{\boldsymbol{\rho}_{s\alpha}\}$ and $\{\boldsymbol{\rho}'_{s\alpha}\}$, based on different clusterings of particles, are related by some linear transformation of the form

$$\boldsymbol{\rho}'_{s\alpha}=\sum_{\beta=1}^{n-1} D_{\alpha\beta}\boldsymbol{\rho}_{s\beta}, \tag{3.22}$$

where D (with components $D_{\alpha\beta}$) is an $(n-1)\times(n-1)$ matrix. But since all choices of mass-weighted Jacobi vectors lead to the same Euclidean form (3.18) of the kinetic energy, D must be orthogonal, i.e., an element of the group $O(n-1)$. We call this group "the democracy group," because it is of use in constructing quantities that are invariant under permutations of particle labels (Smith, 1962; Dragt, 1965; Levy-Leblond and Lévy-Nahas, 1965; Whitten and Smith, 1968; Louck and Galbraith, 1972; del Aguila, 1980; Aquilanti, Cavalli, and Grossi, 1986). In the literature, the "democracy transformations" (3.22) are often referred to as "kinematic rotations" (Smith, 1959) and are usually viewed in the passive sense, as we have done in introducing them above. That is, the matrix D is thought of as connecting two coordinate systems, so that $\{\boldsymbol{\rho}_{s\alpha}\}$ and $\{\boldsymbol{\rho}'_{s\alpha}\}$ are two distinct coordinate representations of the same physical state. Henceforth in this paper, however, we shall usually think of democracy transformations in an active sense; in this point of view, we establish one system of mass-weighted Jacobi coordinates $\{\boldsymbol{\rho}_{s\alpha}\}$ once and for all, based on an arbitrary clustering of the particles, and then we regard the democracy transformations as mapping old configurations into new ones. We shall usually restrict the democracy group to the proper orthogonal matrices in $\mathrm{SO}(n-1)$. This involves little loss of generality, since by changing the sign of one of the Jacobi vectors, if necessary, it is always possible to make $\det\mathsf{D}=+1$.

Certain choices of coordinates $\{\boldsymbol{\rho}_{s\alpha}\}$ which can be reached by democracy transformations treat the particles in a more symmetrical manner than do any of the discrete set of Jacobi coordinates. These include the Radau coordinates, as well as variations on them due to Smith, which are discussed by Aquilanti and Cavalli (1986). Furthermore, in a practical problem, one must pay attention to which choices of Jacobi or other coordinates cause the potential energy to take on the simplest form. Since the potential energy is usually a function of the interparticle distances, one will be interested in the expressions for the distances in terms of the coordinates $\{\boldsymbol{\rho}_{s\alpha}\}$. These issues are discussed by Aquilanti and Cavalli (1986) and by Aquilanti, Cavalli, and Grossi (1990).

Democracy transformations (i.e., kinematic rotations) suggest themselves naturally in the analysis of n-body problems and have been used by many different authors for various purposes over the years. Nevertheless, the democracy group is a symmetry group only of the kinetic energy, not of the potential energy, in general, and we have asked ourselves what its real significance is. The following considerations seem to be relevant to this question.

First, as noted above, the eigenfunctions of the kinetic energy alone (the hyperspherical harmonics) are useful as a basis set in quantum calculations. They also lead to various pseudo-adiabatic approximations, in which the hyperradius is treated as a "slow" variable and the hyperangles are treated by matrix methods (Fano, 1981; Aquilanti, Cavalli, and Sevryuk, 1994). In another approach, involving discrete approximations to the hyperspherical harmonics, one can set up a basis in which the potential energy is diagonal and the kinetic energy matrix is sparse and analytically computable (Aquilanti and Grossi, 1985; Aquilanti, Cavalli, and Grossi, 1991; Aquilanti, Cavalli, and de Fazio, 1995).

In this paper, however, we are interested in another point of view, a geometrical one, which follows from the fact that the rotation group $O(3)$ is the exact symmetry group of the whole Hamiltonian. Because of this exact symmetry, the dynamics of the n-body problem can be reformulated in terms of "shape space" (defined below) and various fields defined upon it. This formulation in terms of shape space is the principal subject of this review. The question then arises, how is the grand symmetry group of the kinetic energy, $O(3n-3)$, expressed in

shape-space language? That is, the group $O(3n-3)$ acts on the (translation reduced) configuration space, not on shape space. Can it be, in effect, projected down onto shape space, and what is the resulting symmetry group? The answer is that only those transformations in $O(3n-3)$ which commute with SO(3) rotations can be regarded as having an action on shape space, because the shape produced by such a transformation is independent of the orientation of the configuration that is acted upon.

As it turns out, the subgroup of $O(3n-3)$ that commutes with all rotations in SO(3) is just the democracy group, $O(n-1)$. We shall prove a related statement, which applies to the connected groups $\mathrm{SO}(3n-3)$ and $\mathrm{SO}(n-1)$. To begin, let us represent an element of $\mathrm{SO}(3n-3)$ by a $(3n-3)\times(3n-3)$ matrix A, which we partition into an $(n-1)\times(n-1)$ array of 3×3 matrices $\mathsf{A}_{\alpha\beta}$. Then the action of this element of $\mathrm{SO}(3n-3)$ on a point of configuration space can be represented by

$$\begin{pmatrix} \boldsymbol{\rho}'_1 \\ \vdots \\ \boldsymbol{\rho}'_{n-1} \end{pmatrix} = \begin{pmatrix} \mathsf{A}_{11} & \mathsf{A}_{12} & \cdots & \mathsf{A}_{1,n-1} \\ \mathsf{A}_{21} & \mathsf{A}_{22} & \cdots & \mathsf{A}_{2,n-1} \\ \vdots & \vdots & \ddots & \vdots \\ \mathsf{A}_{n-1,1} & \mathsf{A}_{n-1,2} & \cdots & \mathsf{A}_{n-1,n-1} \end{pmatrix} \times \begin{pmatrix} \boldsymbol{\rho}_1 \\ \vdots \\ \boldsymbol{\rho}_{n-1} \end{pmatrix}. \tag{3.23}$$

Similarly, the action of $\mathsf{Q}\in\mathrm{SO}(3)$ on a configuration, as indicated by Eq. (3.20), can be represented by a $(3n-3)\times(3n-3)$ block-diagonal matrix,

$$\begin{pmatrix} \boldsymbol{\rho}'_1 \\ \vdots \\ \boldsymbol{\rho}'_{n-1} \end{pmatrix} = \begin{pmatrix} \mathsf{Q} & 0 & \cdots & 0 \\ 0 & \mathsf{Q} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathsf{Q} \end{pmatrix} \begin{pmatrix} \boldsymbol{\rho}_1 \\ \vdots \\ \boldsymbol{\rho}_{n-1} \end{pmatrix}. \tag{3.24}$$

The two matrices in Eqs. (3.23) and (3.24) commute if and only if $[\mathsf{A}_{\alpha\beta},\mathsf{Q}]=0$ for all α, β. But this holds for all $\mathsf{Q}\in\mathrm{SO}(3)$ if and only if $\mathsf{A}_{\alpha\beta}=D_{\alpha\beta}\mathsf{I}$, where I is the 3×3 identity matrix, as follows from Schur's lemma and the fact that the fundamental representation of SO(3) is irreducible. Here $D_{\alpha\beta}$ is a scalar for each value of α, β; the $D_{\alpha\beta}$ can be arranged in an $(n-1)\times(n-1)$ matrix which is an element of $\mathrm{SO}(n-1)$. Then Eq. (3.23) is equivalent to the democracy transformation (3.22), and we see that the democracy group is indeed the largest subgroup of $\mathrm{SO}(3n-3)$ that commutes with all rotations.

Notice that this proof would not work for the n-body problem in a plane, because the fundamental representation of SO(2) is reducible. For the planar problem, the largest subgroup of $\mathrm{SO}(2n-2)$ that commutes with all rotations in SO(2) is $U(n-1)$ [or $\mathrm{SU}(n-1)$, *modulo* minor details], which is larger than the democracy group, $\mathrm{SO}(n-1)$. This fact is responsible for many of the special features of the planar n-body problem, such as the simple forms of the hyperspherical harmonics in that case. We shall report on these aspects of the planar n-body problem in the future; we simply note here the important work of Iwai (1986, 1987b) on the planar problem.

Since in this review we are concentrating on the three-dimensional problem, we can say that the (connected) democracy group $\mathrm{SO}(n-1)$ is the subgroup of the (connected) grand symmetry group of the kinetic energy, $\mathrm{SO}(3n-3)$, which survives projection onto shape space. Therefore the various tensor fields on shape space, which will be introduced below, are invariant under democracy transformations (in an appropriate differential-geometric sense), and the democracy group plays an important role in understanding the symmetries of these fields (the moment-of-inertia tensor, the gauge potential, the Coriolis tensor, and the metric tensor).

B. Shape coordinates in the n-body problem

It requires $3n-6$ coordinates to specify the shape of an n-body system, at least when $n\geq3$, because three degrees of freedom are taken up by the center of mass $\mathbf{R}_s$ and three more by the Euler angles specifying the orientation. The special case $n=2$ will be dealt with separately later (this is ordinary central force motion, which does not follow the patterns established at larger values of n). We shall denote the shape coordinates generally by q^μ, $\mu=1,\ldots,3n-6$, using a contravariant (upper) index. As in Sec. II, we regard two configurations specified by either $\{\boldsymbol{\rho}_{s\alpha}\}$ and $\{\boldsymbol{\rho}'_{s\alpha}\}$ or $\{\mathbf{c}_{s\alpha}\}$ and $\{\mathbf{c}'_{s\alpha}\}$ as having the same shape if they can be mapped into one another by some (now three-dimensional) proper rotation, i.e., if there exists a proper rotation matrix Q such that either of the conditions,

$$\boldsymbol{\rho}_{s\alpha}=\mathsf{Q}\boldsymbol{\rho}'_{s\alpha}, \quad \alpha=1,\ldots,n-1, \tag{3.25}$$

$$\mathbf{c}_{s\alpha}=\mathsf{Q}\mathbf{c}'_{s\alpha}, \quad \alpha=1,\ldots,n, \tag{3.26}$$

holds. By Eq. (3.15), these conditions are equivalent. This definition does not always coincide with the usual meaning of the English word "shape," such as when two configurations are mapped into one another by reflections or other improper rotations, or by scaling operations, but it is the definition we will use. Furthermore, for the sake of this definition, we regard the particles as distinguishable.

Some people we have talked to prefer to include the improper rotations in the definition of "shape." Certainly the potential-energy functions in most problems are invariant under both proper and improper rotations, so if all one wants to do is to label configurations at which the potential could differ, then one does not need to distinguish configurations related by parity. On the other hand, one can define anything one wants to, and we prefer to define "shape" with respect to the proper rotations only. One of our reasons is that, for $n\geq4$, the configurations related by proper plus improper rotations are typically not connected in configuration space,

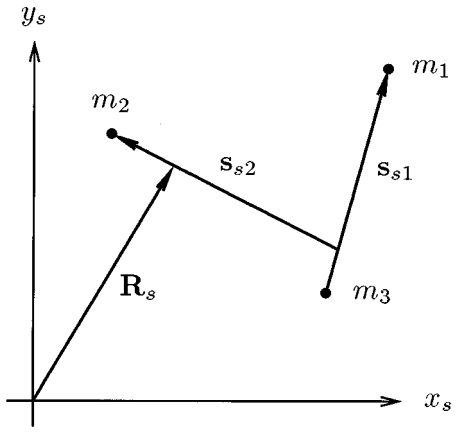

FIG. 8. An example of Jacobi coordinates for the three-body problem. Each vector except the last joins one particle to the center of mass of a cluster of others.

whereas those related by proper rotations are. Since the entire program we are presenting in this review is geometrical, it seems best to respect notions of continuity. In any case, one can conceive of interactions (e.g., the weak ones) that are not invariant under parity, and even for ordinary potentials there is no harm in our definition.

In general, shape coordinates are any $3n-6$ independent functions on configuration space,

$$q^\mu = q^\mu(\boldsymbol{\rho}_{s1}, \ldots, \boldsymbol{\rho}_{s,n-1}), \tag{3.27}$$

that are invariant under proper rotations, i.e., that satisfy

$$q^\mu(\boldsymbol{\rho}_{s1}, \ldots, \boldsymbol{\rho}_{s,n-1}) = q^\mu(\mathsf{Q}\boldsymbol{\rho}_{s1}, \ldots, \mathsf{Q}\boldsymbol{\rho}_{s,n-1}) \tag{3.28}$$

for all rotations $\mathsf{Q} \in \mathrm{SO}(3)$. Examples of such functions are the Jacobi dot products $\boldsymbol{\rho}_{s\alpha} \cdot \boldsymbol{\rho}_{s\beta}$ and triple products $\boldsymbol{\rho}_{s\alpha} \cdot (\boldsymbol{\rho}_{s\beta} \times \boldsymbol{\rho}_{s\gamma})$; in fact, shape coordinates q^μ can always be expressed as some function of the Jacobi dot and triple products. (But, in general, they cannot be expressed as functions of the Jacobi dot products alone, since these cannot distinguish proper from improper rotations.) Alternatively, the q^μ are any $3n-6$ independent functions on the original configuration space $(\mathbf{r}_{s1}, \ldots, \mathbf{r}_{sn})$ that are invariant under both translations and rotations. Relations (3.27) are not invertible because there are $3n-3$ components of the $\boldsymbol{\rho}_{s\alpha}$, but only $3n-6$ of the q^μ.

An interesting question is how to construct shape coordinates in the general n-body problem, preferably in an elegant and symmetrical way. Certainly one answer is given by the Eckart coordinates, discussed more fully below; and the question has also been dealt with by Keating and Mead (1985), who used the theory of the permutation group to construct shape coordinates for the four-body problem. But there is more that can be said about this question, which we have addressed in a recent publication (Littlejohn and Reinsch, 1995).

In the case of the three-body problem, however, many systems of shape coordinates are known and have been used in practice. One is the set (a,b,c), the lengths of the sides of the triangle formed by the three bodies. Closely related to these are the Hylleraas coordinates (s,t,u), used in the classic variational calculations on helium. The three-body problem is special in that shape coordinates, such as (a,b,c), can be chosen to be functions only of the Jacobi dot products $\boldsymbol{\rho}_{s\alpha} \cdot \boldsymbol{\rho}_{s\beta}$ (with no triple products), because the planar shapes that occur in the three-body problem are always invariant under parity.

Another set of coordinates for the three-body problem is (ρ_1, ρ_2, ϕ), defined in terms of Jacobi coordinates $\{\boldsymbol{\rho}_{s\alpha}\}$ by

$$\rho_1 = |\boldsymbol{\rho}_{s1}|, \quad \rho_2 = |\boldsymbol{\rho}_{s2}|, \quad \boldsymbol{\rho}_{s1} \cdot \boldsymbol{\rho}_{s2} = \rho_1 \rho_2 \cos\phi, \tag{3.29}$$

so that ϕ is the angle between $\boldsymbol{\rho}_{s1}$ and $\boldsymbol{\rho}_{s2}$. The angle ϕ is restricted to the range $0 \leqslant \phi \leqslant \pi$ because angles outside this range give shapes that are already represented by angles within this range. Coordinates (ρ_1, ρ_2, ϕ) have been used by Tennyson and Sutcliffe (1982).

Another set of coordinates for the three-body problem treats the kinetic energy in a particularly symmetrical way. These coordinates have been used by many authors (Smith, 1962; Dragt, 1965; Mead and Truhlar, 1979; Pack and Parker, 1987; Iwai, 1987b; Mead, 1992), and they seem to have been rediscovered several times. We denote these coordinates by (w_1, w_2, w_3) or (w, χ, ψ), and define them in terms of (ρ_1, ρ_2, ϕ) by

$$\begin{aligned} w_1 &= w\cos\chi\cos\psi = \rho_1^2 - \rho_2^2, \\ w_2 &= w\cos\chi\sin\psi = 2(\boldsymbol{\rho}_{s1} \cdot \boldsymbol{\rho}_{s2}) = 2\rho_1\rho_2\cos\phi, \\ w_3 &= w\sin\chi = 2|\boldsymbol{\rho}_{s1} \times \boldsymbol{\rho}_{s2}| = 2\rho_1\rho_2\sin\phi. \end{aligned} \tag{3.30}$$

Coordinates (w, χ, ψ) are spherical coordinates in (w_1, w_2, w_3) space, as is evident from the identities,

$$w = \rho_1^2 + \rho_2^2, \tag{3.31}$$

$$w^2 = w_1^2 + w_2^2 + w_3^2. \tag{3.32}$$

Note that χ is the latitude, not the colatitude. The coordinate w is the square of the "hyperradius" (Smith, 1960), and coordinate w_3 is proportional to the area of the parallelogram spanned by the Jacobi vectors, and therefore also to the area of the triangle formed by the three bodies. Coordinates w_1 and w_2 range from $-\infty$ to $+\infty$, but w_3 is strictly non-negative, in accordance with the absolute-value signs and the allowed range of ϕ. A useful relation connecting these coordinates is

$$\tan\chi = \tan\phi\sin\psi, \tag{3.33}$$

which geometrically means that ϕ is the azimuthal angle about the w_1 axis in w space, as illustrated in Fig. 9. In view of this fact and the relations,

$$\rho_1^2 = \tfrac{1}{2}(w + w_1), \quad \rho_2^2 = \tfrac{1}{2}(w - w_1), \tag{3.34}$$

we see that coordinates $(\rho_1^2, \rho_2^2, \phi)$ are essentially confocal parabolic coordinates in w-space, referred to the w_1 axis.

In the case of the four-body problem, the six interparticle distances do not form a proper set of shape coordinates because they cannot in general distinguish two

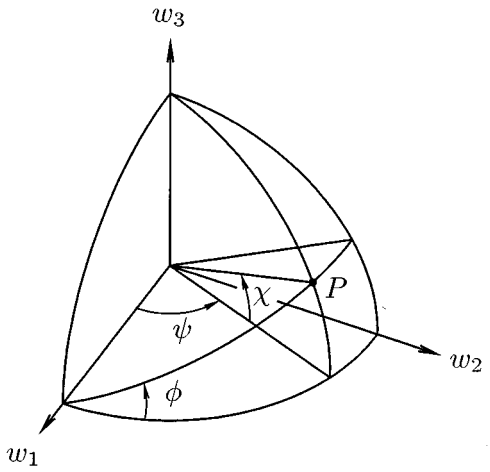

FIG. 9. The angle ϕ, which is the azimuthal angle in w space about the w_1 axis. Coordinates (ρ_1^2,ρ_2^2,ϕ) are confocal parabolic coordinates in w space, referred to the w_1 axis.

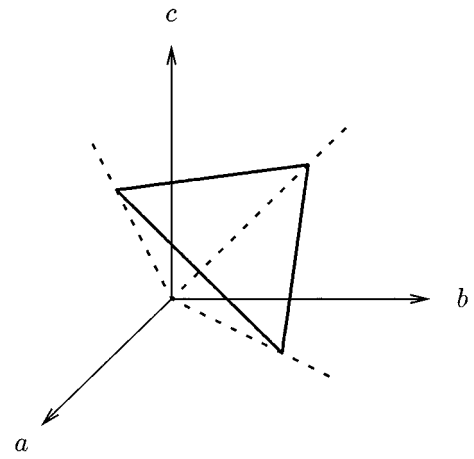

FIG. 10. Shape space for three-body problem—a three-sided pyramid of infinite height, whose vertex is at the origin and whose edges are the dotted lines. Coordinates (a,b,c) are the sides of the triangle. The dotted lines lie in the coordinate planes and run at 45° to the axes defining those planes. Interior points of the pyramid are triangles of nonzero area; the faces are collapsed triangles of zero area in which no two particles coincide; the edges are two-particle collisions; and the vertex is the three-particle collision. The heavy triangle is a slice through the pyramid; points inside the heavy triangle represent shapes of constant perimeter $(a+b+c=\text{const})$.

configurations related by a reflection. There are various ways to resolve this difficulty (Keating and Mead, 1985; Littlejohn and Reinsch, 1995), and to find four-body shape coordinates analogous to the three-body coordinates $\{w_i\}$ introduced above. For $n>4$, the interparticle distances are not even independent, since there must be $3n-6$ shape coordinates and the number of interparticle distances is $n(n-1)/2$.

We now turn to *shape space*, which is the space of all possible shapes, upon which the q^μ are coordinates. Shape space for $n\geqslant 3$ is a manifold of dimensionality $3n-6$, with a boundary in the case $n=3$ and without boundaries for $n\geqslant 4$.

In the three-body problem, it is easy to visualize shape space in the coordinates $q^\mu=(a,b,c)$ (Mead and Truhlar, 1979). The distances (a,b,c) are necessarily non-negative and also satisfy the triangle inequalities, $a\leqslant b+c$, $b\leqslant a+c$, $c\leqslant a+b$. As a result, shape space can be identified with a subset of (a,b,c) space (i.e., $\mathbb{R}^3$) that has the form of a three-sided pyramid of infinite height with its apex at the origin and its three edges lying in the three coordinate planes, running at 45° relative to the two axes in each of the planes. This pyramid is illustrated in Fig. 10. It has four subsets, which can be identified and ranked in order of increasing singularity. First, there is the interior of the pyramid, which is comprised of triangles of nonzero area. Next, there are the faces of the pyramid (excluding the edges), which represent collinear configurations (collapsed triangles of zero area), in which the three particles are spatially separated. Third, there are the edges, indicated by dotted lines in the figure, which represent two-body collisions. Finally, there is the vertex, which represents the three-body collision.

In a different coordinate system, the region of coordinate space representing shape space will be a continuous deformation of the pyramid seen in the (a,b,c) coordinates. For example, in the coordinates (a^2,b^2,c^2), shape space is a circular cone instead of a three-sided pyramid (Mead and Truhlar, 1979). For another example, in the (w_1,w_2,w_3) coordinates given by Eq. (3.30), shape space is the half-space $w_3\geqslant 0$ (Iwai, 1987b), with the collinear configurations occupying the plane $w_3=0$, the two-body collisions lying on three half-lines in this plane radiating out from the origin, and the three-body collision lying at the origin itself. Thus the transformation from (a,b,c) coordinates to (w_1,w_2,w_3) coordinates flattens out the faces of the pyramid and makes them lie in (and fill up) the plane $w_3=0$. One of the half-lines representing two-body collisions is the negative w_1 axis, which consists of collisions between bodies 1 and 3, assuming we use the mass-weighted Jacobi coordinates introduced in Eq. (3.9). The other two radial half-lines, representing the cases in which the ordering of the collinear bodies is permuted, lie at angles in the plane $w_3=0$ which depend on the masses.

These angles and the mass dependencies can be changed by an SO(2) democracy transformation of the type

$$\begin{pmatrix}\boldsymbol{\rho}'_{s1}\\ \boldsymbol{\rho}'_{s2}\end{pmatrix}=\begin{pmatrix}\cos\alpha & -\sin\alpha\\ \sin\alpha & \cos\alpha\end{pmatrix}\begin{pmatrix}\boldsymbol{\rho}_{s1}\\ \boldsymbol{\rho}_{s2}\end{pmatrix}, \tag{3.35}$$

under which the w coordinates transform according to

$$\begin{pmatrix}w'_1\\ w'_2\end{pmatrix}=\begin{pmatrix}\cos 2\alpha & -\sin 2\alpha\\ \sin 2\alpha & \cos 2\alpha\end{pmatrix}\begin{pmatrix}w_1\\ w_2\end{pmatrix}, \tag{3.36}$$

or simply $\psi'=\psi+2\alpha$. Thus the SO(2) democracy rotation (3.35) is equivalent to a rotation (by twice the angle) about the w_3 axis. Such a rotation leaves the boundary of shape space (the plane $w_3=0$) invariant.

An obvious strategy in setting up shape coordinates (for any number of particles) is to use the angles specifying a democracy transformation as shape coordinates. This idea has been developed by Zickendraht (1967, 1969, 1971), Aquilanti, Cavalli, and Grossi (1986), and Littlejohn and Reinsch (1995). In effect, one is foliating shape space under democracy transformations and using democracy-group elements to parametrize the democracy orbits.

Shape space has several interesting subsets. One of these is the set of collinear shapes, upon which the moment-of-inertia tensor is singular. In the three-body problem, the collinear shapes occur on the plane $w_3=0$, i.e., at the boundary of shape space. Another interesting subset is that upon which the moment of inertia tensor is degenerate, since at such shapes the principal axis frame is not unique. In the three-body problem, this degeneracy subset consists of the union of the plane $w_3=0$ with the half-line $w_1=w_2=0$, $w_3\geqslant 0$ (the w_3 axis).

In the four-body problem, shape space can be identified with $\mathbb{R}^6$ and has no boundaries (Narasimhan and Ramadas, 1979). In a separate publication (Littlejohn and Reinsch, 1995), we have discussed coordinates that provide a one-to-one mapping from shape space to points of $\mathbb{R}^6$. In these coordinates, a five-dimensional hyperplane $\mathbb{R}^5$ consisting of planar shapes divides $\mathbb{R}^6$ into two pieces. Shapes not on the hyperplane represent tetrahedra of nonzero volume. One can also identify useful subsets of shape space, such as the three-dimensional submanifold of collinear shapes or the four-dimensional submanifold upon which the moment-of-inertia tensor is degenerate. Many of the important properties of shape space for the four-body problem were apparently first worked out by Zickendraht (1969), from a nongeometrical standpoint.

In the special case of the two-body problem, i.e., ordinary central force motion, there is one shape coordinate that can be taken to be r, the distance between the two bodies. Thus the rule of $3n-6$ shape coordinates does not apply in this case. Shape space itself is the half-line $r\geqslant 0$, the space upon which the ordinary radial Schrödinger equation lives. The point $r=0$ is a singular point in many respects; for example, if the angular momentum is nonzero, the centrifugal potential $L^2/2mr^2$ diverges at $r=0$ and tends to prevent particles from reaching the origin. Analogs of these features for higher values of n occur at the collinear shapes.

C. Orientational coordinates and gauge transformations

Orientational coordinates are some choice of Euler angles or other coordinates on the rotation group manifold, specifying the rotation that maps the space frame into the body frame. Thus orientational coordinates are only defined relative to a convention for body frames, which as we have indicated in Sec. II is considered to be a choice of gauge. Such a convention is established by specifying, for each shape, the positions of the n particles relative to the body frame. These positions can be specified by giving either the n vectors $\{\mathbf{c}_\alpha\}$ or the $n-1$ vectors $\{\boldsymbol{\rho}_\alpha\}$ as functions of the shape coordinates q^μ; of course, the vectors $\{\mathbf{c}_\alpha\}$ must satisfy the constraint (3.14). We shall normally work with the Jacobi vectors and think of the functions,

$$\boldsymbol{\rho}_\alpha=\boldsymbol{\rho}_\alpha(q^\mu),\quad \alpha=1,\ldots,n-1, \tag{3.37}$$

as the specification of a body frame or a gauge convention. Here we introduce the important convention that any vector appearing without the s subscript is referred to the body frame; see Appendix A. Relations (3.37) are not invertible, because there are $3n-3$ components in $\{\boldsymbol{\rho}_\alpha\}$, but only $3n-6$ shape coordinates. In particular, they are not the inverse of the relations $q^\mu=q^\mu(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1})$, which define the shape coordinates.

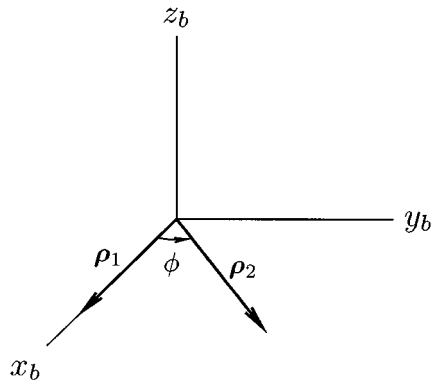

FIG. 11. xxy gauge. We obtain "xxy gauge" for the three-body problem by decreeing that vector $\boldsymbol{\rho}_1$ lies on the body x axis, and vector $\boldsymbol{\rho}_2$ in the body x-y plane.

For example, in the three-body problem, a gauge convention can be established by decreeing that, in the body frame, vector $\boldsymbol{\rho}_1$ lies on the x axis and vector $\boldsymbol{\rho}_2$ lies in the x-y plane with $\rho_{2y}\geqslant 0$, as illustrated in Fig. 11. The condition $\rho_{2y}\geqslant 0$ ensures that there is only one body frame for each shape, since if we allowed $\rho_{2y}<0$ we would obtain a shape already represented by $\rho_{2y}>0$. This gauge convention does not treat the vectors $(\boldsymbol{\rho}_1,\boldsymbol{\rho}_2)$ symmetrically, but it is simple and leads to easy subsequent calculations. We shall call this "xxy gauge," because $\boldsymbol{\rho}_1$ has only an x coordinate and $\boldsymbol{\rho}_2$ has only x and y coordinates. In xxy gauge, the functions in Eq. (3.37) are

$$\begin{aligned}\boldsymbol{\rho}_1&=\rho_1(1,0,0),\\ \boldsymbol{\rho}_2&=\rho_2(\cos\phi,\sin\phi,0),\end{aligned} \tag{3.38}$$

where we use coordinates $q^\mu=(\rho_1,\rho_2,\phi)$. A closely related gauge ("zzx gauge") has been used by Tennyson and Sutcliffe (1982).

Another obvious choice of gauge (for any number of particles) is the principal-axis frame. Later we shall say more about "principal-axis gauge," which has been used by many authors, especially in three-body calculations. In addition, the Eckart conventions, to be discussed later, involve a definite choice of gauge (the Eckart frame, or "Eckart gauge") for any number of particles.

Another example is the gauge used by Bhatia and Temkin (1964). In this gauge, one of the coordinate axes is the angle bisector of the directions of $\boldsymbol{\rho}_1$ and $\boldsymbol{\rho}_2$. This gauge is useful when considering parity and exchange. The original works of Hylleraas and of Breit (1930) contain a definition of a choice of gauge for the helium problem. Pickett (1972) has considered several choices of gauge, and the transformations connecting them (gauge transformations), in problems of molecular vibrations.

A choice of gauge specifies a *reference orientation* for each shape, namely, the orientation in which the body frame coincides with the space frame. In the reference orientation, the body and space positions of the particles are equal, so that $\mathbf{c}_{s\alpha}=\mathbf{c}_\alpha$ and $\boldsymbol{\rho}_{s\alpha}=\boldsymbol{\rho}_\alpha$. Given the reference orientation and some actual orientation of the same shape, there is some rotation (unique for noncollinear shapes) which maps the reference into the actual orientation, carrying the space frame into the body frame. We specify this rotation by a proper rotation matrix R, so that

$$\mathbf{c}_{s\alpha}=\mathsf{R}\mathbf{c}_\alpha, \quad \alpha=1,\ldots,n, \tag{3.39}$$

$$\boldsymbol{\rho}_{s\alpha}=\mathsf{R}\boldsymbol{\rho}_\alpha, \quad \alpha=1,\ldots,n-1. \tag{3.40}$$

(See Appendix A for the choice of R instead of R^{-1} in this formula.)

We shall regard Eq. (3.40) as the specification of a coordinate transformation from $(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1})$ to orientational and shape coordinates (θ^i,q^μ), which we emphasize by writing

$$\boldsymbol{\rho}_{s\alpha}=\mathsf{R}(\theta^i)\boldsymbol{\rho}_\alpha(q^\mu), \quad \alpha=1,\ldots,n-1. \tag{3.41}$$

Here θ^i, $i=1,2,3$, are some set of Euler angles upon which the rotation matrix R depends, and $\boldsymbol{\rho}_\alpha=\boldsymbol{\rho}_\alpha(q^\mu)$ are the functions that specify the gauge convention. Combined with the earlier transformation $(\mathbf{r}_{s1},\ldots,\mathbf{r}_{sn})\to(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1},\mathbf{R}_s)$ which introduced the center-of-mass position $\mathbf{R}_s$, Eq. (3.41) gives us an overall transformation of the form $(\mathbf{r}_{s1},\ldots,\mathbf{r}_{sn})\to(\mathbf{R}_s,\theta^i,q^\mu)$. This transformation achieves a separation of the three center-of-mass degrees of freedom from the remaining degrees of freedom, in the sense of classical Hamiltonian mechanics, but it does not, as we shall see, separate all three rotational degrees of freedom (only two rotational degrees of freedom are separated).

The transformation (3.41) is a proper coordinate transformation only if it is invertible, i.e., if the Euler angles θ^i are uniquely determined by a given reference and actual orientation. This will be the case if the particles are noncollinear, since any two noncollinear configurations of the same shape are related by a unique rotation. However, for collinear shapes the rotation is not unique, since a rotation about the line of collinearity has no effect. Therefore the coordinate transformation specified by Eq. (3.41) is singular at the collinear configurations (in the sense that the Euler angles are not unique). For $n=3$, the collinear configurations are at the boundaries of shape space, whereas for $n\geqslant 4$ they are in the interior of shape space, which has no boundary. For $n=2$, all configurations are collinear and Eq. (3.41) does not apply.

Next we consider changes in body-frame convention, i.e., gauge transformations, which are specified by some shape-dependent, proper rotation $\mathsf{S}=\mathsf{S}(q^\mu)\in\mathrm{SO}(3)$ that maps an old body frame into a new one. Under a redefinition of body frames, the body-referred vectors such as $\mathbf{c}_\alpha$ change their components due to the change of frame to which they are referred,

$$\mathbf{c}_\alpha=\mathsf{S}(q^\mu)\mathbf{c}'_\alpha, \tag{3.42}$$

where primes indicate the components in the new gauge. (See Appendix A for the choice of S instead of S^{-1} in this formula.) Likewise, the matrix R representing the rotation that maps the space frame into the body frame changes according to

$$\mathsf{R}=\mathsf{R}'\mathsf{S}^T, \tag{3.43}$$

which is the generalization of Eq. (2.19) to three dimensions. These transformation laws imply

$$\mathbf{c}_{s\alpha}=\mathsf{R}\mathbf{c}_\alpha=\mathsf{R}'\mathbf{c}'_\alpha, \quad \alpha=1,\ldots,n, \tag{3.44}$$

$$\boldsymbol{\rho}_{s\alpha}=\mathsf{R}\boldsymbol{\rho}_\alpha=\mathsf{R}'\boldsymbol{\rho}'_\alpha, \quad \alpha=1,\ldots,n-1, \tag{3.45}$$

so that the space-referred vectors $\mathbf{c}_{s\alpha}$ or $\boldsymbol{\rho}_{s\alpha}$ are gauge invariant (i.e., their components are gauge invariant), as they must be since the determination of these components does not involve body-frame conventions.

In most of the traditional atomic and molecular literature, it is the custom to commit oneself at the beginning of a calculation to a specific choice of shape coordinates and a specific convention for body frame. Often it is not clearly stated that these two choices are distinct and independent of one another. For example, the Eckart conventions provide a gauge convention (the Eckart frame) as well as a coordinate system on shape space (essentially normal-mode coordinates for small vibrations). In our presentation we emphasize the independence of these two choices and we develop the transformation properties of various quantities under both changes of convention.

D. The fiber-bundle formulation of shape and orientation

For some time now (Lubkin, 1963; Wu and Yang, 1975) it has been recognized that the mathematical theory of fiber bundles is natural for the description of gauge theories. There are currently a number of books and review articles available (e.g., Eguchi, Gilkey, and Hanson, 1980; Nash and Sen, 1983; Göckeler and Schücker, 1987; Nakahara, 1990; Visconti, 1992) which explain the mathematics of fiber bundles in some detail, including physical applications (usually to particle theory). Nevertheless, it is a substantial investment to master this material, and many of the essential geometrical ideas can be understood without the official abstract formalism. In this spirit, we shall now present some of the basic geometrical constructions associated with the fiber-bundle structure induced on configuration space by the action of rotations.

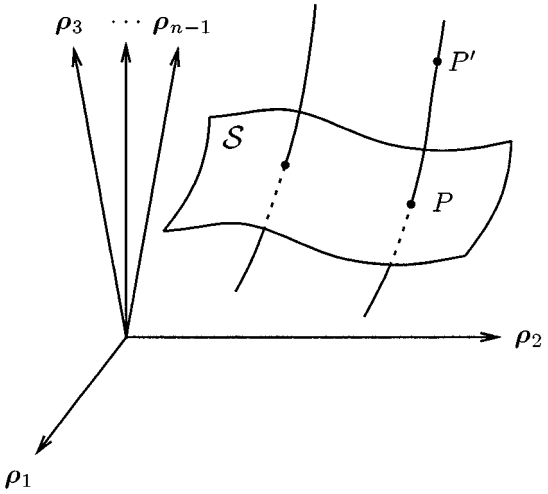

FIG. 12. The $(3n-3)$-dimensional translation-reduced configuration space for the n-body problem, is represented schematically by several axes. A typical configuration is P, on which the rotation group SO(3) acts, producing the orbit indicated schematically by the line passing through P. Actually, the orbit has either zero, two, or three dimensions (usually three, for $n\geqslant 3$). P' is another configuration on the orbit passing through P. The surface $\mathcal{S}$ is a $(3n-6)$-dimensional surface of reference orientations, specifying a gauge convention.

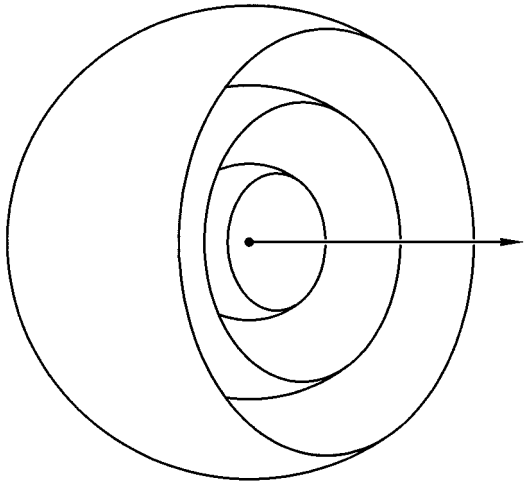

FIG. 13. Orbits for the two-body problem, shown as concentric spheres about the origin of the (translation-reduced) configuration space, which is $\mathbb{R}^3$. Shape space is the radial halfline, $r\geqslant 0$.

We begin by considering the $(3n-3)$-dimensional configuration space, as illustrated schematically in Fig. 12, upon which the Jacobi vectors $\boldsymbol{\rho}_{s\alpha}$ are coordinates. We let P be some specific configuration, and we consider the set of configurations $\{\mathsf{Q}P|\mathsf{Q}\in \mathrm{SO}(3)\}$, which are generated by letting all proper rotations Q act on P. These configurations are all those with the same shape as P, and they form a surface in configuration space passing through P. This surface is represented schematically by a line in Fig. 12, but in fact its dimensionality is either 0, 2, or 3. This surface is the orbit of the point P under the action of the rotation group (in the mathematical sense of the word "orbit," not to be confused with particle trajectories in mechanics). If the configuration P is noncollinear, then the orbit is a copy of the three-dimensional rotation group SO(3) itself, since any two noncollinear configurations, such as P and P' in the figure, are related by a unique rotation. Thus, for noncollinear configurations, the points of the orbit can be placed in one-to-one correspondence with rotations, and rotations or their Euler angles can be used as coordinates along the orbit. For collinear shapes that are not collapsed to a point, the orbit is two-dimensional and is a copy of the two-sphere S^2, since rotations can only change the direction in which the linear shape is pointing. Finally, for configurations in which all particles coincide at a single point (an n-body collision), the orbit is just the point P itself, since $\mathsf{Q}P=P$ for all Q; in this case the orbit is zero-dimensional.

For $n\geqslant 3$, the collinear configurations form a set of measure zero. If we exclude these, then the remainder of the $(3n-3)$-dimensional configuration space is divided up or foliated into a $(3n-6)$-parameter family of three-dimensional orbits, each of which is a copy of SO(3). Shape space is the family itself, i.e., it is the quotient space $\mathbb{R}^{3n-3}/\mathrm{SO}(3)$, the space in which a single point represents a whole orbit in $\mathbb{R}^{3n-3}$, i.e., an equivalence class of configurations of the same shape. Shape space is, properly speaking, not a subset of configuration space, although it can be identified with various subsets (submanifolds) in a nonunique way. The construction of shape space as a quotient space has previously been considered by Mezey (1987, 1993).

In the special case $n=2$, all shapes are collinear and the orbits are concentric spheres surrounding the origin, since rotations cause the vector $\boldsymbol{\rho}_{s1}$ (there is only one) to sweep out the surface of a sphere while holding r fixed. In this case we have a sphere bundle over shape space instead of an SO(3) bundle, and the foliation is worth a picture (Fig. 13) because a realistic drawing can be made. Because the spheres are two-dimensional instead of three-dimensional, the count of shape coordinates in the two-body problem is $3n-5$, i.e., 1, instead of $3n-6$.

Returning to the case $n\geqslant 3$, if we exclude the collinear configurations, then the orbit structure imposed on configuration space by rotations qualifies this space as a *principal fiber bundle*, in which shape space is the *base space*, the *structure group* is SO(3), and the *fibers* are the orbits. Of course, the collinear configurations are not excluded on physical grounds, since collinear configurations can and do occur; rather, it is a matter of identifying a standard mathematical construction. We shall henceforth often refer to the orbits as fibers, partly to avoid confusion with the usual physical meaning of the word "orbit," although properly speaking only the orbits of noncollinear configurations are fibers.

The fiber-bundle picture also provides a geometrical interpretation for a choice of gauge. To see how, we refer to Fig. 12 and declare that configuration P specifies the reference orientation for the shape represented by

the fiber passing through P. Thus a body frame is defined at P to be identical to the space frame, and at other points P' on the same fiber the body frame is defined by demanding that the rotation that maps P into P' also map the space frame into the body frame. Having done this for one fiber, we extend the definition of the reference orientation to neighboring fibers, proceeding in a continuous way until all fibers (at least in some neighborhood) have been covered. In this way, a $(3n-6)$-dimensional surface $\mathcal{S}$ of reference orientations is swept out, and body frames are defined for all noncollinear configurations. The surface $\mathcal{S}$ is known as a *section* of the fiber bundle, because of the way it cuts through the fibers. Thus the section $\mathcal{S}$ is a geometrical representation of a gauge convention. Any other gauge convention is specified by the choice of a different section; sections can be chosen in many ways, but they should cut transversally to the fibers, i.e., be nowhere tangent to the fibers, so that small changes in shape do not lead to large changes in the reference orientation. We do not require the section $\mathcal{S}$ to be perpendicular to the fibers; indeed, it turns out that it is impossible to choose a section that is everywhere perpendicular to the fibers. This is an issue that arises in the establishment of the Eckart conventions, and we shall have more to say about it later.

There are two ways of specifying a surface such as $\mathcal{S}$ in practice. One is to write down a set of $3n-6$ functions of the form $\boldsymbol{\rho}_\alpha(q^\mu)$, which are the same functions introduced in Eq. (3.37), whereupon the section $\mathcal{S}$ is the graph of these functions in configuration space, i.e., it is the surface $\boldsymbol{\rho}_{s\alpha}=\boldsymbol{\rho}_\alpha(q^\mu)$. Notice that by setting space components equal to body components we are specifying the reference orientation. These functions specify a mapping from the $(3n-6)$-dimensional space of coordinates q^μ to configuration space, so that the q^μ serve as coordinates on the section $\mathcal{S}$. The only conditions imposed on the functions $\boldsymbol{\rho}_\alpha(q^\mu)$ are that they be independent and that the surface $\mathcal{S}$ be transverse to the fibers; these are mild conditions, so that most functions $\boldsymbol{\rho}_\alpha(q^\mu)$ written down at random would work in principle. The specification of the functions $\boldsymbol{\rho}_\alpha(q^\mu)$ establishes both a gauge convention and a coordinate system on shape space, although afterwards either of these can be changed independently at will.

A complementary way to specify the $(3n-6)$-dimensional section $\mathcal{S}$ in the $(3n-3)$-dimensional configuration space is to specify three constraints on the coordinates $\{\boldsymbol{\rho}_{s\alpha}\}$, i.e., three functions of the form

$$F_i(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1})=0, \quad i=1,2,3. \tag{3.46}$$

These functions should be independent and yield a surface $\mathcal{S}$ that is transverse to the fibers; again, these are mild conditions. The specification of such a set of constraints establishes a gauge convention but not a system of shape coordinates; in practice some additional choice has to be made for the latter. An example of such a set of constraints are the equations defining the Eckart gauge (Eckart, 1935; Louck, 1976; Louck and Galbraith, 1976; Biedenharn and Louck, 1981); these are

$$\sum_{\alpha=1}^{n-1}\boldsymbol{\rho}_{s\alpha}\times\boldsymbol{\rho}_{0s\alpha}=\sum_{\alpha=1}^{n}m_\alpha\mathbf{c}_{s\alpha}\times\mathbf{c}_{0s\alpha}=0, \tag{3.47}$$

where the 0 subscript refers to some equilibrium configuration of a molecule, i.e., some orientation of an equilibrium shape (we assume there is only one). The many equilibrium configurations of the molecule are related by rotations (they lie on an "equilibrium fiber"), and the choice of one of them to use in Eq. (3.47) is equivalent to the choice of a body frame for the equilibrium shape. Once this is done, Eq. (3.47) determines the body frames for all other shapes. Notice that Eckart gauge specifies a section $\mathcal{S}$ by means of linear constraints on the coordinates $\{\boldsymbol{\rho}_{s\alpha}\}$; the section $\mathcal{S}$ is actually a $(3n-6)$-dimensional vector subspace of the (translation-reduced) configuration space.

The section $\mathcal{S}$ (by any convention) can be loosely identified with shape space itself, and thus shape space can be loosely identified with a submanifold of configuration space. It is easy to see this, since the q^μ are coordinates on shape space and since the equations $\boldsymbol{\rho}_{s\alpha}=\boldsymbol{\rho}_\alpha(q^\mu)$ also allow the q^μ to be taken as coordinates on $\mathcal{S}$. The geometry of this association is that a point of shape space represents a fiber, and a fiber presumably intersects the section at a single point. But the identification is only loose, because it may not be possible to define a smooth section that intersects all the fibers (see below) and because the section in any case is not unique, but rather may be pushed "up" and "down" along the fibers by means of a gauge transformation. Thus any feature that derives from identifying shape space with a submanifold of configuration space will not be gauge invariant. Many of the non-gauge-invariant features of the Eckart conventions arise in this way.

A standard question in fiber-bundle theory is whether it is possible to choose a section that cuts through all the fibers and that is smooth (free of singularities) everywhere. If so (in the case of a principal fiber bundle), the bundle is said to be trivial. In the present example, the issue is whether it is possible to choose a convention for body frame that is smooth over all of shape space. For the sake of this discussion, we exclude the collinear configurations, so that shape space is an open set. (We can worry later about what happens as we approach a collinear configuration.) Then it turns out that, for $n=3$, it is possible to choose such a smooth convention for body frame, so that the bundle is trivial (Iwai, 1987b); this follows from the contractability of shape space. Our xxy gauge given by Eq. (3.38) is an explicit example of a smooth gauge convention for the three-body problem. For $n\geq 4$, globally smooth sections no longer exist, and the bundle is nontrivial. Even for the three-body problem, however, we may wish to choose a gauge that is not globally smooth. An example is the principal-axis gauge, as we shall see later.

The relevance of singularities in the convention for body frame is that they lead to singularities in the gauge potential $\mathbf{A}_\mu$, which appears in a classical canonical Hamiltonian description of the reduced dynamics, as well as in the Schrödinger equation. These singularities

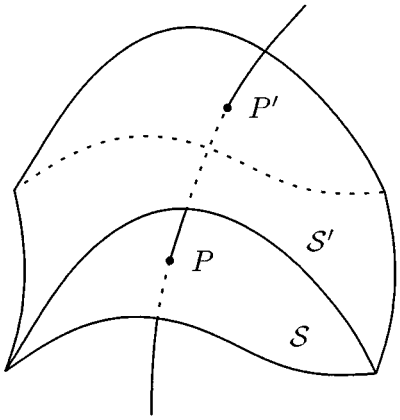

FIG. 14. A gauge transformation viewed geometrically as the replacement of one section $\mathcal{S}$ by another $\mathcal{S}'$. One can imagine pushing the old section "up" along the fibers to create the new section.

are mathematically of the same form as monopole strings (Wu and Yang, 1975; Sakurai, 1985), and on this analogy we shall call them "string singularities." String singularities force the wave function on shape space to be represented in overlapping patches, with different patches belonging to different gauges. For example, in the four-body problem, the Schrödinger wave function on shape space cannot be defined in a globally smooth manner (at least for nonzero values of angular momentum). String singularities are less of a problem in classical mechanics; although they appear in the canonical Hamiltonian, they do not appear in the classical equations of motion. They can even be removed from the Hamiltonian by the use of noncanonical variables. We shall say more about these issues later.

The fiber-bundle picture also provides a geometrical interpretation of gauge transformations. If a choice of gauge is a choice of a section $\mathcal{S}$, as illustrated in Fig. 14, then a change of gauge is the selection of a new section $\mathcal{S}'$. For example, as illustrated in the figure, we may decide that instead of configuration P as the reference for its fiber we may prefer configuration P'. Then the rotation S is that which maps P into P', i.e., it represents the "distance" (really a rotation) along the fiber between the old and new sections. This "distance" can differ from one fiber to the next, i.e., S is a function of q^μ.

Finally, the fiber-bundle picture illuminates the useful concept of a "democratic gauge." In a democratic gauge, the components of the eigenvectors of the moment-of-inertia tensor in the body frame are democratic invariants, i.e., they take on the same values at any two shapes related by a democracy transformation. For example, in the three-body problem, a democratic gauge is one in which the body-referred eigenvectors of the moment-of-inertia tensor are azimuthally symmetric about the w_3 axis, as indicated by Eq. (3.36). The principal-axis gauge is an example of a democratic gauge, since the eigenvectors in the principal-axis frame are just the unit vectors (1,0,0), etc., which have constant components. On the other hand, xxy gauge is not democratic. It turns out that the geometrical meaning of a democratic gauge is that it is one in which the section $\mathcal{S}$ is invariant under the democracy group, i.e., the transformations (3.22) map points of $\mathcal{S}$ into other such points. Democratic gauges are especially important for the case $n \geqslant 4$, and we shall have more to say about them in future publications.

E. The gauge potential in the n-body problem

The gauge potential emerges when we express the angular momentum about the center of mass in terms of shape and orientational coordinates. In this calculation we can work with either the vector $\{\boldsymbol{\rho}_\alpha\}$ or the vector $\{\mathbf{c}_\alpha\}$; we choose $\{\boldsymbol{\rho}_\alpha\}$ and present alternatives in the $\{\mathbf{c}_\alpha\}$ form to key expressions below.

We begin by defining the $\boldsymbol{\rho}$-space velocities $\mathbf{v}_{s\alpha} = \dot{\boldsymbol{\rho}}_{s\alpha}$, which we express in terms of shape and orientation by differentiating Eq. (3.41) with respect to time. We obtain

$$\mathbf{v}_{s\alpha} = \dot{\boldsymbol{\rho}}_{s\alpha} = \dot{\mathsf{R}}\boldsymbol{\rho}_\alpha + \mathsf{R}\frac{\partial \boldsymbol{\rho}_\alpha}{\partial q^\mu}\dot{q}^\mu. \tag{3.48}$$

Referring these velocities to the body frame, we have

$$\mathbf{v}_\alpha = \mathsf{R}^T\mathbf{v}_{s\alpha} = \Omega\boldsymbol{\rho}_\alpha + \frac{\partial \boldsymbol{\rho}_\alpha}{\partial q^\mu}\dot{q}^\mu = \boldsymbol{\omega}\times\boldsymbol{\rho}_\alpha + \frac{\partial \boldsymbol{\rho}_\alpha}{\partial q^\mu}\dot{q}^\mu, \tag{3.49}$$

where Ω is the antisymmetric matrix,

$$\Omega = \mathsf{R}^T\dot{\mathsf{R}} = -\dot{\mathsf{R}}^T\mathsf{R}, \tag{3.50}$$

and where we associate Ω with the vector $\boldsymbol{\omega}$ according to the notation explained in Appendix B,

$$\Omega \leftrightarrow \boldsymbol{\omega}, \tag{3.51}$$

so that $\Omega\boldsymbol{\rho}_\alpha = \boldsymbol{\omega}\times\boldsymbol{\rho}_\alpha$.

Here $\boldsymbol{\omega}$ is the angular velocity vector referred to the body frame (the angular velocity referred to the space frame is $\boldsymbol{\omega}_s$). The angular velocity is defined as the instantaneous rate of rotation of the body frame with respect to the space frame; this is the usual definition in the physics, chemistry, and engineering literature, but it is at variance with the definition used in several recent mathematical works on the n-body problem, including those of Iwai, 1986, 1987b; Tachibana and Iwai, 1986; Lin and Marsden, 1992; and Marsden, 1992. These authors prefer to define the angular velocity by $\boldsymbol{\omega} = \mathsf{M}^{-1}\mathbf{L}$, so that $\boldsymbol{\omega}$ and the angular momentum $\mathbf{L}$ satisfy the rigid-body relation; this definition has considerable appeal due to features of fiber-bundle theory. (It is the angular velocity of the parallel-translated frame with respect to the space frame; see Appendix D.) This definition of the angular velocity is also used by Jellinek and Li, 1989, in a context described in Sec. V.F. However, we shall stick to the definition given by Eqs. (3.50) and (3.51).

Now we refer the angular momentum about the center of mass to the body frame and express it in terms of shape and orientational coordinates. We have

$$\mathbf{L}=\mathsf{R}^T\mathbf{L}_s=\mathsf{R}^T\sum_{\alpha=1}^{n-1}\boldsymbol{\rho}_{s\alpha}\times\mathbf{v}_{s\alpha}$$
$$=\sum_{\alpha=1}^{n-1}\boldsymbol{\rho}_\alpha\times\mathbf{v}_\alpha$$
$$=\sum_{\alpha=1}^{n-1}\boldsymbol{\rho}_\alpha(\boldsymbol{\omega}\times\boldsymbol{\rho}_\alpha)+\boldsymbol{\rho}_\alpha\times\frac{\partial\boldsymbol{\rho}_\alpha}{\partial q^\mu}\dot{q}^\mu, \tag{3.52}$$

where we use Eqs. (3.19) and (3.49). Into this we introduce the usual moment-of-inertia tensor M,

$$M_{ij}=M_{ij}(q)=\sum_{\alpha=1}^{n-1}(|\boldsymbol{\rho}_\alpha|^2\delta_{ij}-\rho_{\alpha i}\rho_{\alpha j})$$
$$=\sum_{\alpha=1}^{n}m_\alpha[|\mathbf{c}_\alpha|^2\delta_{ij}-c_{\alpha i}c_{\alpha j}], \tag{3.53}$$

and another quantity (De Celles and Darling, 1969),

$$\mathbf{a}_\mu=\mathbf{a}_\mu(q)=\sum_{\alpha=1}^{n-1}\boldsymbol{\rho}_\alpha\times\frac{\partial\boldsymbol{\rho}_\alpha}{\partial q^\mu}=\sum_{\alpha=1}^{n}m_\alpha\mathbf{c}_\alpha\times\frac{\partial\mathbf{c}_\alpha}{\partial q^\mu}, \tag{3.54}$$

so that the angular momentum becomes

$$\mathbf{L}=\mathsf{M}\boldsymbol{\omega}+\mathbf{a}_\mu\dot{q}^\mu. \tag{3.55}$$

Both $\mathsf{M}=\mathsf{M}(q)$ and $\mathbf{a}_\mu=\mathbf{a}_\mu(q)$ are fields over shape space. The field $\mathbf{a}_\mu$ can be thought of as a collection of $3n-6$ 3-vectors, indexed by μ.

More useful than $\mathbf{a}_\mu$ is the gauge potential $\mathbf{A}_\mu$, defined by

$$\mathbf{A}_\mu=\mathbf{A}_\mu(q)=\mathsf{M}^{-1}\mathbf{a}_\mu. \tag{3.56}$$

It is also thought of as a collection of $3n-6$ 3-vectors, or as a tensorlike field over shape space with $3(3n-6)$ components A_μ^i. In terms of $\mathbf{A}_\mu$ the angular momentum takes on an especially useful form,

$$\mathbf{L}=\mathsf{M}(\boldsymbol{\omega}+\mathbf{A}_\mu\dot{q}^\mu). \tag{3.57}$$

The two terms on the right-hand side of this equation are sometimes thought of as the rotational and internal (or vibrational) contributions to the angular momentum; but, as we shall see, this decomposition is not gauge invariant.

To see the physical and geometrical meaning of the gauge potential, we think of the falling cat and set $\mathbf{L}=0$, so that

$$\boldsymbol{\omega}=-\mathbf{A}_\mu\dot{q}^\mu. \tag{3.58}$$

Then we write the angular velocity in terms of its magnitude and direction, $\boldsymbol{\omega}=\omega\hat{\mathbf{n}}$, and multiply through by dt to obtain

$$\hat{\mathbf{n}}\delta\alpha=-\mathbf{A}_\mu dq^\mu, \tag{3.59}$$

where $\delta\alpha=\omega dt$. Thus the gauge potential $\mathbf{A}_\mu$ provides the mapping between an infinitesimal change in shape dq^μ and the corresponding infinitesimal rotation, represented in terms of its axis $\hat{\mathbf{n}}$ and infinitesimal angle $\delta\alpha$, under conditions of vanishing angular momentum. This is a clear generalization of Eq. (2.9), the main difference being that infinitesimal rotations in three dimensions are specified by a vector that can be referred to any frame. In the present formulation, all the vectors, $\boldsymbol{\omega}$, $\hat{\mathbf{n}}$, and $\mathbf{A}_\mu$, are referred to the body frame (hence the absence of the subscript s).

For finite times, the infinitesimal rotations specified by Eq. (3.59) compound upon one another to generate a finite rotation. Of course, the axis changes in general as a function of time, so the elementary rotations do not commute. To find $\mathsf{R}(t)$ for finite times, we suppose $\boldsymbol{\omega}(t)$ is known so that $\Omega(t)$ is also known. Then Eq. (3.50) gives

$$\dot{\mathsf{R}}=\mathsf{R}\Omega(t), \tag{3.60}$$

a system of nine coupled, linear differential equations for the components of R with time-dependent coefficients. The solution can be written as a time-ordered product,

$$\mathsf{R}(t)=\mathsf{R}_0T\exp\left[\int_{t_0}^{t_1}\Omega(t')dt'\right], \tag{3.61}$$

where T represents the time ordering. Mathematically, this is just another notation for the solution of Eq. (3.60), but it is supposed to suggest the composition of the infinitesimal rotations mentioned above. Of course, Eq. (3.60) can also be expressed in terms of Euler angles (whereupon it becomes nonlinear and rather unattractive), or Cayley-Klein parameters, etc.

Equations (3.60) and (3.61) apply to any problem in which $\boldsymbol{\omega}(t)$ is given, e.g., rigid-body mechanics, and merely determine the rotation connecting two frames, regardless of the context. But when $\boldsymbol{\omega}(t)$ is generated by the falling cat with vanishing angular momentum, then Eq. (3.58) applies, which we rewrite in the form

$$\Omega=-\mathsf{A}_\mu\dot{q}^\mu, \tag{3.62}$$

where

$$\mathsf{A}_\mu\leftrightarrow\mathbf{A}_\mu. \tag{3.63}$$

Here we use sans serif A to indicate the antisymmetric matrix A_μ, in contrast to the vector $\mathbf{A}_\mu$ (in boldface). Substituting Eq. (3.62) into Eq. (3.61), we obtain a path-ordered product,

$$\mathsf{R}(t)=\mathsf{R}_0P\exp\left[-\int_{q_0}^{q_1}\mathsf{A}_\mu dq^\mu\right], \tag{3.64}$$

where now the integral is taken along the path $q^\mu(t)$ in shape space, with $q(t_0)=q_0$ and $q(t_1)=q_1$. Again, this is just notation, but it suggests correctly that the rotation $\mathsf{R}(t)$ is independent of the rate of traversal of the path, i.e., that $\mathsf{R}(t)$ is "geometrical." This is the same conclusion we reached for our planar models in Sec. II, here generalized to non-Abelian rotations. Alternatively, we can write Eq. (3.60) in the form

$$d\mathsf{R}=-\mathsf{R}\mathsf{A}_\mu dq^\mu, \tag{3.65}$$

in which the time parameter has dropped out. The geometrical meaning of the gauge potential $\mathbf{A}_\mu$ was apparently first appreciated by Guichardet (1984) and later

independently by Shapere and Wilczek (1989b), whose presentation is similar to ours.

To define the "net rotation" of a deformable body during some time interval, we imagine some vector $\mathbf{k}$ that is fixed in the body frame (e.g., it could be one of the unit vectors defining the body frame). Thus its body components are constant in time. But the space components $\mathbf{k}_s$ are time dependent, since $\mathbf{k}_s(t)=\mathsf{R}(t)\mathbf{k}$. If we now consider $\mathbf{k}_s$ at some initial and final times, $\mathbf{k}_{s0}=\mathsf{R}_0\mathbf{k}$ and $\mathbf{k}_{s1}=\mathsf{R}_1\mathbf{k}$, then it is logical to define the net rotation between the two given times in terms of the operator that maps $\mathbf{k}_{s0}$ into $\mathbf{k}_{s1}$, for any choice of $\mathbf{k}$. Since $\mathbf{k}_{s1}=\mathsf{R}_1\mathsf{R}_0^T\mathbf{k}_{s0}$, we take the matrix representing this operator in the space frame as $\mathsf{R}_1\mathsf{R}_0^T$. This matrix is the analog of the angle $\Delta\theta$ introduced in Eq. (2.11).

Next we consider the behavior of the net rotation under gauge transformations. Letting the two times be t_0 and t_1, corresponding to shapes q_0 and q_1, then by Eq. (3.43) we have

$$\mathsf{R}_1\mathsf{R}_0^T=\mathsf{R}_1'\mathsf{S}_1^T\mathsf{S}_0\mathsf{R}_0'^T, \tag{3.66}$$

where $\mathsf{S}_0=\mathsf{S}(q_0)$, $\mathsf{S}_1=\mathsf{S}(q_1)$. If $q_0\neq q_1$ (an open curve in shape space), then $\mathsf{R}_1\mathsf{R}_0^T\neq\mathsf{R}_1'\mathsf{R}_0'^T$ and the net rotation is gauge dependent; but if $q_0=q_1$ (a closed curve), then the S matrices drop out and the net rotation is gauge invariant. This is the same conclusion reached for our planar models in Sec. II, and the reason is the same: for an open curve, the two frames at the two times are attached to different shapes and can be redefined independently of one another under a gauge transformation, but for closed curves there is only one shape and the frame redefinition drops out of the computation.

F. Gauge invariance and gauge covariance

We now begin a systematic program to examine how the various quantities of the theory transform under gauge transformations. First we note that the shape coordinates q^μ, their time derivatives $\dot q^\mu$, accelerations $\ddot q^\mu$, etc., are all gauge invariant, because their definitions do not depend on a body frame. Likewise, the space components of any vector that has a meaning independent of body frame, such as $\mathbf{r}_{s\alpha}$, $\boldsymbol{\rho}_{s\alpha}$, $\mathbf{c}_{s\alpha}$, $\mathbf{L}_s$, and their time derivatives, are all gauge invariant. Orientational coordinates θ^i or $\mathsf{R}(\theta^i)$ are gauge dependent, as indicated by Eq. (3.43).

If any of the vectors whose space components are gauge invariant are transformed to the body frame, then naturally the new (body) components will be gauge dependent, because a redefinition of body frame will change the frame to which they are referred. But the transformation law is just that expected when we change the basis to which a vector is referred, namely,

$$\mathbf{c}_\alpha=\mathsf{S}\mathbf{c}_\alpha',\quad \boldsymbol{\rho}_\alpha=\mathsf{S}\boldsymbol{\rho}_\alpha',\quad \mathbf{v}_\alpha=\mathsf{S}\mathbf{v}_\alpha',\quad \mathbf{L}=\mathsf{S}\mathbf{L}', \tag{3.67}$$

etc. Similarly, the moment-of-inertia tensor transforms under a gauge transformation exactly as a second-rank tensor should under change of basis, namely,

$$\mathsf{M}=\mathsf{S}\mathsf{M}'\mathsf{S}^T, \tag{3.68}$$

as follows from the definition (3.53). The inverse moment-of-inertia tensor M^{-1} transforms similarly. Thus, although it is not customary to refer the moment-of-inertia tensor to the space frame, we would obtain gauge-invariant components if we did so. We shall refer to quantities that transform as in Eqs. (3.67) or (3.68), with one copy of the S matrix for each index i,j, etc., as *gauge covariant.*

But not everything is gauge covariant. On transforming the body angular velocity, we find

$$\boldsymbol{\omega}\leftrightarrow\Omega=\mathsf{R}^T\dot{\mathsf{R}}=\mathsf{S}\mathsf{R}'^T(\dot{\mathsf{R}}'\mathsf{S}^T+\mathsf{R}'\dot{\mathsf{S}}^T)=\mathsf{S}(\Omega'+\dot{\mathsf{S}}^T\mathsf{S})\mathsf{S}^T, \tag{3.69}$$

where we use $\mathsf{R}=\mathsf{R}'\mathsf{S}^T$ and $\Omega'=\mathsf{R}'^T\dot{\mathsf{R}}'$. Next we note that $\dot{\mathsf{S}}^T\mathsf{S}$ is antisymmetric and we follow the pattern of relations between $\boldsymbol{\omega}$ and Ω to write

$$\dot{\mathsf{S}}^T\mathsf{S}=-\mathsf{S}^T\dot{\mathsf{S}}=-\mathsf{S}^T\frac{\partial\mathsf{S}}{\partial q^\mu}\dot q^\mu=-\Gamma_\mu\dot q^\mu, \tag{3.70}$$

where the antisymmetric matrix Γ_μ can be associated with a vector $\boldsymbol{\gamma}_\mu$,

$$\Gamma_\mu=\mathsf{S}^T\frac{\partial\mathsf{S}}{\partial q^\mu}\leftrightarrow\boldsymbol{\gamma}_\mu. \tag{3.71}$$

Then the transformation law takes the form

$$\Omega=\mathsf{S}(\Omega'-\Gamma_\mu\dot q^\mu)\mathsf{S}^T, \tag{3.72}$$

or, if we convert back to vectors,

$$\boldsymbol{\omega}=\mathsf{S}(\boldsymbol{\omega}'-\boldsymbol{\gamma}_\mu\dot q^\mu), \tag{3.73}$$

where we use Eq. (B5). Thus the angular velocity $\boldsymbol{\omega}$ is not gauge covariant, due to the second term on the right in Eq. (3.73).

The geometrical reason for this more complicated transformation law is the following. The angular velocity represents the relation between the space and body frames at two times t and $t+dt$. But since the shape can change during the infinitesimal time increment dt, the body frames attached to the two shapes can be redefined independently of one another under a gauge transformation. Thus $\boldsymbol{\omega}$ is not gauge covariant. Nor for that matter is the space-referred vector $\boldsymbol{\omega}_s$ gauge invariant; it does not represent a vector in a geometrical sense that has any meaning independent of conventions for body frame, so even its space components are gauge dependent.

If the angular velocity is not gauge covariant, then by Eq. (3.58) the gauge potential $\mathbf{A}_\mu$ cannot be either. Indeed, appealing directly to the definition (3.56), we find the transformation law

$$\mathbf{A}_\mu=\mathsf{S}(\mathbf{A}_\mu'+\boldsymbol{\gamma}_\mu). \tag{3.74}$$

On the other hand, the vector $\boldsymbol{\omega}+\mathbf{A}_\mu\dot q^\mu$ is gauge covariant, as follows from Eq. (3.57), since both $\mathbf{L}$ and M are gauge covariant. Thus we see that the decomposition of $\mathbf{L}$ into the two terms seen in Eq. (3.57) is gauge depen-

dent, even though it is tempting to think of them as the "rotational" and "internal" contributions to the angular momentum.

In tensor analysis it is traditional not to consider an object a tensor just because it has indices, but to require in addition certain transformation laws under coordinate transformations. In particular, a true tensor is multilinear in its indices, transforming by one copy of the Jacobian matrix or its inverse for each index, depending on whether the index is contravariant or covariant. Not all the objects of interest in tensor analysis are true tensors by this definition.

The various quantities of our theory have two kinds of indices, Latin ones i,j,k, etc., which we shall call R indices, and Greek ones μ,ν, etc., which we shall call q indices. Gauge transformations involve only the R indices, whereas coordinate transformations on shape space involve only the q indices. Regarding the R indices, it is not necessary to distinguish contravariant and covariant indices, because our transformation matrices S are always orthogonal. But it is necessary to distinguish those objects which transform multilinearly in the R indices, i.e., with one copy of the S matrix for each index, from objects that have more complicated transformation laws. We have called the former kind of object "gauge covariant;" we shall also call them "true R tensors." The word tensor includes both scalars and vectors, so in particular, a true R scalar is an object without R indices that is invariant under gauge transformations. All the quantities in our theory that are independent of convention must be true R scalars. So far we have determined that q^μ, $\dot{q}^\mu$, etc., are true R scalars; $\mathbf{c}_\alpha$, $\boldsymbol{\rho}_\alpha$, $\mathbf{L}$, etc. are true R vectors; M, M^{-1} are true R tensors of second rank; but $\boldsymbol{\omega}$ and $\mathbf{A}_\mu$ are not true R tensors (of any rank).

Similar considerations apply to the q indices. We shall pay less attention to these because the rules and transformation laws for the q indices under coordinate transformations in shape space are exactly as in ordinary tensor analysis. For example, the quantity $\dot{q}^\mu$ transforms as a contravariant vector,

$$\dot{q}^\mu=\frac{\partial q^\mu}{\partial q'^\nu}\dot{q}'^\nu, \tag{3.75}$$

under the change of coordinates $q^\mu\to q'^\nu$. Thus $\dot{q}^\mu$ is a true R scalar and a true q-contravariant vector. Similarly, the gauge potential, although not a true R vector, is a true q-covariant vector,

$$\mathbf{A}_\mu=\frac{\partial q'^\nu}{\partial q^\mu}\mathbf{A}'_\nu, \tag{3.76}$$

where now the prime refers to the new components of $\mathbf{A}_\mu$ after the coordinate transformation.

There are several advantages of true R tensors. First, as we have noted, true R tensors have gauge-invariant components when referred to the space frame; we may therefore think of them as having an absolute geometrical meaning. Second, true R tensors can be contracted to form true R scalars, which are gauge invariant. Thus, for example, the quantity $(1/2)\mathbf{L}\cdot\mathsf{M}^{-1}\cdot\mathbf{L}$ is a true R scalar, whereas $(1/2)\boldsymbol{\omega}\cdot\mathsf{M}\cdot\boldsymbol{\omega}$ is not. [In rigid-body theory, these would be equal to each other and to the kinetic energy of rotation; but here they are unequal and have different transformation laws. Altogether, $(1/2)\mathbf{L}\cdot\mathsf{M}^{-1}\cdot\mathbf{L}$ is a more fundamental quantity.]

A third property of true R tensors is that if they vanish in one gauge, they vanish in all gauges. For example, the statement $\mathbf{L}=0$ is gauge invariant. The same is not true for $\boldsymbol{\omega}=0$, for by a gauge transformation it is possible to make $\boldsymbol{\omega}$ take on any desired value (zero or nonzero) at a given instant in time. One can even do this along an entire curve segment $q^\mu(t)$ in shape space, so long as the curve does not cross itself. For example, by establishing a gauge that just happens to make the body frames turn at the right rate as the motion proceeds along a given curve $q^\mu(t)$, one can make $\boldsymbol{\omega}=0$. However, the scheme will fail if the curve crosses itself, for then the curve returns to a shape in which the body frame was already defined to make $\boldsymbol{\omega}=0$ on an earlier part of itself.

Similarly, it is possible to make $\mathbf{A}_\mu$ vanish at a single point of shape space by means of a gauge transformation, or even along a curve that does not intersect itself. Indeed, one of the objects of the Eckart conventions is to make $\mathbf{A}_\mu=0$ at the equilibrium configuration of a molecule. In this way, the "Coriolis terms" in the Lagrangian or Hamiltonian are first order in the small displacements from equilibrium (Casimir, 1931; Eckart, 1935; Wilson, Decius, and Cross, 1955), since $\mathbf{A}_\mu$ deviates linearly from zero in the small displacement. This convention has about the same significance as one that causes the phase of the wave function for a charged particle in a magnetic field to take on some particular value at a specified spatial point; such conventions may be convenient, but in neither case do they have any physical significance.

G. The curvature form or Coriolis tensor

Now we introduce the curvature form or Coriolis tensor $\mathbf{B}_{\mu\nu}$ by considering small cycles in shape space under conditions of vanishing angular momentum. For our planar models in Sec. II, we introduced the curvature form by means of Stokes' theorem, but in the three-dimensional, non-Abelian gauge theory Stokes' theorem cannot be used. Thus it is not possible to transform path-ordered integrals such as (3.64) into integrals over some enclosed region, at least if the region is finite. But for infinitesimal regions, something like an infinitesimal version of Stokes' theorem can be applied, and it leads to the curvature form. The following construction is standard in gauge theories; only the physical and geometrical meaning of the quantities involved differs from other gauge theories.

We begin by considering an infinitesimal parallelogram in shape space, spanned by infinitesimal vectors ξ^μ and η^μ, as illustrated in Fig. 15. The quantities ξ^μ and η^μ are regarded as infinitesimal increments in the coordinates q^μ, so that the parallelogram closes exactly (to all orders of infinitesimals). We imagine going around

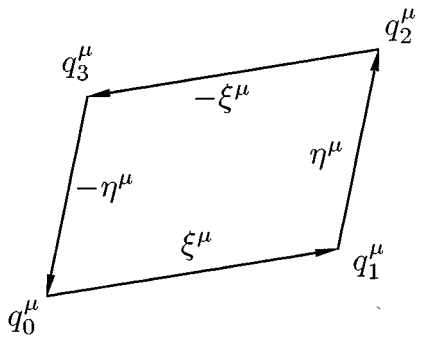

FIG. 15. An infinitesimal parallelogram in shape space.

this infinitesimal parallelogram under conditions of vanishing angular momentum, starting at point q_0^μ and proceeding to q_1^μ, q_2^μ, q_3^μ, and back to the starting point, and we wish to compute the rotation generated. We let the values of the orientation, specified by R, be $\mathsf{R}_0,\ldots,\mathsf{R}_4$ as we go around the parallelogram; although q^μ returns to its starting value, R does not; $\mathsf{R}_4 \neq \mathsf{R}_0$, since in general some net rotation is generated.

For the first leg $q_0 \to q_1$ we parametrize the curve by

$$q^\mu(t) = q_0^\mu + t\xi^\mu, \tag{3.77}$$

so that $q(0)=q_0$ and $q(1)=q_1$. Since the rotation generated does not depend on the time parametrization, we can use any parametrization we like. We solve Eq. (3.60) by expanding in a Taylor series in time and set $t=1$ to obtain $\mathsf{R}_1=\mathsf{R}(1)$. We have

$$\mathsf{R}(t) = \mathsf{R}(0) + t\dot{\mathsf{R}}(0) + \frac{t^2}{2}\ddot{\mathsf{R}}(0) + \cdots,$$

$$\mathsf{R}_1 = \mathsf{R}_0 + \dot{\mathsf{R}}_0 + \frac{1}{2}\ddot{\mathsf{R}}_0 + \cdots, \tag{3.78}$$

where we carry things only through second order because that is where the first nonvanishing effect is found. To obtain R and its derivatives at $t=0$ we combine Eqs. (3.60) and (3.62) and differentiate,

$$\dot{\mathsf{R}} = -\mathsf{R}\mathsf{A}_\mu \dot{q}^\mu,$$

$$\ddot{\mathsf{R}} = -\dot{\mathsf{R}}\mathsf{A}_\mu \dot{q}^\mu - \mathsf{R}\mathsf{A}_{\mu,\nu}\dot{q}^\mu \dot{q}^\nu - \mathsf{R}\mathsf{A}_\mu \ddot{q}^\mu, \tag{3.79}$$

where we use comma notation for derivatives (see Appendix A). But by Eq. (3.77) we have $\dot{q}^\mu = \xi^\mu$ and $\ddot{q}^\mu = 0$, so

$$\dot{\mathsf{R}} = -\mathsf{R}\mathsf{A}_\mu \xi^\mu,$$

$$\ddot{\mathsf{R}} = \mathsf{R}(\mathsf{A}_\nu \mathsf{A}_\mu - \mathsf{A}_{\mu,\nu})\xi^\mu \xi^\nu, \tag{3.80}$$

where we have used the first equation to eliminate $\dot{\mathsf{R}}$ in the second. Substituting these into Eq. (3.78) gives us an equation for the rotation produced along leg $q_0 \to q_1$.

Equations valid for leg $q_1 \to q_2$ are obtained from those for leg $q_0 \to q_1$ by changing subscripts $0\to 1$, $1\to 2$, and $\xi^\mu \to \eta^\mu$; equations for the next leg are obtained by subsequently changing subscripts $1\to 2$, $2\to 3$, and $\eta^\mu \to -\xi^\mu$, etc. Summarizing these, we have

$$\mathsf{R}_1 = \mathsf{R}_0[\mathsf{I} - \mathsf{A}_{0\mu}\xi^\mu + \tfrac{1}{2}(\mathsf{A}_{0\nu}\mathsf{A}_{0\mu} - \mathsf{A}_{0\mu,\nu})\xi^\mu \xi^\nu + \cdots] = \mathsf{R}_0\mathsf{F}_0,$$

$$\mathsf{R}_2 = \mathsf{R}_1[\mathsf{I} - \mathsf{A}_{1\mu}\eta^\mu + \tfrac{1}{2}(\mathsf{A}_{1\nu}\mathsf{A}_{1\mu} - \mathsf{A}_{1\mu,\nu})\eta^\mu \eta^\nu + \cdots] = \mathsf{R}_1\mathsf{F}_1,$$

$$\mathsf{R}_3 = \mathsf{R}_2[\mathsf{I} + \mathsf{A}_{2\mu}\xi^\mu + \tfrac{1}{2}(\mathsf{A}_{2\nu}\mathsf{A}_{2\mu} - \mathsf{A}_{2\mu,\nu})\xi^\mu \xi^\nu + \cdots] = \mathsf{R}_2\mathsf{F}_2,$$

$$\mathsf{R}_4 = \mathsf{R}_3[\mathsf{I} + \mathsf{A}_{3\mu}\eta^\mu + \tfrac{1}{2}(\mathsf{A}_{3\nu}\mathsf{A}_{3\mu} - \mathsf{A}_{3\mu,\nu})\eta^\mu \eta^\nu + \cdots] = \mathsf{R}_3\mathsf{F}_3, \tag{3.81}$$

where the symbols F_i are abbreviations for the matrices in the square brackets and where the numeric subscripts, e.g., the 3 in $\mathsf{A}_{3\mu}$, indicate the point, e.g., q_3^μ, at which the quantity in question is evaluated. Combining these, we have for the net rotation generated on going around the whole loop,

$$\mathsf{R}_4\mathsf{R}_0^T = \mathsf{R}_0(\mathsf{F}_0\mathsf{F}_1\mathsf{F}_2\mathsf{F}_3)\mathsf{R}_0^T. \tag{3.82}$$

To compute the product of the F_i, it is convenient first to have all the fields appearing in the F_i evaluated at a common point, say, q_0. Expanding everything about q_0, we have

$$\mathsf{A}_{1\mu} = \mathsf{A}_\mu(q_0+\xi) = \mathsf{A}_{0\mu} + \mathsf{A}_{0\mu,\nu}\xi^\nu + \cdots,$$

$$\mathsf{A}_{2\mu} = \mathsf{A}_\mu(q_0+\xi+\eta) = \mathsf{A}_{0\mu} + \mathsf{A}_{0\mu,\nu}(\xi^\nu + \eta^\nu) + \cdots,$$

$$\mathsf{A}_{3\mu} = \mathsf{A}_\mu(q_0+\eta) = \mathsf{A}_{0\mu} + \mathsf{A}_{0\mu,\nu}\eta^\nu + \cdots. \tag{3.83}$$

Then the expressions for the F_i become

$$\mathsf{F}_0 = \mathsf{I} - \mathsf{A}_\mu\xi^\mu + \tfrac{1}{2}(\mathsf{A}_\nu\mathsf{A}_\mu - \mathsf{A}_{\mu,\nu})\xi^\mu\xi^\nu + \cdots,$$

$$\mathsf{F}_1 = \mathsf{I} - \mathsf{A}_\mu\eta^\mu - \mathsf{A}_{\mu,\nu}\eta^\mu\xi^\nu + \tfrac{1}{2}(\mathsf{A}_\nu\mathsf{A}_\mu - \mathsf{A}_{\mu,\nu})\eta^\mu\eta^\nu + \cdots,$$

$$\mathsf{F}_2 = \mathsf{I} + \mathsf{A}_\mu\xi^\mu + \mathsf{A}_{\mu,\nu}\xi^\mu\eta^\nu + \tfrac{1}{2}(\mathsf{A}_\nu\mathsf{A}_\mu + \mathsf{A}_{\mu,\nu})\xi^\mu\xi^\nu + \cdots,$$

$$\mathsf{F}_3 = \mathsf{I} + \mathsf{A}_\mu\eta^\mu + \tfrac{1}{2}(\mathsf{A}_\nu\mathsf{A}_\mu + \mathsf{A}_{\mu,\nu})\eta^\mu\eta^\nu + \cdots, \tag{3.84}$$

where now we omit the numeric subscripts on the fields A_μ, it being understood that everything is evaluated at q_0.

When we multiply these together, carrying the product out to second order and being careful about the order of noncommuting matrices, and substitute into Eq. (3.82), we find

$$\mathsf{R}_4\mathsf{R}_0^{-1} = \mathsf{R}_0(\mathsf{I} - \mathsf{B}_{\mu\nu}\xi^\mu\eta^\nu + \cdots)\mathsf{R}_0^T, \tag{3.85}$$

where

$$\mathsf{B}_{\mu\nu} = \frac{\partial \mathsf{A}_\nu}{\partial q^\mu} - \frac{\partial \mathsf{A}_\mu}{\partial q^\nu} - [\mathsf{A}_\mu, \mathsf{A}_\nu]. \tag{3.86}$$

Here the square brackets indicate the matrix commutator. The field $\mathsf{B}_{\mu\nu}$ is the matrix version of the curvature form or Coriolis tensor. Since the matrix $\mathsf{B}_{\mu\nu}$ (for fixed values of $\mu\nu$) is antisymmetric, it can be converted into the vector version of the curvature form,

$$\mathsf{B}_{\mu\nu} \leftrightarrow \mathbf{B}_{\mu\nu} = \frac{\partial \mathbf{A}_\nu}{\partial q^\mu} - \frac{\partial \mathbf{A}_\mu}{\partial q^\nu} - \mathbf{A}_\mu \times \mathbf{A}_\nu, \tag{3.87}$$

where we use Eq. (B6). In either form, the Coriolis tensor is antisymmetric in the indices μ,ν,

$$\mathsf{B}_{\mu\nu}=-\mathsf{B}_{\nu\mu}, \quad \mathbf{B}_{\mu\nu}=-\mathbf{B}_{\nu\mu}. \tag{3.88}$$

To see the geometrical meaning of the Coriolis tensor, we note that $\mathsf{R}_4\mathsf{R}_0^T$ is an infinitesimal rotation which we can write in axis-angle form. We denote the axis, referred to the space frame, by $\hat{\mathbf{n}}_s$ and the angle by $\delta\alpha$, and, as before, we write $\mathbf{k}$ for a vector fixed in the body frame, with space components $\mathbf{k}_{s0}=\mathsf{R}_0\mathbf{k}$ at the beginning of the excursion around the parallelogram and $\mathbf{k}_{s4}=\mathsf{R}_4\mathbf{k}$ at the end. Then we have

$$\begin{aligned}\mathbf{k}_{s4}&=(\mathsf{R}_4\mathsf{R}_0^{-1})\mathbf{k}_{s0}=\mathbf{k}_{s0}+\delta\alpha\hat{\mathbf{n}}_s\times\mathbf{k}_{s0}\\&=(\mathsf{I}+\delta\alpha\mathsf{N}_s)\mathbf{k}_{s0}=\mathsf{R}_0(\mathsf{I}+\delta\alpha\mathsf{N})\mathsf{R}_0^T\mathbf{k}_{s0},\end{aligned} \tag{3.89}$$

where $\hat{\mathbf{n}}_s\leftrightarrow\mathsf{N}_s=\mathsf{R}_0\mathsf{N}\mathsf{R}_0^T$, $\hat{\mathbf{n}}_s=\mathsf{R}_0\hat{\mathbf{n}}$, $\hat{\mathbf{n}}\leftrightarrow\mathsf{N}$, so that $(\hat{\mathbf{n}}_s,\mathsf{N}_s)$ and $(\hat{\mathbf{n}},\mathsf{N})$ are, respectively, the space and body versions of the axis of rotation, in both vector and antisymmetric matrix form. Comparing Eq. (3.89) with Eq. (3.85), we see that (with a conventional minus sign) $\mathsf{B}_{\mu\nu}\xi^\mu\eta^\nu$ and $\mathbf{B}_{\mu\nu}\xi^\mu\eta^\nu$ are, respectively, the matrix and vector versions of the infinitesimal rotation generated by going around the parallelogram under conditions of vanishing angular momentum, represented in axis-angle form and referred to the body frame. That is, we have

$$\hat{\mathbf{n}}\delta\alpha=-\mathbf{B}_{\mu\nu}\xi^\mu\eta^\nu. \tag{3.90}$$

We chose a minus sign in the definition of $\mathsf{B}_{\mu\nu}$ in Eq. (3.86) in order to make a minus sign come out here, so that this equation would look like Eq. (3.59).

Equations (3.59) and (3.90) have a similar structure, but there is an important difference: the rotation generated by the open infinitesimal line segment dq^μ in Eq. (3.59) is gauge dependent, while the rotation generated by the closed infinitesimal parallelogram spanned by ξ^μ,η^μ in Eq. (3.90) is gauge invariant. This means that if the axis of the rotation in Eq. (3.90) is referred to the space frame, it is gauge invariant, whereas if referred to the body frame, as in Eq. (3.90), it is gauge covariant. Therefore the Coriolis tensor $\mathbf{B}_{\mu\nu}$, unlike the gauge potential $\mathbf{A}_\mu$, is a true R vector.

The gauge covariance of $\mathbf{B}_{\mu\nu}$ is an important fact which can be verified directly by subjecting the definition to a gauge transformation. To do this it is easier to work with the matrix version, as in Eq. (3.86). We use the transformation law for the gauge potential, Eq. (3.74), which in matrix form is

$$\mathsf{A}_\mu=\mathsf{S}(\mathsf{A}'_\mu+\Gamma_\mu)\mathsf{S}^T=\mathsf{S}\mathsf{A}'_\mu\mathsf{S}^T+\frac{\partial\mathsf{S}}{\partial q^\mu}\mathsf{S}^T, \tag{3.91}$$

which we substitute into Eq. (3.86). Eighteen terms result, of which fourteen cancel, leaving us with

$$\mathsf{B}_{\mu\nu}=\mathsf{S}\left(\frac{\partial\mathsf{A}'_\nu}{\partial q^\mu}-\frac{\partial\mathsf{A}'_\mu}{\partial q^\nu}-\mathsf{A}'_\mu\mathsf{A}'_\nu+\mathsf{A}'_\nu\mathsf{A}'_\mu\right)\mathsf{S}^T=\mathsf{S}\mathsf{B}'_{\mu\nu}\mathsf{S}^T, \tag{3.92}$$

or simply

$$\mathbf{B}_{\mu\nu}=\mathsf{S}\mathbf{B}'_{\mu\nu}. \tag{3.93}$$

The gauge covariance of the Coriolis tensor has several important consequences. Unlike the gauge potential $\mathbf{A}_\mu$, $\mathbf{B}_{\mu\nu}$ cannot be made to vanish at a point of shape space by means of a gauge transformation unless it is already zero there, which in fact never happens. For example, at the equilibrium shape of a molecule, $\mathbf{B}_{\mu\nu}$ has a nonzero value that can be referred to various body frames but that otherwise cannot be changed. Another consequence of the gauge covariance of $\mathbf{B}_{\mu\nu}$ is that it is impossible to choose a convention for body frame that will cause $\mathbf{A}_\mu$ to vanish over a finite region of shape space. If this were possible, then the "Coriolis coupling" terms in the molecular Hamiltonian would vanish and there would be a separation of rotational and vibrational degrees of freedom at lowest order in the Born-Oppenheimer ordering parameter. Therefore the possibility of finding a convention to make $\mathbf{A}_\mu$ vanish in a finite neighborhood of the equilibrium position was considered in early studies by Eckart (1935). Eckart did not think it was possible to transform away $\mathbf{A}_\mu$, but he was not sure and did not supply a proof. This same doubt has persisted into more recent reviews of the subject (Sutcliffe, 1980). But it is easy to put it to rest. If there were a gauge for which $\mathbf{A}_\mu$ were zero over a finite region, then we would have $\mathbf{B}_{\mu\nu}=0$ over that same region, a gauge-invariant result. But in fact $\mathbf{B}_{\mu\nu}\neq 0$, as we find by a direct calculation, which can be carried out in any gauge (see below); therefore making $\mathbf{A}_\mu=0$ over a finite region is impossible.

H. Examples of fields and gauges in the three-body problem

In the case of the three-body problem, it is easy to compute some of the fields we have defined. These can be put into different forms, depending on the choice of gauge convention and shape coordinates. Three-body problems are common in the literature and much is known about them, although gauge transformations are seldom contemplated. There are many special features of the three-body problem, some of which we point out here, which limit its utility for illustrating general properties of n-body systems. On the other hand, not only does the computational effort increase for $n>3$, but also a proper treatment of the fields on shape space for $n\geqslant 4$ requires due attention to the democracy group and other considerations. Therefore we shall restrict our examples here to the three-body problem and present calculations for $n>3$ in future publications.

We begin with the xxy gauge defined by Eq. (3.38) and use coordinates (ρ_1,ρ_2,ϕ). Since the triangle formed by the three bodies lies in the body xy plane, the moment-of-inertia tensor block diagonalizes,

$$M_{ij}=\begin{pmatrix}\rho_2^2\sin^2\phi & -\rho_2^2\sin\phi\cos\phi & 0\\ -\rho_2^2\sin\phi\cos\phi & \rho_1^2+\rho_2^2\cos^2\phi & 0\\ 0 & 0 & \rho_1^2+\rho_2^2\end{pmatrix}. \tag{3.94}$$

Because the figure is planar, the two moments of inertia

in the plane add up to the third moment of inertia, i.e., the trace of the upper 2×2 block is equal to the component M_{33}.

It is now a short calculation to find the gauge potential in the xyy gauge and (ρ_1,ρ_2,ϕ) coordinates, working from the definition (3.54) and (3.56). The result is

$$\mathbf{A}_{\rho_1}=0,\quad \mathbf{A}_{\rho_2}=0,\quad \mathbf{A}_{\phi}=\frac{\rho_2^2}{\rho_1^2+\rho_2^2}\hat{\mathbf{z}}, \tag{3.95}$$

where $\hat{\mathbf{z}}$ is the unit vector in the body frame. Instead of listing the components of $\mathbf{A}_\mu$, it is more compact and convenient to use a differential form,

$$\mathbf{A}_\mu dq^\mu=\frac{\rho_2^2}{\rho_1^2+\rho_2^2}d\phi\hat{\mathbf{z}}. \tag{3.96}$$

From the gauge potential we easily compute the Coriolis tensor, using Eq. (3.87); the cross product cancels. Because of the antisymmetry, we only have to list the components of $\mathbf{B}_{\mu\nu}$ for which $\mu<\nu$; these are

$$\mathbf{B}_{\rho_1\phi}=-\frac{2\rho_1\rho_2^2}{(\rho_1^2+\rho_2^2)^2}\hat{\mathbf{z}},\quad \mathbf{B}_{\rho_2\phi}=+\frac{2\rho_1^2\rho_2}{(\rho_1^2+\rho_2^2)^2}\hat{\mathbf{z}}, \tag{3.97}$$

or, in terms of the associated differential form,

$$\sum_{\mu<\nu}\mathbf{B}_{\mu\nu}dq^\mu\wedge dq^\nu$$

$$=\frac{2\rho_1\rho_2}{(\rho_1^2+\rho_2^2)^2}(\rho_1 d\rho_2\wedge d\phi-\rho_2 d\rho_1\wedge d\phi)\hat{\mathbf{z}}. \tag{3.98}$$

The most striking aspect of these results is that the gauge potential and curvature form have only a z component. This is related to the elementary fact (Whittaker, 1960) that three-body motion is planar when $\mathbf{L}=0$, so all rotations generated by shape deformations under conditions of vanishing angular momentum must take place in the plane of the triangle formed by the three bodies. [The holonomy group for the three-body problem is SO(2).] This special form of $\mathbf{A}_\mu$ means that the cross-product term in the definition of $\mathbf{B}_{\mu\nu}$, the characteristic of non-Abelian gauge theories, vanishes (in gauges that place the three particles in a constant plane in the body frame, such as xyy gauge). Thus the gauge theory of the three-body problem is pseudo-Abelian, in a sense. For example, the different matrices A_μ in the path-ordered product (3.64) commute at different q points, the path-ordering operator P can be dropped, and Stokes' theorem can be applied. One can also think in terms of the "field lines" of $\mathbf{B}_{\mu\nu}$ as in ordinary electromagnetic theory, since effectively $\mathbf{A}_\mu$ and $\mathbf{B}_{\mu\nu}$ become scalars in their R indices, having only a z component. These are all special features of the three-body problem that do not generalize to higher values of n. On the other hand, three-body motion for $\mathbf{L}\neq 0$ does not take place in a constant plane as viewed from the space frame, and the time-ordered integration in Eq. (3.61) will involve noncommuting matrices.

Obviously the gauge fields $\mathbf{A}_\mu$ and $\mathbf{B}_\mu$ are singular when $\rho_1=\rho_2=0$, i.e., at the three-body collision, located at the vertex of the pyramid in Fig. 10. What is less obvious is that in a certain sense the gauge potential $\mathbf{A}_\mu$ has a singularity when $\rho_1=0$, regardless of the value of ρ_2, as will be explained momentarily. In fact, the Coriolis tensor $\mathbf{B}_{\mu\nu}$ has the form of a Dirac monopole, with field lines radiating out from the three-body collision, and the singularity in $\mathbf{A}_\mu$ just referred to is a monopole string. This monopole was apparently first discovered by Iwai (1987a) in his treatment of the planar three-body problem (some details are different in the planar case). We shall call it the "Iwai monopole."

To see the Iwai monopole more explicitly, it helps to transform to the (w_1,w_2,w_3) coordinates, defined in Eq. (3.30). We stay in the xyy gauge. The moment-of-inertia tensor has no q indices and does not change, but $\mathbf{A}_\mu$ transforms as a covariant vector, as in Eq. (3.76). We find

$$\mathbf{A}_\mu dq^\mu=\frac{w_2dw_3-w_3dw_2}{2w(w+w_1)}\hat{\mathbf{z}}. \tag{3.99}$$

From this we easily find the Coriolis tensor, which we present in the form

$$\frac{1}{2}\mathbf{B}_{\mu\nu}dq^\mu\wedge dq^\nu=\epsilon_{ijk}\frac{w_i}{4w^3}dw_j\wedge dw_k\hat{\mathbf{z}}. \tag{3.100}$$

The Coriolis tensor has the form of a monopole at the origin of shape space, as we shall now explain by analogy with the ordinary Dirac monopole.

To compare the Iwai monopole with an ordinary Dirac monopole, it is necessary first to be careful of notation, since the index i in the components A_i, B_i of the magnetic vector potential $\mathbf{A}$ and magnetic field $\mathbf{B}$ in ordinary space are analogous to the q indices on the gauge potential $\mathbf{A}_\mu$ and curvature form $\mathbf{B}_{\mu\nu}$. The boldface on the latter symbols represents the R indices, which have no analog in the case of ordinary magnetic fields and vector potentials. Thus the boldface has a different meaning in the two cases.

The magnetic field of a Dirac monopole in ordinary three-dimensional space is

$$\mathbf{B}=\kappa\frac{\mathbf{r}}{r^3}, \tag{3.101}$$

where κ is the strength of the monopole. A vector potential that places the string on the negative z axis is

$$\mathbf{A}=\kappa\frac{1-\cos\theta}{r\sin\theta}\hat{\boldsymbol{\phi}}=\kappa\frac{x\hat{\mathbf{y}}-y\hat{\mathbf{x}}}{r(r+z)}, \tag{3.102}$$

where (r,θ,ϕ) are ordinary spherical coordinates. Although the ϕ component of the vector potential, in the sense of $\hat{\phi}\cdot\mathbf{A}$, diverges on the negative z axis, the covariant ϕ component, defined by $\mathbf{A}\cdot d\mathbf{r}=A_r dr+A_\theta d\theta+A_\phi d\phi$, does not, for we have

$$A_\phi=\kappa(1-\cos\theta). \tag{3.103}$$

Instead, what is singular on the z axis is the differential form $d\phi$, since ϕ is not defined there and its gradient has no direction. On the positive z axis, the factor $1-\cos\theta$ cancels out the singularity in $d\phi$, but on the

negative z axis it remains. Similarly, the (covariant) components of the gauge potential $\mathbf{A}_\mu$ in Eq. (3.95) are not themselves singular when $\rho_1=0$, $\rho_2\neq 0$, but the differential form $\mathbf{A}_\mu dq^\mu$ in Eq. (3.96) is, due to the singularity of $d\phi$ (now with a different meaning for ϕ). This is why the monopole string is difficult to see in the coordinates (ρ_1,ρ_2,ϕ).

The string of the Dirac vector potential $\mathbf{A}$ in Eq. (3.102) can be rotated to place it in any direction we like. In particular, to place it on the negative x axis, we simply permute indices xyz in Eq. (3.102), to obtain

$$\mathbf{A}=\kappa\frac{y\hat{\mathbf{z}}-z\hat{\mathbf{y}}}{r(r+x)}. \tag{3.104}$$

On comparing this with Eq. (3.99), we see that the gauge potential represented there does indeed have a string singularity on the negative w_1 axis and that the strength of the monopole is $\kappa=1/2$. As for the magnetic field of the Dirac monopole, we write it in terms of its dual tensor,

$$B_{ij}=\epsilon_{ijk}B_k=\kappa\epsilon_{ijk}\frac{x_k}{r^3}, \tag{3.105}$$

in which form the comparison with the curvature form $\mathbf{B}_{\mu\nu}$ in Eq. (3.100) is immediate.

In the case of the Dirac monopole, the vector $\mathbf{B}$ defines the field lines radiating out from the monopole, whereas the dual tensor $\Sigma_{i<j}B_{ij}dx_i\wedge dx_j$ represents κ times the element of solid angle $d\Omega$. Thus the total flux emanating from the monopole is $4\pi\kappa$. In the case of the Iwai monopole, the differential form (3.100) represents the element of "angle flux" emanating from the monopole (the angle representing rotations about the z axis); the total angle flux is π, since $\kappa=1/2$ and since only the region $w_3\geqslant 0$ (one hemisphere) is physical. A triangle deforming its shape by running around the edge of the solid triangle in Fig. 10 encircles all of this flux and rotates by an angle π, as elementary considerations will show. On the other hand, if we want to view the Iwai monopole in terms of field lines, we need to construct a contravariant vector field on shape space, say, $\mathbf{B}^\mu$, which is dual to the tensor (two-form) $\mathbf{B}_{\mu\nu}$. This requires the use of a metric on shape space, i.e.,

$$\mathbf{B}^\mu=\frac{1}{2\sqrt{g}}\epsilon^{\mu\nu\sigma}\mathbf{B}_{\nu\sigma}, \tag{3.106}$$

where g is the determinant of the covariant metric tensor. Shape space has such a metric tensor (see below), but it is non-Euclidean. Fortunately for the symmetry of this problem, the metric is invariant under rotations in w space, because otherwise the vector field $\mathbf{B}^\mu$ would not be rotationally symmetric. As it is, g turns out to be a function only of the radial coordinate w, and the radial field lines present exactly the same picture as in the case of a Dirac monopole, although the space is non-Euclidean and we must use the right coordinates to see the field lines as straight. Several special features of the three-body problem and the w coordinates make this picture of the Iwai monopole possible. The construction of field lines works only for the three-body problem, in which shape space is three-dimensional and the gauge field is pseudo-Abelian; for larger values of n, the Coriolis tensor cannot be transformed into a vector field as in Eq. (3.106).

The Coriolis tensor $\mathbf{B}_{\mu\nu}$ is invariant under three-dimensional rotations in (w_1,w_2,w_3) space, as is evident from Eq. (3.100), but the gauge potential $\mathbf{A}_\mu$ of Eq. (3.99) is invariant only under rotations about the w_1 axis. It is to be expected that the potential whould have less symmetry than the field itself, but for some purposes it would be more convenient if the gauge potential were invariant under rotations about the w_3 axis instead, since such rotations do not carry the physical region $w_3\geqslant 0$ into the nonphysical region $w_3<0$. In addition, we recall that rotations about the w_3 axis belong to the democracy group [see Eq. (3.36)].

It turns out that the gauge transformation to move the string onto the w_3 axis can be "discovered" by considering the principal-axis gauge. Principal-axis gauge is very popular in the literature; here we follow the notation of Smith (1962), Dragt (1965), and Iwai (1987b). The transformation from xxy gauge to principal-axis gauge is merely that which diagonalizes the moment-of-inertia tensor (3.94), and the diagonalizing matrix $\mathsf{S}=\mathsf{S}(q^\mu)$ is that which appears in the formulas for gauge transformations such as (3.42), (3.68), etc. The calculation is conveniently carried out in the coordinates (w,χ,ψ) defined in Eq. (3.30). We shall not display the diagonalizing matrix S (containing the eigenvectors of M), but the eigenvalues of M are

$$I_1=w\sin^2\frac{\chi}{2},\quad I_2=w\cos^2\frac{\chi}{2},\quad I_3=w. \tag{3.107}$$

On transforming the vectors $\boldsymbol{\rho}_\alpha(q^\mu)$ to the new body frame, we find

$$\boldsymbol{\rho}_1=\sqrt{w}\left(\cos\frac{\chi}{2}\cos\frac{\psi}{2},-\sin\frac{\chi}{2}\sin\frac{\psi}{2},0\right),$$
$$\boldsymbol{\rho}_2=\sqrt{w}\left(\cos\frac{\chi}{2}\sin\frac{\psi}{2},\sin\frac{\chi}{2}\cos\frac{\psi}{2},0\right). \tag{3.108}$$

The appearance of the angle $\psi/2$ in these formulas indicates a branch cut in shape space, say, along the half-plane $\psi=\pi$. The gauge is not continuous along the cut and has branch points on the w_3 axis. Finally, the gauge potential in principal-axis gauge can be computed either directly from the definition (3.56) in the new gauge or by carrying out the gauge transformation according to Eq. (3.74). We find

$$\mathbf{A}_\mu dq^\mu=\frac{w_3}{2w(w_1^2+w_2^2)}(w_2dw_1-w_1dw_2)\hat{\mathbf{z}}. \tag{3.109}$$

The Coriolis tensor does not change under the transformation to principal-axis gauge because the gauge transformation merely rotates the body axes in the body xy plane, and $\mathbf{B}_{\mu\nu}$ has only a z component. Thus Eq. (3.100) is valid in any gauge that leaves the three par-

ticles in the body xy plane (as if $\mathbf{B}_{\mu\nu}$ were an R scalar, another reflection of the pseudo-Abelian nature of the three-body gauge fields).

Equation (3.109) reveals a string singularity on the w_3 axis, but it is on both the positive and negative sides. The meaning of this is more clear in the spherical (w,χ,ψ) coordinates, where we find

$$\mathbf{A}_\mu dq^\mu = -\tfrac{1}{2}\sin\chi\, d\psi\hat{\mathbf{z}}. \tag{3.110}$$

Thus it is as if in the case of the Dirac monopole we were to use the vector potential

$$\mathbf{A} = -\kappa\frac{\cos\theta}{r\sin\theta}\hat{\boldsymbol{\phi}}, \quad \mathbf{A}\cdot d\mathbf{r} = -\kappa\cos\theta\, d\phi. \tag{3.111}$$

The geometrical meaning of this string singularity is interesting. The w_3 axis is where the mass-weighted vectors $\boldsymbol{\rho}_1$ and $\boldsymbol{\rho}_2$ are of equal magnitude and perpendicular, which is exactly the condition that the moment-of-inertia tensor be degenerate in the body xy plane. But when the moment-of-inertia tensor is degenerate, the principal-axis frame is not uniquely defined, nor does it approach a unique value as we approach a given point on the w_3 axis from different directions in shape space. Thus the functions $\boldsymbol{\rho}_\alpha(q^\mu)$ are singular at the degenerate shapes; the singularity has the form of a branch point, as noted previously, and it produces a corresponding singularity in the gauge potential.

The string singularity on the w_3 axis and the branch cut in the functions $\boldsymbol{\rho}_\alpha(q^\mu)$ on the half-plane $\psi=\pi$ in the principal-axis gauge also have interesting analogs in Born-Oppenheimer theory, in which one deals with an electronic Hamiltonian that is parametrized by the nuclear coordinates (Mead and Truhlar, 1979; Mead, 1992). If the electronic Hamiltonian is represented with respect to some fixed electronic basis, then it can be seen as a field of Hermitian matrices over nuclear configuration space and is analogous to the moment-of-inertia tensor in the present problem, a real, symmetric matrix field over shape space. In both cases, the eigenvectors of the field of matrices cannot be defined in a continuous manner as one goes around the codimension 2 manifold of degeneracies, but rather the two eigenvectors corresponding to the degenerate subspace change sign. In Born-Oppenheimer theory, this gives rise to a π phase shift of the electronic wave function (''Berry's phase''), and in the present case, it gives rise to an inversion of the axes of the principal-axis frame in the plane of the triangle. This inversion is sometimes called the ''Eckart paradox'' (Pack and Parker, 1987), and it causes some authors, e.g., Johnson (1983b), to use a ''coordinate system'' on shape space that goes around the line of degeneracy twice, by doubling the range of the angle ψ. Actually, it would be clearer to use a proper, single-valued coordinate system on shape space but to view the gauge as double valued, which geometrically would mean a section $\mathcal{S}$ that cuts each fiber at two points.

Curvature forms with the form of monopole fields are common in examples of Berry's phase (e.g., Berry, 1984) and are usually due to some rotational symmetry of the problem. In the case of the three-body problem, there is such a rotational symmetry in shape space. It is due to the fact that the holonomy group for the three-body problem in three-dimensional space is SO(2), just like the planar three-body problem. In the planar n-body problem there are symmetry groups of the kinetic energy in shape space larger than the democracy group.

The string singularity in the physical region of shape space which occurs in principal-axis gauge causes the Schrödinger wave function to become singular on the string, even though there is nothing singular about the physics at such shapes. As a result, principal-axis gauge has definite drawbacks for certain applications, at least for nonzero angular momentum. A gauge such as xxy gauge, which places the string singularity at the boundary of shape space, might be better, but better still would be a gauge that removes it to the nonphysical region $w_3<0$.

In fact, it is easy to perform a further gauge transformation on principal-axis gauge to eliminate the singularity from the positive half of the w_3 axis. It is as if, in the case of the Dirac monopole, we were to add the gradient of $\kappa\phi$ to the vector potential (3.111) to produce the vector potential (3.102); in the language of our SO(3) gauge fields, we wish to perform a gauge transformation specified by a rotation matrix S that rotates about the body z axis by an angle of $-\psi/2$. When we have done this, the vectors $\boldsymbol{\rho}_\alpha(q^\mu)$ have the form

$$\boldsymbol{\rho}_1 = \sqrt{\frac{w}{2}}\left(\cos\frac{\chi'}{2}+\sin\frac{\chi'}{2}\cos\psi, \sin\frac{\chi'}{2}\sin\psi, 0\right),$$

$$\boldsymbol{\rho}_2 = \sqrt{\frac{w}{2}}\left(\sin\frac{\chi'}{2}\sin\psi, \cos\frac{\chi'}{2}-\sin\frac{\chi'}{2}\cos\psi, 0\right), \tag{3.112}$$

where $\chi'=\pi/2-\chi$. We see that the branch cut has disappeared, as evidenced by the absence of the half-angles $\psi/2$. In addition, the string singularity has been removed from the positive w_3 axis, as indicated by the new gauge potential,

$$\mathbf{A}_\mu dq^\mu = \frac{1}{2}(1-\sin\chi)\, d\psi\hat{\mathbf{z}} = \frac{w_1 dw_2 - w_2 dw_1}{2w(w+w_3)}\hat{\mathbf{z}}. \tag{3.113}$$

The string singularity now lies on the negative w_3 axis, outside the physical region. Of course, the moment of inertia tensor is no longer diagonal in this gauge (a price we may wish to pay), but it has the interesting form

$$\mathsf{M} = \begin{pmatrix} \rho_2^2 & -\boldsymbol{\rho}_1\cdot\boldsymbol{\rho}_2 & 0 \\ -\boldsymbol{\rho}_1\cdot\boldsymbol{\rho}_2 & \rho_1^2 & 0 \\ 0 & 0 & \rho_1^2+\rho_2^2 \end{pmatrix}. \tag{3.114}$$

We shall call the gauge represented by Eqs. (3.112), (3.113), and (3.114) ''north regular gauge,'' because it is well behaved over the northern hemisphere $(w_3>0)$ of w space, becoming singular only at the south pole. As noted by Pack (1995), this gauge is also an Eckart gauge, in which the equilibrium position as in Eq. (3.47) is $\boldsymbol{\rho}_{0s1}=(1,0,0)$, $\boldsymbol{\rho}_{0s2}=(0,1,0)$.

IV. GAUGE DYNAMICS OF THE n-BODY PROBLEM

Up to this point we have considered shape deformations or histories in shape space $q^\mu(t)$ that could have been generated by any means, e.g., by the willful actions of a falling cat. Henceforth, however, we shall assume that they are generated by the time evolution of the n-body system itself. It turns out that the gauge fields, whose kinematical significance was explained in Sec. III, have a dynamical significance as well, i.e., the field $\mathbf{A}_\mu$ enters into the Lagrangian and the Hamiltonian (both classical and quantum) for the dynamics on shape space, and the field $\mathbf{B}_{\mu\nu}$ enters into the classical equations of motion and the quantum commutation relations.

To show how this comes about, we first transform the Lagrangian for an n-body system to orientational and shape coordinates and put it into manifestly gauge-invariant form. This involves a discussion of "horizontal" and "vertical" velocities in the fiber bundle and the notion of holonomy, and it results in a decomposition of the kinetic energy into a vertical, or purely rotational, part and a horizontal, or zero-angular-momentum, part. The kinetic energy is block diagonalized at this stage, and the classical Lagrangian is in its most convenient form. We then make a digression, to discuss the notions of left and right group actions and the invariance of the horiztonal-vertical decomposition under the left group action. Next we discuss a certain pseudo-metric, which is not gauge invariant but which is common in the molecular physics literature, as well as the true, gauge-invariant metric on shape space. We supply the geometrical meaning of the true metric (in terms of projecting the kinetic-energy metric down onto shape space in a geometrically natural way). It turns out that the true metric is non-Euclidean. We also give various explicit forms for this metric in the three-body problem. Next we work out the classical equations of motion and examine their consequences. This involves the use of anholonomic frames, in particular, the frame of left-invariant vector fields on the rotation-group manifold. We find that the equations of motion are naturally expressed in terms of covariant derivatives. We also develop the classical Hamiltonian formulation of the equations of motion. We first write the Hamiltonian in manifestly gauge-invariant form and then contrast that with the form common in the molecular physics literature, in which the gauge invariance is effectively hidden. Finally, we transform the quantum Hamiltonian to shape and orientational coordinates and obtain the reduced or internal Schrödinger equation. In this discussion, we display a novel form for the "Watsonian" term (arising from nonclassical commutators in the kinetic energy). We also show how the quantum Hamiltonian and wave function transform under gauge transformations.

A. The classical Lagrangian and the metric tensor on shape space

The Lagrangian for the n-body system in the original coordinates $\{\mathbf{r}_{s\alpha}\}$ is

$$L=\frac{1}{2}\sum_{\alpha=1}^{n} m_\alpha|\dot{\mathbf{r}}_{s\alpha}|^2-V(\mathbf{r}_{s1},\ldots,\mathbf{r}_{sn}), \tag{4.1}$$

where the potential energy V is assumed to be invariant under translations and rotations. On transforming this to coordinates $(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1},\mathbf{R}_s)$ and dropping the kinetic energy of the center of mass (3.17), we find that the Lagrangian becomes

$$L=\frac{1}{2}\sum_{\alpha=1}^{n-1} |\dot{\boldsymbol{\rho}}_{s\alpha}|^2-V(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1}). \tag{4.2}$$

Finally, when the Lagrangian is transformed to shape and orientational coordinates, the potential energy becomes simply a function of shape, $V=V(q^\mu)$, whereas by Eq. (3.49) the kinetic energy in Eq. (3.2) (physically, the kinetic energy about the center of mass) becomes

$$\begin{aligned}K&=\frac{1}{2}\sum_{\alpha=1}^{n-1} |\dot{\boldsymbol{\rho}}_\alpha|^2\\&=\frac{1}{2}\sum_{\alpha=1}^{n-1}\left[|\boldsymbol{\omega}\times\boldsymbol{\rho}_\alpha|^2+2\boldsymbol{\omega}\cdot\left(\boldsymbol{\rho}_\alpha\times\frac{\partial\boldsymbol{\rho}_\alpha}{\partial q^\mu}\right)\dot{q}^\mu\right.\\&\quad\left.+\left(\frac{\partial\boldsymbol{\rho}_\alpha}{\partial q^\mu}\cdot\frac{\partial\boldsymbol{\rho}_\alpha}{\partial q^\nu}\right)\dot{q}^\mu\dot{q}^\nu\right].\end{aligned} \tag{4.3}$$

We write this in the form

$$K=\tfrac{1}{2}(\boldsymbol{\omega}\cdot\mathsf{M}\cdot\boldsymbol{\omega})+(\boldsymbol{\omega}\cdot\mathsf{M}\cdot\mathbf{A}_\mu)\dot{q}^\mu+\tfrac{1}{2}h_{\mu\nu}\dot{q}^\mu\dot{q}^\nu, \tag{4.4}$$

where $h_{\mu\nu}$ is a new field over shape space, defined by

$$h_{\mu\nu}=h_{\mu\nu}(q)=\sum_{\alpha=1}^{n-1}\frac{\partial\boldsymbol{\rho}_\alpha}{\partial q^\mu}\cdot\frac{\partial\boldsymbol{\rho}_\alpha}{\partial q^\nu}=\sum_{\alpha=1}^{n} m_\alpha\frac{\partial\mathbf{c}_\alpha}{\partial q^\mu}\cdot\frac{\partial\mathbf{c}_\alpha}{\partial q^\nu}. \tag{4.5}$$

The field $h_{\mu\nu}$ looks like a metric tensor on shape space, but it is not the true metric, as we shall see.

Of course the kinetic energy K, the sum of the three terms on the right-hand side of Eq. (4.4), is gauge invariant, although none of the three terms is individually. This is clear in the case of the first and second terms, since neither $\boldsymbol{\omega}$ nor $\mathbf{A}_\mu$ is a true R vector, so their contractions with the true R tensor M are not true R scalars. The final term in Eq. (4.4) is not gauge-invariant either, for although $h_{\mu\nu}$ appears to be an R scalar (it has no R indices), it is not a true R scalar. To show this, we subject the definition (4.5) to a gauge transformation, using Eqs. (3.67), (3.68), and (3.71). We find

$$h_{\mu\nu}=h'_{\mu\nu}+\boldsymbol{\gamma}_\mu\cdot\mathsf{M}'\cdot\mathbf{A}'_\nu+\boldsymbol{\gamma}_\nu\cdot\mathsf{M}'\cdot\mathbf{A}'_\mu+\mathbf{A}'_\mu\cdot\mathsf{M}'\cdot\mathbf{A}'_\nu. \tag{4.6}$$

On the other hand, $h_{\mu\nu}$ is a true covariant, symmetric q tensor in the indices μ,ν. Although it has been traditional (Wilson and Howard, 1936) to call the first term of Eq. (4.4) the rotational energy, the third the vibrational energy, and the second the coupling between rotation and vibration, this terminology has no gauge-invariant meaning and we shall not use it.

Because of the lack of gauge invariance of its constituent terms, the kinetic energy K in Eq. (4.4) is not in

satisfactory form. Indeed, if we use this form of the kinetic energy in the Lagrangian and compute the equations of motion, we find complicated expressions for the accelerations $\ddot{q}^\mu$, quantities which we know to be gauge invariant. The expressions that result are by no means manifestly gauge invariant. Therefore before tackling the equations of motion we shall put K itself into manifestly gauge-invariant form.

We begin by writing $|v\rangle$ for a $(3n-3)$-dimensional velocity vector in configuration space, using a Dirac notation for linear algebra on such vectors (i.e., tangent vectors to configuration space). Thus, in the $\{\boldsymbol{\rho}_{s\alpha}\}$ coordinates, we write

$$|v\rangle=(\dot{\boldsymbol{\rho}}_{s1},\ldots,\dot{\boldsymbol{\rho}}_{s,n-1}), \tag{4.7}$$

whereas in orientational and shape coordinates we would have $|v\rangle=(\dot{\theta}^i,\dot{q}^\mu)$. Actually, for the construction of the Lagrangian it is more convenient to work with the components of the body angular velocity $\boldsymbol{\omega}$ than the time derivatives of the Euler angles $\dot{\theta}^i$, so we write instead

$$|v\rangle=(\boldsymbol{\omega},\dot{q}^\mu). \tag{4.8}$$

In this form, the system velocity $|v\rangle$ is represented with respect to an anholonomic frame in configuration space (actually in the tangent bundle). We shall say more about this later, but for now we shall refer to the form (4.8) as the velocity with respect to the "angular velocity and shape basis."

We use the kinetic energy to define the scalar product of velocity vectors, so that in $\{\boldsymbol{\rho}_{s\alpha}\}$ coordinates we have

$$\langle v|v\rangle=2K=\sum_{\alpha=1}^{n-1}|\dot{\boldsymbol{\rho}}_{s\alpha}|^2. \tag{4.9}$$

To express the scalar product in terms of the angular velocity and shape basis, we use Eq. (4.4) and write $\langle v|v\rangle$ in matrix form,

$$\langle v|v\rangle=2K=(\boldsymbol{\omega}^T\quad\dot{q}^\mu)\begin{pmatrix}\mathsf{M} & \mathsf{M}\mathbf{A}_\nu\\ \mathbf{A}_\mu^T\mathsf{M} & h_{\mu\nu}\end{pmatrix}\begin{pmatrix}\boldsymbol{\omega}\\ \dot{q}^\nu\end{pmatrix}, \tag{4.10}$$

where the $(3n-3)\times(3n-3)$ matrix shown is partitioned according to $3n-3=3+(3n-6)$ and where the T indicates the transpose (see Appendix A). More generally, we shall write the components of $|v\rangle$, with respect to any basis, as v^a, where $a=1,\ldots,3n-3$ (see Appendix A), and we shall write the scalar product in the form

$$\langle v|v\rangle=G_{ab}v^a v^b, \tag{4.11}$$

so that G_{ab} is the metric tensor on configuration space in the given basis. Then in the $\{\boldsymbol{\rho}_{s\alpha}\}$ coordinates we have $G_{ab}=\delta_{ab}$, the form of a manifestly Euclidean metric, and we see that the matrix in Eq. (4.10) is the component matrix G_{ab} with respect to the angular velocity and shape basis.

If the system velocity $|v\rangle$ in the angular velocity and shape basis has the form $(\boldsymbol{\omega},0)$, i.e., with $\dot{q}^\mu=0$, then we shall call it "purely rotational," an obvious terminology, since the shape is not changing. We note that the condition $\dot{q}^\mu=0$ is gauge invariant, so this terminology has a gauge-invariant meaning. In the fiber-bundle picture, purely rotational velocity vectors are tangent to the fibers, as illustrated in Fig. 16. In fiber-bundle language, such vectors are also called *vertical*, because of the suggestion made by such figures. The vector space of vertical vectors is three dimensional, the same as the fibers themselves.

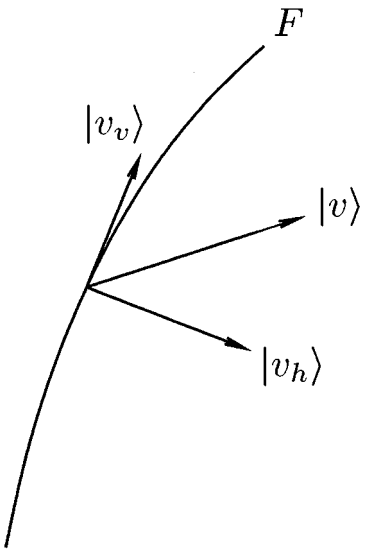

FIG. 16. Velocity vectors. A vertical velocity vector $|v_v\rangle$ is one that is tangent to the fiber (F in the figure); it represents motion that is purely rotational. A horizontal velocity vector $|v_h\rangle$ is orthogonal to every vertical vector in the metric imposed by the kinetic energy. Such a vector represents physically a motion of vanishing angular momentum. An arbitrary velocity $|v\rangle$ can be represented uniquely as a linear combination of a vertical and a horizontal velocity vector.

One might suppose that we should call a system velocity vector of the form $|v\rangle=(0,\dot{q}^\mu)$, i.e., with $\boldsymbol{\omega}=0$, "purely internal" or "purely vibrational." But the condition $\boldsymbol{\omega}=0$ is not gauge invariant, so such terminology has no meaning independent of conventions, and we will not use it.

But there is a notion complementary to "purely rotational." We define a system velocity $|v\rangle=(\boldsymbol{\omega},\dot{q}^\mu)$ to be *horizontal* if it is perpendicular to all vertical velocity vectors, in the sense of the scalar product (4.10). That is, suppose $|v_v\rangle=(\boldsymbol{\omega}_v,0)$ is a vertical velocity vector, let $|v_h\rangle=(\boldsymbol{\omega}_h,\dot{q}_h^\mu)$, and suppose $\langle v_v|v_h\rangle=0$ for all $\boldsymbol{\omega}_v$. Then by Eq. (4.10) we have

$$\begin{aligned}\langle v_v|v_h\rangle&=\begin{pmatrix}\boldsymbol{\omega}_v^T & 0\end{pmatrix}\begin{pmatrix}\mathsf{M} & \mathsf{M}\mathbf{A}_\nu\\ \mathbf{A}_\mu^T\mathsf{M} & h_{\mu\nu}\end{pmatrix}\begin{pmatrix}\boldsymbol{\omega}_h\\ \dot{q}_h^\nu\end{pmatrix}\\ &=\boldsymbol{\omega}_v\cdot\mathsf{M}\cdot(\boldsymbol{\omega}_h+\mathbf{A}_\nu\dot{q}_h^\nu)=\boldsymbol{\omega}_v\cdot\mathbf{L}_h,\end{aligned} \tag{4.12}$$

where $\mathbf{L}_h$ is the angular momentum associated with system velocity $|v_h\rangle$. But if this vanishes for all $\boldsymbol{\omega}_v$, we have $\mathbf{L}_h=0$, so we see that a system velocity is horizontal if and only if the associated angular momentum vanishes. Thus the geometrical significance in the fiber-bundle pic-

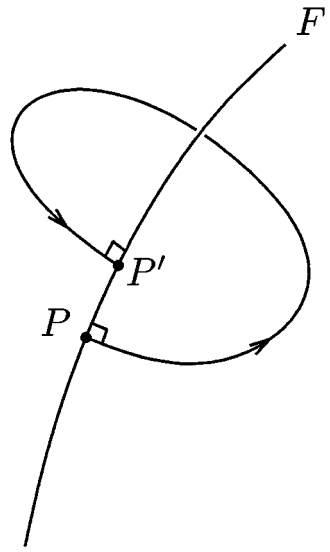

FIG. 17. A motion taking place with zero angular momentum, represented as a trajectory in the configuration space which is everywhere horizontal, i.e., perpendicular to the fibers. Nevertheless, when the motion returns to its original fiber F, there is a shift or holonomy along the fiber which has taken place, i.e., a rotation transforming the original configuration P into the final one P'.

ture of motions of vanishing angular momentum, which have played such a large role in our development so far of the gauge theory of the n-body problem, is that the corresponding velocities are perpendicular to the fibers. The vector space of horizontal velocity vectors is $(3n-6)$ dimensional, since the conditions $\mathbf{L}=0$ impose three constraints on the $3n-3$ velocity components, or since the space of horizontal motions is perpendicular to the three-dimensional space of vertical motions.

We have considered several examples of motions of vanishing angular momentum, such as the falling cat. It is interesting that such a motion, if viewed in the fiber bundle as in Fig. 17, is everywhere perpendicular to the fibers, and yet if it returns to its original shape, there appears a displacement along the original fiber. That is, the trajectory may be closed in shape space, but in configuration space it does not close, as illustrated in the figure, but rather it carries the original configuration P to a final one P' on the same fiber. The rotation taking P into P' is the net rotation of the system, also referred to as the *holonomy*, which the cat uses to turn itself over. The existence of this effect in n-body systems such as molecules was first noted by Guichardet (1984).

The failure of purely horizontal curves to close in the fiber bundle, i.e., in configuration space, even after closing in shape space, is related to the fact that there do not exist surfaces in configuration space of dimensionality $3n-6$ which are everywhere perpendicular to the fibers. For if such a surface did exist, every closed curve lying in it would represent a closed cycle in shape space of zero angular momentum, which would generate no net rotation. But we know such rotations do occur, as evidenced by the falling cat. Furthermore, if such a surface were interpreted as the section $\mathcal{S}$ of the fiber bundle specifying a gauge convention, then we would find $\mathbf{A}_\mu=0$ in the region of shape space over which the surface $\mathcal{S}$ was defined. This follows because a trajectory lying in $\mathcal{S}$ satisfies $\dot{\mathsf{R}}=0$ or $\boldsymbol{\omega}=0$, and a horizontal trajectory satisfies $\mathbf{L}=0$; the two are consistent for all possible trajectories lying in $\mathcal{S}$ only if $\mathbf{A}_\mu=0$. But we know that it is impossible to choose a gauge to make $\mathbf{A}_\mu=0$ over a finite region. It is possible to make $\mathbf{A}_\mu$ vanish at a point, which means geometrically that $\mathcal{S}$ is orthogonal to the fibers at that point; this is what the Eckart conventions do at the equilibrium shape of a molecule.

Some authors (Guichardet, 1984) have referred to a horizontal velocity vector as "purely vibrational." We do not feel this terminology is justified, since any physical picture associated with these words will suggest $\dot{\mathsf{R}}=0$, i.e., $\boldsymbol{\omega}=0$, a condition that is not gauge invariant. In any case, the physics of horizontal motion is the vanishing of angular momentum. Therefore we confine ourselves to "horizontal" or "vanishing angular momentum" to describe such vectors.

An arbitrary system velocity is neither horizontal nor vertical, but can be represented as a unique linear combination of horizontal and vertical velocities, as illustrated in Fig. 16. For if we write $|v\rangle=|v_v\rangle+|v_h\rangle$, or

$$(\boldsymbol{\omega},\dot{q}^\mu)=(\boldsymbol{\omega}_v,\dot{q}_v^\mu)+(\boldsymbol{\omega}_h,\dot{q}_h^\mu), \tag{4.13}$$

then the vertical condition on $|v_v\rangle$ implies $\dot{q}_v^\mu=0$, and the horizontal condition on $|v_h\rangle$ implies $\boldsymbol{\omega}_h+\mathbf{A}_\nu\dot{q}_h^\nu=0$. From these we find the explicit form of the decomposition,

$$(\boldsymbol{\omega},\dot{q}^\mu)=(\boldsymbol{\omega}+\mathbf{A}_\nu\dot{q}^\nu,0)+(-\mathbf{A}_\nu\dot{q}^\nu,\dot{q}^\mu), \tag{4.14}$$

where the first term is vertical and the second horizontal.

Now the kinetic energy about the center of mass can be written

$$K=\tfrac{1}{2}\langle v|v\rangle=\tfrac{1}{2}\langle v_v|v_v\rangle+\tfrac{1}{2}\langle v_h|v_h\rangle, \tag{4.15}$$

with no cross terms, since $\langle v_v|v_h\rangle=0$. By Eq. (4.10), the vertical contribution is

$$K_v=\tfrac{1}{2}(\boldsymbol{\omega}+\mathbf{A}_\mu\dot{q}^\mu)\cdot\mathsf{M}\cdot(\boldsymbol{\omega}+\mathbf{A}_\nu\dot{q}^\nu), \tag{4.16}$$

and the horizontal contribution is

$$K_h=\tfrac{1}{2}g_{\mu\nu}\dot{q}^\mu\dot{q}^\nu, \tag{4.17}$$

where $g_{\mu\nu}$ is a new metric on shape space (De Celles and Darling, 1969), defined by

$$g_{\mu\nu}=h_{\mu\nu}-\mathbf{A}_\mu\cdot\mathsf{M}\cdot\mathbf{A}_\nu. \tag{4.18}$$

The vertical and horizontal contributions to the kinetic energy are individually gauge invariant. As for the vertical contribution, this is obvious because $\boldsymbol{\omega}+\mathbf{A}_\mu\dot{q}^\mu$ is a true R vector, or by noting the equivalent formula,

$$K_v=\tfrac{1}{2}\mathbf{L}\cdot\mathsf{M}^{-1}\cdot\mathbf{L}. \tag{4.19}$$

As for the horizontal contribution, its gauge invariance follows by combining the transformation law for $h_{\mu\nu}$,

Eq. (4.6), with that of $\mathbf{A}_\mu \cdot \mathsf{M} \cdot \mathbf{A}_\nu$. The six correction terms all cancel, and we are left with

$$g_{\mu\nu} = g'_{\mu\nu}. \tag{4.20}$$

Thus the metric $g_{\mu\nu}$ is a true R scalar, and is to be interpreted as the true metric on shape space. (It is also a true, symmetric, covariant q tensor.) Altogether, we can now write the Lagrangian in manifestly gauge-invariant form,

$$L = \tfrac{1}{2}(\boldsymbol{\omega} + \mathbf{A}_\mu \dot{q}^\mu) \cdot \mathsf{M} \cdot (\boldsymbol{\omega} + \mathbf{A}_\nu \dot{q}^\nu) + \tfrac{1}{2} g_{\mu\nu} \dot{q}^\mu \dot{q}^\nu - V(q). \tag{4.21}$$

This is the most useful form of the Lagrangian. We shall return to it after two digressions one on the mathematics of connections and one on the metrics $h_{\mu\nu}$ and $g_{\mu\nu}$.

B. Left and right actions and the connection

We shall now use the fiber bundle in the n-body problem to illustrate certain general features of principal fiber bundles, including the left and right group actions and the geometrical meaning of a connection. In standard mathematical theory, a fiber bundle is a differentiable manifold upon which a group acts, which also has several other properties. In the case of a principal fiber bundle, the group acts freely, so that the orbits of the group action (the fibers) are diffeomorphic to the group itself, i.e., they are effectively copies of the group. In the n-body problem (if we assume $n \geq 3$ and exclude the collinear configurations), configuration space is a principal fiber bundle, and of course the group in question is SO(3).

A group action (on any space) can either be from the right or from the left. In the case of a principal fiber bundle, both kinds of actions can be defined, but only one can be defined independently of a choice of section or gauge, which is effectively a choice of an origin or reference in each of the fibers. This is the group action referred to in the preceding paragraph. In most mathematics books on fiber-bundle theory, it is customary to say that the group action that can be defined independently of any section is a right action. Insofar as the mathematics is concerned, this is purely a matter of convention, and one could just as well develop equivalent mathematics by insisting that the group action from the left is the one defined independently of any section. But in a specific physical problem, the nature of the two group actions is determined by the physics. In the n-body problem, for example, it turns out that the group action that is defined independently of any section is a left action, opposite the usual custom in mathematics. Therefore, when comparing the present discussion of the n-body problem to typical mathematics texts, it is usually necessary to reverse the words "right" and "left." In any case, the group action that is defined independently of any section (right in the case of most mathematics texts and left in the case of the n-body problem) is defined in a gauge-independent manner. We shall call it the "gauge-invariant action."

In the case of the n-body problem, the gauge-invariant left action of SO(3) on configuration space is physically just the rigid rotation of the n-body system about the center of mass, which has already been illustrated in Eq. (3.20). To state this action in a slightly different way, we let $\mathsf{Q} \in \mathsf{SO(3)}$ be a proper rotation and define its action by

$$(\boldsymbol{\rho}_{s1}, \ldots, \boldsymbol{\rho}_{s,n-1}) \mapsto (\mathsf{Q}\boldsymbol{\rho}_{s1}, \ldots, \mathsf{Q}\boldsymbol{\rho}_{s,n-1}). \tag{4.22}$$

This is a left action, because the action of Q_1 followed by that of Q_2 is equivalent to the action of $\mathsf{Q}_2\mathsf{Q}_1$. The definition (4.22) works with the space components of the Jacobi vectors and is therefore independent of any section or gauge convention (a definition of a body frame, in our case). If, however, a body-frame convention is chosen, we can just as well represent a point of configuration space by (R, q^μ), where R is a function of the Euler angles θ^i. Then a statement equivalent to Eq. (4.22) is

$$(\mathsf{R}, q^\mu) \mapsto (\mathsf{QR}, q^\mu). \tag{4.23}$$

If a convention for body frame is chosen, we can also define a right action of SO(3) on the bundle by

$$(\mathsf{R}, q^\mu) \mapsto (\mathsf{RQ}, q^\mu), \tag{4.24}$$

for $\mathsf{Q} \in \mathrm{SO}(3)$. This is a right action, because the action of Q_1 followed by the action of Q_2 is equivalent to the action of $\mathsf{Q}_1\mathsf{Q}_2$. The definition of this action depends on a choice of gauge and cannot be expressed purely in terms of space components. This right action is obviously closely related to a gauge transformation, as shown by Eq. (3.43), but the interpretations are somewhat different: in a gauge transformation, we change the definition of the reference point on each fiber, which can be thought of as a (passive) coordinate transformation on the fibers, whereas we think of the right action in Eq. (4.24) as taking place in an active sense, so that an old configuration is mapped into a new one, with the gauge convention or body frame held fixed.

In a principal fiber bundle, one can always define the "vertical" subspace of the tangent space at any point of the fiber bundle as consisting of those vectors which are tangent to the fiber passing through the given point. The dimensionality of the vertical subspace is the same as the group itself, and often useful basis vectors in this subspace are the infinitesimal generators of left or right group actions. We shall make extensive use of these basis vectors below.

However, the fiber bundle may or may not have a definition of "horizontal" subspaces. If horizontal subspaces are defined, they are subspaces in the tangent spaces which are required to be transverse to the vertical subspaces and complementary to them in dimensionality. If the fiber bundle is endowed with a metric, as is the fiber bundle in the n-body problem, one will often define the horizontal subspaces as those perpendicular to the vertical subspaces, as we have done. If, in addition, the definition of horizontal subspaces is invariant under the gauge-invariant action of the group (the right action

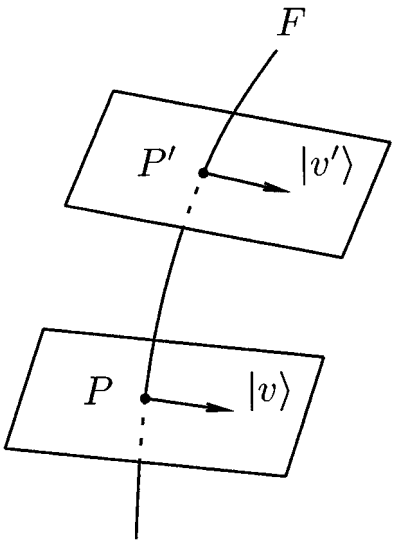

FIG. 18. Horizontal subspaces in the fiber bundle of the n-body problem. The horizontal subspaces constitute a connection because they are invariant under the left action of the group. A trajectory passing through configuration P on fiber F with horizontal velocity $|v\rangle$ is mapped by left rotations into another trajectory whose velocity $|v'\rangle$ is also horizontal. Physically, motions of vanishing angular momentum are mapped by rotations into other motions of vanishing angular momentum.

in most mathematics books, but the left action in our problem), then the horizontal subspaces are said to constitute a "connection."

We shall now illustrate what is meant by the invariance of the definition of the horizontal subspaces under the gauge-invariant group action by the example of the n-body problem. The essential geometry is illustrated in Fig. 18. In the figure, F is a fiber passing through configuration P. The subspace of horizontal vectors at point P is illustrated schematically by a plane, and $|v\rangle$ is a horizontal velocity vector in this subspace. A proper rotation Q has a left action on P as shown by Eq. (4.22), which we imagine maps P into configuration P', and velocity $|v\rangle$ at P into velocity $|v'\rangle$ at P'. If it should happen that $|v'\rangle$ is horizontal for all horizontal choices of $|v\rangle$, then the left action of the group carries horizontal subspaces into other horizontal subspaces, and we can say that the definition of the horizontal subspaces is invariant under the left action of the group.

In fact, this is the case for the n-body problem. To show this, let us imagine that velocity $|v\rangle$ is the velocity of a trajectory $\boldsymbol{\rho}_{s\alpha}=\boldsymbol{\rho}_{s\alpha}(t)$ passing through P at some time, so that $|v\rangle$ is represented by the quantities $\{\dot{\boldsymbol{\rho}}_{s\alpha}\}$, as in Eq. (4.7). Then since $|v\rangle$ is horizontal we have

$$\sum_{\alpha} \boldsymbol{\rho}_{s\alpha}\times\dot{\boldsymbol{\rho}}_{s\alpha}=0. \tag{4.25}$$

The velocity $|v'\rangle$ is the velocity of the rotated trajectory $\boldsymbol{\rho}'_{s\alpha}(t)=\mathsf{Q}\boldsymbol{\rho}_{s\alpha}(t)$ at the same instant in time, so that P' has coordinates $\{\mathsf{Q}\boldsymbol{\rho}_{s\alpha}\}$, and $|v'\rangle$ is represented by the quantities $\{\mathsf{Q}\dot{\boldsymbol{\rho}}_{s\alpha}\}$. Then the angular momentum of the rotated trajectory is given by

$$\sum_{\alpha} (\mathsf{Q}\boldsymbol{\rho}_{s\alpha})\times(\mathsf{Q}\dot{\boldsymbol{\rho}}_{s\alpha})=\mathsf{Q}\sum_{\alpha} \boldsymbol{\rho}_{s\alpha}\times\dot{\boldsymbol{\rho}}_{s\alpha}=0, \tag{4.26}$$

so that $|v'\rangle$ is also horizontal.

Thus, in the n-body problem, the invariance of the horizontal subspaces under the left action of the group is simply due to the fact that the angular momentum of a rotated trajectory is just the rotated angular momentum, so that, in particular, trajectories of vanishing angular momentum are mapped into other trajectories of vanishing angular momentum.

The geometrical significance of the connection is that it allows a given vector to be projected into its horizontal and vertical components. Furthermore, this decomposition is invariant under the group action.

C. Discussion of the pseudo-metric $h_{\mu\nu}$ and true metric $g_{\mu\nu}$

The geometrical significance of the pseudo-metric $h_{\mu\nu}$ is that it is the restriction of the Euclidean metric G_{ab} on the $(3n-3)$-dimensional configuration space, defined in Eq. (4.11), to the $(3n-6)$-dimensional section $\mathcal{S}$, regarded as a submanifold of configuration space. Since the section can be bent and moved in many ways by gauge transformations, the pseudo-metric $h_{\mu\nu}$ also changes and is not gauge-invariant. From a gauge-theoretical standpoint, one should pay no attention to $h_{\mu\nu}$, but it figures prominently in the traditional literature on molecular vibrations. Indeed, one of the effects of the Eckart conventions is to choose a section $\mathcal{S}$ and shape coordinates q^{μ} such that $h_{\mu\nu}=\delta_{\mu\nu}$, which might seem to imply that shape space is Euclidean. Actually, this form of $h_{\mu\nu}$ tells us nothing about the intrinsic metrical geometry of shape space, but only something about that of the section $\mathcal{S}$. Under the Eckart gauge, the geometry of $\mathcal{S}$ is indeed Euclidean, for the Eckart conventions specify a section $\mathcal{S}$ which is a vector subspace of configuration space. Naturally, a flat subspace of a Euclidean space is itself Euclidean, and linear coordinates q^{μ} can be chosen on it to make the metric have the form $h_{\mu\nu}=\delta_{\mu\nu}$. The Eckart conventions are primarily useful for small-amplitude vibrations about the equilibrium position; since the conventions specify $\mathbf{A}_{\mu}=0$ at this position, by Eq. (4.18) we also have $h_{\mu\nu}=g_{\mu\nu}$ there, and for small-amplitude vibrations the two metrics differ only by quantities that are second order in the vibrational amplitude.

The geometrical significance of the true metric $g_{\mu\nu}$ is that it is the projection of the metric G_{ab} on configuration space onto shape space in accordance with the quotient operation $\mathbb{R}^{3n-3}/\mathrm{SO}(3)$. The projection process is carried out in an essentially unique, geometrically "natural" way, which guarantees that the projected metric is gauge invariant. The projection process relies on the fact that the original metric G_{ab} is invariant under rotations.

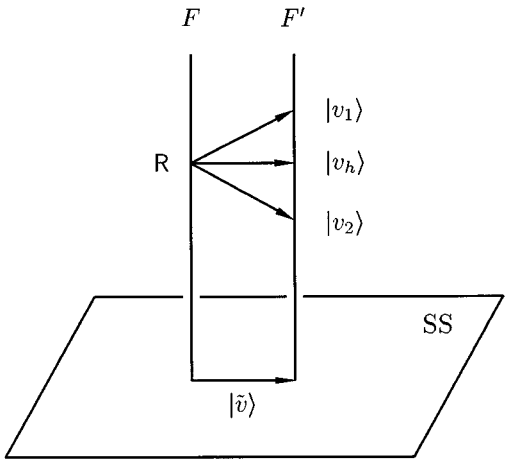

FIG. 19. The geometrical sense in which the shape-space metric $g_{\mu\nu}$ is the projection of the configuration-space metric G_{ab}. The vector $|\tilde{v}\rangle$ in shape space joins two nearby points, corresponding to two nearby fibers F and F' in configuration space. Associated with $|\tilde{v}\rangle$ on shape space is the unique horizontal vector $|v_h\rangle$ on configuration space, in terms of which the scalar product of vectors on shape space is defined.

The following is a simplified statement of the essential ideas in the projection process. Let $|\tilde{v}\rangle$ be a velocity vector on shape space, in which the tilde distinguishes velocities on shape space (with $3n-6$ components) from velocities $|v\rangle$ on configuration space (with $3n-3$ components). Thus we can associate $|\tilde{v}\rangle$ with components $\dot{q}^\mu$. We wish to define a scalar product $\langle\tilde{v}_1|\tilde{v}_2\rangle$ of shape-space velocities in terms of the original scalar product $\langle v_1|v_2\rangle$ of configuration-space velocities. A given vector $|\tilde{v}\rangle$ on shape space can be thought of as taking us from one fiber F with coordinates q^μ to a neighboring fiber F' with coordinates $q^\mu+dq^\mu$ in time dt, as illustrated in Fig. 19. But the vector $|\tilde{v}\rangle$ does not uniquely determine the vector $|v\rangle$ on configuration space, because an arbitrary vertical vector can be added to the latter and it will still connect the two fibers F and F' (and therefore project onto the given $|\tilde{v}\rangle$). For example, vectors $|v_1\rangle$ and $|v_2\rangle$ in the figure both project onto $|\tilde{v}\rangle$. In fact, the only gauge-invariant way to associate a vector on configuration space with a given vector $|\tilde{v}\rangle=\dot{q}^\mu$ on shape space is to use the horizontal vector $|v_h\rangle$ connecting the two fibers, which by Eq. (4.14) is $|v_h\rangle=(-\mathbf{A}_\mu\dot{q}^\mu,\dot{q}^\mu)$ in the angular velocity and shape basis. Then we can define the metric $g_{\mu\nu}$ on shape space by

$$\langle\tilde{v}_1|\tilde{v}_2\rangle=g_{\mu\nu}\dot{q}_1^\mu\dot{q}_2^\nu=\langle v_{1h}|v_{2h}\rangle=G_{ab}v_{1h}^a v_{2h}^b. \tag{4.27}$$

This leads directly to the definition (4.18). The fact that the components of $g_{\mu\nu}$, according to this definition, are independent of orientation R and depend only on shape is due to the invariance of G_{ab} under rotations. Equivalently, the scalar product turns out to be independent of the base point of the vectors $|v\rangle$, marked by R in Fig. 19, due to the rotational invariance of G_{ab}.

Another point of view concerning the projection of the metric onto shape space centers on the contravariant versions of the tensors, G^{ab} and $g^{\mu\nu}$, and is based on the fact that contravariant tensors are projected in a natural way under the quotient operation. In terms of the component matrices, this means that if the contravariant metric tensor G^{ab} on configuration space is expressed in orientational and shape coordinates (θ^i,q^μ), then the $(3n-6)\times(3n-6)$ block corresponding to the q's is just the contravariant metric $g^{\mu\nu}$ on shape space.

To prove this, we shall first express the covariant tensor G_{ab} in the coordinates (θ^i,q^μ). It is not necessary to do this, but it makes the following presentation less abstract. The tensor G_{ab} is displayed in the angular velocity and shape basis in Eq. (4.10); effectively, we must express the kinetic energy in terms of $(\dot{\theta}^i,\dot{q}^\mu)$ instead of $(\boldsymbol{\omega},\dot{q}^\mu)$. The relation between $\boldsymbol{\omega}$ and $\dot{\theta}^i$ is a linear one of the form

$$\omega^i=\Lambda_j^{(i)}\dot{\theta}^j, \tag{4.28}$$

where the coefficients $\Lambda_j^{(i)}$ are functions of the Euler angles θ^i and where the notation is explained more fully in Appendix C. We shall also write this in matrix form,

$$\boldsymbol{\omega}=\Lambda\dot{\boldsymbol{\theta}}, \tag{4.29}$$

$$\dot{\boldsymbol{\theta}}=\mathsf{X}\boldsymbol{\omega}, \tag{4.30}$$

where X is the matrix inverse to Λ,

$$\mathsf{X}=\Lambda^{-1}. \tag{4.31}$$

Relations of the form (4.28) are familiar from rigid-body theory, and an example of Eq. (4.28) for a particular choice of Euler angles is displayed in Eq. (B8). Our policy, however, will be to avoid explicit conventions for Euler angles as much as possible and to use instead the general properties of the coefficients $\Lambda_j^{(i)}$. In particular, we note that the linear relation between $\boldsymbol{\omega}$ and $\dot{\theta}^i$ follows from

$$\boldsymbol{\omega}\leftrightarrow\Omega=\mathsf{R}^T\dot{\mathsf{R}}=\mathsf{R}^T\frac{\partial\mathsf{R}}{\partial\theta^j}\dot{\theta}^j, \tag{4.32}$$

so that

$$\Lambda_j^{(i)}=-\frac{1}{2}\epsilon_{ik\ell}\mathsf{R}_{mk}\frac{\partial\mathsf{R}_{m\ell}}{\partial\theta^j}, \tag{4.33}$$

$$\frac{\partial\mathsf{R}_{ij}}{\partial\theta^k}=\epsilon_{j\ell m}\mathsf{R}_{i\ell}\Lambda_k^{(m)}. \tag{4.34}$$

It is now easy to write G_{ab} in the coordinate basis (θ^i,q^μ); it is

$$G_{ab}=\begin{pmatrix}\Lambda^T\mathsf{M}\Lambda & \Lambda^T\mathsf{M}\mathbf{A}_\nu\\ \mathbf{A}_\mu^T\mathsf{M}\Lambda & h_{\mu\nu}\end{pmatrix}. \tag{4.35}$$

We invert this to find the contravariant metric tensor in the coordinate basis (θ^i,q^μ); it is

$$G^{ab}=\begin{pmatrix}\mathsf{X}\tilde{\mathsf{M}}^{-1}\mathsf{X}^T & -\mathsf{X}\mathbf{A}_\sigma g^{\sigma\nu}\\ -g^{\mu\sigma}\mathbf{A}_\sigma^T\mathsf{X}^T & g^{\mu\nu}\end{pmatrix}, \tag{4.36}$$

where $\tilde{\mathsf{M}}$ is a "modified" moment of inertia tensor, defined by

$$\tilde{\mathsf{M}}^{-1}=\mathsf{M}^{-1}+\mathbf{A}_\mu g^{\mu\nu}\mathbf{A}_\nu^T. \tag{4.37}$$

Here we use dyadic notation, in which the juxtaposition of the two vectors $\mathbf{A}_\mu$ and $\mathbf{A}_\nu^T$ is the tensor with i,j components $A_\mu^i A_\nu^j$, as explained in Appendix A. To check Eq. (4.36), we may directly multiply matrices and show that $G_{ac}G^{cb}=\delta_a^b$.

The lower $(3n-6)\times(3n-6)$ block of G^{ab} is $g^{\mu\nu}$, as claimed, and this fact gives us an alternative way of computing $g^{\mu\nu}$ or $g_{\mu\nu}$. For if we write out the transformation law of the contravariant tensor G^{ab} under the coordinate transformation $\{\boldsymbol{\rho}_{s\alpha}\}\rightarrow(\theta^i,q^\mu)$, noting that $G^{ab}=\delta_{ab}$ in the coordinates $\{\boldsymbol{\rho}_{s\alpha}\}$, then we find

$$g^{\mu\nu}=\sum_{\alpha=1}^{n-1}\frac{\partial q^\mu}{\partial\boldsymbol{\rho}_{s\alpha}}\cdot\frac{\partial q^\nu}{\partial\boldsymbol{\rho}_{s\alpha}}. \tag{4.38}$$

Once we have found $g^{\mu\nu}$ by this equation, $g_{\mu\nu}$ follows by matrix inversion. This is often easier in practice than using Eq. (4.18). Equation (4.38) makes it obvious that $g^{\mu\nu}$ and hence $g_{\mu\nu}$ is gauge invariant, since it is the space components $\boldsymbol{\rho}_{s\alpha}$ which appear.

Let us now consider examples of the metric and pseudo-metric in various coordinate systems for the three-body problem. First, in coordinates (ρ_1,ρ_2,ϕ), a direct application of Eqs. (4.5) and (4.38) gives

$$h_{\mu\nu}=\begin{pmatrix}1&0&0\\0&1&0\\0&0&\rho_2^2\end{pmatrix}. \tag{4.39}$$

Here we use the xxy gauge. (It is necessary to specify this, since $h_{\mu\nu}$ is not gauge invariant.) We now apply Eqs. (4.18), (3.94), and (3.96) to obtain

$$g_{\mu\nu}=\begin{pmatrix}1&0&0\\0&1&0\\0&0&\dfrac{\rho_1^2\rho_2^2}{\rho_1^2+\rho_2^2}\end{pmatrix}. \tag{4.40}$$

A more compact way of writing this is in terms of the "arc length" in shape space,

$$ds^2=g_{\mu\nu}dq^\mu dq^\nu=d\rho_1^2+d\rho_2^2+\frac{\rho_1^2\rho_2^2}{\rho_1^2+\rho_2^2}d\phi^2. \tag{4.41}$$

We see that the metric is diagonal in the (ρ_1,ρ_2,ϕ) coordinates. This fact simplifies the Lagrangian and Hamiltonian (both classical and quantum).

There are several other coordinate systems for the three-body problem which yield a diagonal metric, but the one that produces the greatest overall symmetry is the (w_1,w_2,w_3) system of coordinates. To find the metric in these coordinates, we can transform $g_{\mu\nu}$ as a covariant tensor, starting with Eq. (4.40), or, what is easier, work with Eqs. (4.38) and (3.30). This quickly yields

$$g^{\mu\nu}=\begin{pmatrix}4w&0&0\\0&4w&0\\0&0&4w\end{pmatrix} \tag{4.42}$$

or

$$\begin{aligned}ds^2&=g_{\mu\nu}dq^\mu dq^\nu\\&=\frac{1}{4w}(dw_1^2+dw_2^2+dw_3^2)\\&=\frac{1}{4w}(dw^2+w^2d\chi^2+w^2\cos^2\chi d\psi^2).\end{aligned} \tag{4.43}$$

These expressions in the coordinates (w_1,w_2,w_3) make it obvious that the metric is conformally flat, i.e., proportional to a Euclidean metric (Iwai, 1987b). This is another special property of the three-body problem; the metric for $n=4$ is not conformally flat, as one can prove by computing the Weyl tensor (Eguchi, Gilkey, and Hanson, 1980; Nakahara, 1990).

What is more remarkable than the conformal flatness of the metric is the fact that it is invariant under SO(3) rotations in shape space, i.e., ordinary orthogonal transformations applied to the shape coordinates (w_1,w_2,w_3). That is, not only is the metric tensor proportional to the identity matrix, but also the factor of proportionality (namely, $1/4w$) is rotationally invariant. It was to be expected that the metric would be invariant under democracy transformations; as indicated by Eq. (3.36), these are SO(2) rotations about the w_3 axis. But we see that $g_{\mu\nu}$ is also invariant with respect to rotations about the w_1 and w_2 axes. Of course, unlike the democracy rotations about the w_3 axis, the latter rotations carry parts of the physical region $w_3\geqslant 0$ into the nonphysical region $w_3<0$, but the SO(3) symmetry still exists in a local sense. As noted earlier, the Coriolis tensor $\mathbf{B}_{\mu\nu}$ is symmetric under the same SO(3) group.

We have been able to show, in a calculation we shall present elsewhere, that in the four-body problem the metric $g_{\mu\nu}$ has no larger symmetry group than the democracy group. Thus the existence of a symmetry group of the metric in the three-body problem that is larger than the democracy group is another special feature of the three-body problem.

The true metric $g_{\mu\nu}$ on shape space is non-Euclidean. To prove this in the general case, we must show that the Riemann tensor does not vanish, or even that the Riemann scalar does not vanish. In fact, as shown by Eq. (4.61), the Riemann scalar R can be written in terms of the Coriolis tensor and the moment-of-inertia tensor,

$$R=\tfrac{3}{4}\mathbf{B}^{\mu\nu}\cdot\mathsf{M}\cdot\mathbf{B}_{\mu\nu}, \tag{4.44}$$

which is a nonvanishing quantity. (Here we raise indices on $\mathbf{B}^{\mu\nu}$ with the metric $g^{\mu\nu}$.) For example, in the three-body problem, we find

$$R=\frac{6}{w}. \tag{4.45}$$

The non-Euclidean nature of shape space is an intrinsic feature of this space and is not a matter that can be defined away, due to the gauge invariance of $g_{\mu\nu}$ and the coordinate invariance of conditions such as (4.45). Thus even simple questions regarding dynamics on shape space will quickly lead into the standard machinery of

non-Euclidean geometry. For example, Christoffel symbols arise in the equations of motion for free particles and the Riemann tensor in equations of deviation of two nearby classical trajectories. Similarly, quantum mechanics on shape space has many of the features of quantum mechanics on curved space-time.

D. Derivation of the classical equations of motion

There are two issues that arise in computing the classical equations of motion from the Lagrangian (4.21) which are not altogether elementary. One is the fact that the components of the angular velocity $\boldsymbol{\omega}$ cannot be written as the time derivatives of any coordinates on the rotation-group manifold, i.e., they are anholonomic velocity components. These components can be expressed in terms of the Euler angles and their time derivatives, but since the explicit use of Euler angles is unattractive, this is to be avoided. Instead, we shall work with an anholonomic or *vielbein* formalism insofar as the orientational variables are concerned. The second issue is the appearance of covariant derivatives in the equations of motion, which are necessary to put those equations into manifestly gauge-invariant form.

As far as the shape degrees of freedom are concerned, the Lagrangian of Eq. (4.21) is a proper function of generalized coordinates q^μ and their time derivatives $\dot{q}^\mu$, but the orientational degrees of freedom are expressed through the medium of the angular velocity $\boldsymbol{\omega}$. The relation between the angular velocity and the $\dot{\theta}^i$ was given in Eqs. (4.28)–(4.33). We shall write the components of the matrix X as $X^i_{(j)}$ (row i, column j), so that

$$X^i_{(k)}\Lambda^{(k)}_j=\delta^i_j, \quad \Lambda^{(i)}_k X^k_{(j)}=\delta^i_j. \tag{4.46}$$

The reason for this notation, as explained more fully in Appendix C, is that we regard $X^i_{(j)}$ as a set of three contravariant vector fields on the group manifold SO(3), labeled by j, whose components are indexed by i; the parentheses around j are a reminder that this index labels the vector fields and is not a component index. We think of these vector fields as constituting a *vielbein* (perhaps we should say "*dreibein*," since there are three of them), so that the components of the angular velocity ω^i are seen as the anholonomic components of the rotational velocity with respect to this *vielbein*. The use of *vielbeins* or anholonomic frames in Lagrangian and Hamiltonian mechanics is explained in Appendix C; we shall call freely on the formulas of that Appendix, making the notational changes $x^\mu\to\theta^i$, $\underline{L}\to L$, etc. In particular, $\Lambda^{(i)}_j$ are regarded as the components of a set of three covectors, members of the basis of covectors $\Lambda^{(i)}$ are dual to the *vielbein* $X_{(j)}$, and the notation v^α of Appendix C for the anholonomic components of the velocity is identified here with ω^i.

In a recent paper, Lukka (1995) has simplified earlier methods of deriving the molecular rovibrational Hamiltonian, in part by eliminating all explicit references to Euler angles. It seems to us that this must be equivalent to working with the geometrical properties of the *vielbein* $X_{(j)}$, such as the property that these vector fields are left invariant on the group manifold and represent through the Lie bracket the Lie algebra of the group.

According to Eq. (C17), the anholonomic components of the momenta conjugate to ω^i are given by $\partial L/\partial\omega^i$, which we recognize as the components of the body angular momentum,

$$\mathbf{L}=\frac{\partial L}{\partial\boldsymbol{\omega}}=\mathsf{M}(\boldsymbol{\omega}+\mathbf{A}_\mu\dot{q}^\mu). \tag{4.47}$$

Thus the notation π_α of Appendix C is here identified with L_i. We also have

$$L_i=X^j_{(i)}p_j, \quad p_i=\Lambda^{(j)}_i L_j, \tag{4.48}$$

the analog of Eq. (C4), where p_i is the momentum conjugate to the Euler angle θ^i.

The momenta conjugate to the shape coordinates are

$$p_\mu=\frac{\partial L}{\partial\dot{q}^\mu}=g_{\mu\nu}\dot{q}^\nu+\mathbf{L}\cdot\mathbf{A}_\mu. \tag{4.49}$$

The momenta p_μ are gauge dependent, because of the term $\mathbf{L}\cdot\mathbf{A}_\mu$ on the right; this is analogous to the gauge dependence of $\mathbf{p}=m\mathbf{v}+(e/c)\mathbf{A}$ in ordinary electromagnetic theory. The quantity $p_\mu-\mathbf{L}\cdot\mathbf{A}_\mu$, however, is gauge invariant. Our original sign convention for $\mathbf{A}_\mu$, and the minus sign appearing in Eq. (3.58), were chosen because of this electromagnetic analogy.

In order to find the equations of motion, we must apply Eq. (C19), the anholonomic version of the Euler-Lagrange equations. But these involve the structure constants c^i_{jk} associated with the *vielbein* $X^i_{(j)}$, which we must compute first. To do this we first compute the exterior derivatives of the dual basis covectors $\Lambda^{(i)}$ and then use Eq. (C13). The components of these exterior derivatives are

$$d\Lambda^{(i)}_{jk}=\Lambda^{(i)}_{k,j}-\Lambda^{(i)}_{j,k}. \tag{4.50}$$

But by Eq. (4.28) we have

$$\frac{\partial\boldsymbol{\omega}^i}{\partial\dot{\theta}^k}=\Lambda^{(i)}_k, \quad \frac{\partial^2\boldsymbol{\omega}^i}{\partial\dot{\theta}^k\partial\theta^j}=\Lambda^{(i)}_{k,j}. \tag{4.51}$$

Therefore the right-hand side of Eq. (4.50) is the ith component of the vector,

$$\frac{\partial^2\boldsymbol{\omega}}{\partial\dot{\theta}^k\partial\theta^j}-\frac{\partial^2\boldsymbol{\omega}}{\partial\dot{\theta}^j\partial\theta^k}\leftrightarrow\frac{\partial^2\Omega}{\partial\dot{\theta}^k\partial\theta^j}-\frac{\partial^2\Omega}{\partial\dot{\theta}^j\partial\theta^k}. \tag{4.52}$$

But in view of Eq. (4.32), we have

$$\frac{\partial\Omega}{\partial\dot{\theta}^k}=\mathsf{R}^T\mathsf{R}_{,k}=-\mathsf{R}^T_{,k}\mathsf{R}, \quad \frac{\partial^2\Omega}{\partial\dot{\theta}^k\partial\theta^j}=\mathsf{R}^T_{,j}\mathsf{R}_{,k}+\mathsf{R}^T\mathsf{R}_{,kj}, \tag{4.53}$$

so that

$$\begin{aligned}\frac{\partial^2\Omega}{\partial\dot{\theta}^k\partial\theta^j}-\frac{\partial^2\Omega}{\partial\dot{\theta}^j\partial\theta^k}&=\mathsf{R}^T_{,j}\mathsf{R}\mathsf{R}^T\mathsf{R}_{,k}-\mathsf{R}^T_{,k}\mathsf{R}\mathsf{R}^T\mathsf{R}_{,j}\\&=\left[\frac{\partial\Omega}{\partial\dot{\theta}^k},\frac{\partial\Omega}{\partial\dot{\theta}^j}\right]\leftrightarrow\frac{\partial\boldsymbol{\omega}}{\partial\dot{\theta}^k}\times\frac{\partial\boldsymbol{\omega}}{\partial\dot{\theta}^j},\end{aligned} \tag{4.54}$$

where the square bracket is the matrix commutator. But by Eq. (4.51), the ith component of this final vector is

$$d\Lambda^{(i)}_{jk} = \epsilon_{i\ell m}\Lambda^{(\ell)}_{k}\Lambda^{(m)}_{j}. \tag{4.55}$$

Therefore $d\Lambda^{(i)}(X_{(r)}, X_{(s)}) = -\epsilon_{irs}$, or,

$$c^{i}_{jk} = \epsilon_{ijk}. \tag{4.56}$$

The nonvanishing of this result proves incidentally that the angular velocity components ω^i cannot be written as the time derivatives of any coordinates on the rotation-group manifold, i.e., the *vielbein* $X^i_{(j)}$ is genuinely anholonomic.

The simplicity of the result (4.56) is a reflection of the fundamental geometrical significance of the vector fields constituting the *vielbein* $X^i_{(j)}$, which we have ignored in this calculation. These vector fields are left-invariant vector fields on the group manifold, whose commutation relations under the Lie bracket reproduce the structure constants of the Lie algebra of the group itself. The significance of the left invariance, rather than right invariance, is that we worked with the body components of the angular velocity, rather than the space components.

The space components of the angular velocity give rise to a distinct *vielbein* on the group manifold SO(3), the *vielbein* of right-invariant vector fields. To define the space or right-invariant version of the dual basis we write

$$\omega^i_s = \Lambda^{(i)}_{sj}\dot{\theta}^j, \tag{4.57}$$

so that

$$\Lambda^{(i)}_{sj} = \mathsf{R}_{ik}\Lambda^{(k)}_{j}, \tag{4.58}$$

and we define the *vielbein* itself by $X^i_{s(j)}\Lambda^{(j)}_{sk} = \delta^i_k$. The calculation of the structure constants for the new *vielbein* proceeds as above and yields

$$(c_s)^i_{jk} = -\epsilon_{ijk}, \tag{4.59}$$

with a minus sign relative to the body, or left-invariant, *vielbein*.

The two *vielbeins* we have introduced and their dual bases of covectors can be written in the standard notation of differential geometry, in which a vector field is represented as a differential operator and a covector field as a differential form. For the left-invariant fields, the relations are

$$X_{(i)} = X^j_{(i)}\frac{\partial}{\partial\theta^j}, \quad \Lambda^{(i)} = \Lambda^{(i)}_j d\theta^j, \tag{4.60}$$

and for the right-invariant fields they are

$$X_{s(i)} = X^j_{s(i)}\frac{\partial}{\partial\theta^j}, \quad \Lambda^{(i)}_s = \Lambda^{(i)}_{sj} d\theta^j. \tag{4.61}$$

The two classes of vector fields (left- and right-invariant) can be viewed either as vector fields on the group manifold or as vector fields on the fiber bundle. For if we choose a section, then the Euler angles θ^i or associated rotation matrices $\mathsf{R} = \mathsf{R}(\theta^i)$ serve as coordinates on each of the fibers and also provide a one-to-one mapping between the rotation-group manifold and each of the fibers. This mapping allows vector fields on the rotation-group manifold to be mapped into vector fields on the fibers. Since this can be done for each fiber individually, the result is a set of vector fields on the bundle. These vector fields are vertical, i.e., their q^μ components vanish, and their θ^j components are given by $X^j_{(i)}$ or $X^j_{s(i)}$. The right-invariant vector fields on the fiber bundle, constructed in this manner, are in fact independent of the choice of section (they are gauge invariant), but the left-invariant fields do depend on the choice of section.

It also happens that the right-invariant vector fields are the infinitesimal generators of the left group action, as in Eq. (4.23), and the left-invariant fields are the infinitesimal generators of the right action, as in Eq. (4.24). For example, if the matrix Q in Eq. (4.22) is infinitesimal, having the form, say,

$$\mathsf{Q} = \mathsf{I} + \delta\phi\mathsf{N}_s, \tag{4.62}$$

for some antisymmetric matrix $\mathsf{N}_s \leftrightarrow \mathbf{n}_s$ and some infinitesimal angle $\delta\phi$, then the infinitesimal motions generated by Eq. (4.22) or (4.23) trace out the right-invariant vector field $n_{si}X_{s(i)}$. This is an infinitesimal "space" rotation, in which the Jacobi vectors are mapped according to

$$\boldsymbol{\rho}_{s\alpha} \mapsto \boldsymbol{\rho}_{s\alpha} + \delta\phi\,\mathbf{n}_s \times \boldsymbol{\rho}_{s\alpha}. \tag{4.63}$$

Similarly, if the matrix Q in Eq. (4.24) has the form

$$\mathsf{Q} = \mathsf{I} + \delta\phi\mathsf{N}, \tag{4.64}$$

for some antisymmetric matrix $\mathsf{N} \leftrightarrow \mathbf{n}$ and some infinitesimal angle $\delta\phi$, then the infinitesimal motions generated by Eq. (4.24) trace out the left-invariant vector field $n_i X_{(i)}$. This is an infinitesimal "body" rotation (viewed here in an active sense, not as a gauge transformation), in which the space components of the Jacobi vectors transform according to

$$\boldsymbol{\rho}_{s\alpha} = \mathsf{R}\boldsymbol{\rho}_\alpha \mapsto \mathsf{R}(\mathsf{I} + \delta\phi\mathsf{N})\boldsymbol{\rho}_\alpha = \mathsf{R}(\boldsymbol{\rho}_\alpha + \delta\phi\,\mathbf{n}\times\boldsymbol{\rho}_\alpha). \tag{4.65}$$

[This equation should be interpreted properly. We are adopting here an active point of view, in which right, or body, rotations map old configurations into new ones. These rotations map a point on a given fiber into another point on the same fiber; thus the q^μ coordinates of the point do not change. Only R changes, as indicated by Eq. (4.24). Furthermore, the gauge convention is considered to be held fixed. Therefore the body components of the Jacobi vectors $\boldsymbol{\rho}_\alpha$ are the same at the old and new points, since these are functions only of q^μ. Although Eq. (4.65) looks like the mapping

$$\boldsymbol{\rho}_\alpha \mapsto \boldsymbol{\rho}_\alpha + \delta\phi\,\mathbf{n}\times\boldsymbol{\rho}_\alpha, \tag{4.66}$$

in fact the quantities $\{\boldsymbol{\rho}_\alpha\}$ do not change. On the other hand, if we were to perform an infinitesimal gauge transformation, it would be possible to make the body Jacobi vectors change as in Eq. (4.66). If at the same time we were to adjust the space Jacobi vectors $\{\boldsymbol{\rho}_{s\alpha}\}$ so that R remained fixed, then the changes in the space Jacobi vectors would be exactly the same as indicated by Eq.

(4.65). This would give us a passive interpretation of Eq. (4.65), which, however, we shall not adopt in this review.]

We now proceed to apply Eq. (C19), obtaining the equations of motion. We trust there will be no confusion between the Lagrangian L and the angular momentum $\mathbf{L}$ or its components L_i. For the orientational variables, we have

$$\dot{L}_i = X^j_{(i)} \frac{\partial L}{\partial \theta^j} - c^k_{ij} \omega^j L_k \tag{4.67}$$

or, since the Lagrangian does not depend on the Euler angles,

$$\dot{\mathbf{L}} = -\boldsymbol{\omega} \times \mathbf{L}. \tag{4.68}$$

This of course is an elementary result, which merely expresses the constancy of the space components of the angular momentum, $\dot{\mathbf{L}}_s = 0$. It is true both for rigid bodies and for deformable ones, as long as angular momentum is conserved. On the other hand, for rigid bodies it is possible to use the relation $\mathbf{L} = \mathsf{M}\boldsymbol{\omega}$ to eliminate either $\mathbf{L}$ or $\boldsymbol{\omega}$ from Eq. (4.68), to obtain an autonomous system of equations (Euler's equations for a torque-free rigid body). This cannot be done in the case of deformable bodies, because the relation (3.57) between $\mathbf{L}$ and $\boldsymbol{\omega}$ involves the shape coordinates. Thus, for deformable bodies, Eq. (4.68) is not autonomous, but is coupled to the evolution of the shape variables. In either case, we have the conservation law

$$\frac{d|\mathbf{L}|^2}{dt} = 0, \tag{4.69}$$

so that the motion of the body angular momentum vector can be viewed as taking place on the surface of a sphere $|\mathbf{L}|^2 = \text{const}$ in body angular momentum space. In the case of rigid bodies, this motion usually follows closed orbits, but for deformable bodies the orbits will not close due to the coupling to the shape degrees of freedom. The body angular momentum sphere is a two-dimensional surface, but counts for only a single degree of freedom, since it is a phase space, not a configuration space.

Since $\boldsymbol{\omega}$ is not gauge covariant, it is desirable to use Eq. (3.57) to eliminate $\boldsymbol{\omega}$ from Eq. (4.68). We write the result in a notation to be explained momentarily,

$$\frac{D\mathbf{L}}{Dt} = \dot{\mathbf{L}} - \mathbf{A}_\mu \times \mathbf{L}\dot{q}^\mu = -(\mathsf{M}^{-1}\mathbf{L}) \times \mathbf{L}. \tag{4.70}$$

Because of the term $\mathbf{A}_\mu \times \mathbf{L}\dot{q}^\mu$, we see that $\dot{\mathbf{L}}$ is not gauge covariant. This may be surprising, since $\mathbf{L}$ itself is gauge covariant. The reason is that, in computing $\dot{\mathbf{L}}$, we are taking a limit of the form

$$\lim_{\epsilon \to 0} \frac{1}{\epsilon} [\mathbf{L}(t+\epsilon) - \mathbf{L}(t)], \tag{4.71}$$

so that $\mathbf{L}$ is evaluated at two distinct times. But $\mathbf{L}$ stands for the body components of the angular momentum, and during the time interval between t and $t+\epsilon$ the shape will have changed by some amount dq^μ. The two vectors $\mathbf{L}$ in the limit are referred to two distinct body frames, which can be changed independently of one another under a gauge transformation. Therefore $\dot{\mathbf{L}}$ is not a true R vector. On the other hand, if we subtract the term $\mathbf{A}_\mu \times \mathbf{L}\dot{q}^\mu$, then the result is gauge covariant, as we see from the right-hand side of Eq. (4.70). We note that $\mathsf{M}^{-1}\mathbf{L}$ is essentially the vertical component of the system velocity, as indicated by Eqs. (3.57) and (4.14). The subtracted term is a correction, which accounts for the changing body frame and converts the noncovariant vector $\dot{\mathbf{L}}$ into a covariant result. We write $D\mathbf{L}/Dt$ for the result, where D/Dt stands for the covariant time derivative.

As for the shape coordinates, the Euler-Lagrange equations in the usual sense can be applied, since the Lagrangian is a proper function of $(q^\mu, \dot{q}^\mu)$. A special case of interest is that of a system of free particles of vanishing angular momentum ($V = 0$, $\mathbf{L} = 0$); in this case the Lagrangian is that of a free particle on a non-Euclidean manifold with metric $g_{\mu\nu}$, $L = (1/2) g_{\mu\nu} \dot{q}^\mu \dot{q}^\nu$, so that the equations of motion are simply those of a geodesic,

$$\frac{D\dot{q}^\mu}{Dt} = \ddot{q}^\mu + \Gamma^\mu_{\sigma\tau} \dot{q}^\sigma \dot{q}^\tau = 0, \tag{4.72}$$

where the Christoffel symbols are the usual ones,

$$\Gamma^\mu_{\sigma\tau} = \frac{1}{2} g^{\mu\nu} (g_{\nu\sigma,\tau} + g_{\nu\tau,\sigma} - g_{\sigma\tau,\nu}), \tag{4.73}$$

and where we again use the notation D/Dt for the covariant time derivative. In this case the covariant time derivative is the usual one in the differential geometry of Riemannian manifolds, i.e., it indicates covariance with respect to arbitrary coordinate transformations on shape space.

Now we deal with the general case. We apply the Euler-Lagrange equations, $\dot{p}_\mu = \partial L / \partial q^\mu$, and we collect the geodesic terms on the left and everything else on the right. We find

$$g_{\mu\nu} \frac{D\dot{q}^\nu}{Dt} = -\dot{\mathbf{L}} \cdot \mathbf{A}_\mu + \mathbf{L} \cdot (\mathbf{A}_{\nu,\mu} - \mathbf{A}_{\mu,\nu}) \dot{q}^\nu + \tfrac{1}{2} \mathbf{L} \cdot \mathsf{M}^{-1} (\mathsf{M}_{,\mu}) \mathsf{M}^{-1} \cdot \mathbf{L} - V_{,\mu}, \tag{4.74}$$

after eliminating $\boldsymbol{\omega}$ in favor of $\mathbf{L}$. But by Eq. (4.70), the first term on the right-hand side becomes

$$-\dot{\mathbf{L}} \cdot \mathbf{A}_\mu = -\mathbf{L} \cdot (\mathbf{A}_\mu \times \mathbf{A}_\nu) \dot{q}^\nu + \mathbf{L} \cdot [\mathbf{A}_\mu \times (\mathsf{M}^{-1}\mathbf{L})]. \tag{4.75}$$

The final term of this expression in turn becomes

$$\mathbf{L} \cdot [\mathbf{A}_\mu \times (\mathsf{M}^{-1}\mathbf{L})] = \mathbf{L} \cdot \mathsf{A}_\mu \mathsf{M}^{-1} \cdot \mathbf{L} = \tfrac{1}{2} \mathbf{L} \cdot [\mathsf{A}_\mu, \mathsf{M}^{-1}] \cdot \mathbf{L}, \tag{4.76}$$

where $\mathsf{A}_\mu \leftrightarrow \mathbf{A}_\mu$ and where we use the antisymmetry of A_μ to express the result as a commutator. Finally, shifting a derivative from M to M^{-1}, we have

$$g_{\mu\nu}\frac{D\dot{q}^{\nu}}{Dt}=g_{\mu\nu}(\ddot{q}^{\nu}+\Gamma^{\nu}_{\sigma\tau}\dot{q}^{\sigma}\dot{q}^{\tau})$$

$$=\mathbf{L}\cdot\mathbf{B}_{\mu\nu}\dot{q}^{\nu}-\tfrac{1}{2}\mathbf{L}\cdot(\mathsf{M}^{-1})_{;\mu}\cdot\mathbf{L}-V_{,\mu}, \quad (4.77)$$

where

$$\mathsf{M}^{-1}_{;\mu}=\mathsf{M}^{-1}_{,\mu}-[\mathsf{A}_{\mu},\mathsf{M}^{-1}]. \quad (4.78)$$

The notation $\mathsf{M}^{-1}_{;\mu}$ represents the covariant derivative of the inverse moment-of-inertia tensor. Although M^{-1} is a true R tensor, the ordinary derivative $\mathsf{M}^{-1}_{,\mu}$ is not, since shape derivatives involve a limit of the form

$$\lim_{\epsilon\to 0}\frac{1}{\epsilon}[\mathsf{M}^{-1}(q^{\mu}+\epsilon\xi^{\mu})-\mathsf{M}^{-1}(q^{\mu})]=\xi^{\mu}\frac{\partial\mathsf{M}^{-1}}{\partial q^{\mu}}, \quad (4.79)$$

where ξ^{μ} is some fixed vector, so that M^{-1} (i.e., its components) are evaluated with respect to two distinct body frames attached to two distinct shapes. Since these frames can be redefined independently under a gauge transformation, the quantity $\mathsf{M}^{-1}_{,\mu}$ is not a true R tensor. This is the same theme as in the computation of $\dot{\mathbf{L}}$ in Eq. (4.71), except that here we are discussing the partial derivative with respect to q^{μ} of a field $\mathsf{M}^{-1}(q)$ over shape space, and there we were discussing the time derivative of a quantity $\mathbf{L}(t)$ defined only along an orbit. We can also see the noncovariance of $\mathsf{M}^{-1}_{,\mu}$ directly, by differentiating $\mathsf{M}^{-1}=\mathsf{S}\mathsf{M}'^{-1}\mathsf{S}^{T}$ to obtain

$$\mathsf{M}^{-1}_{,\mu}=\mathsf{S}(\mathsf{M}'^{-1}_{,\mu}+[\Gamma_{\mu},\mathsf{M}^{-1}])\mathsf{S}^{T}. \quad (4.80)$$

But if we add the correction term $-[\mathsf{A}_{\mu},\mathsf{M}^{-1}]$, then all terms involving Γ_{μ} cancel and we are left with

$$\mathsf{M}^{-1}_{;\mu}-[\mathsf{A}_{\mu},\mathsf{M}^{-1}]=\mathsf{S}(\mathsf{M}'^{-1}_{,\mu}-[\mathsf{A}'_{\mu},\mathsf{M}'^{-1}])\mathsf{S}^{T} \quad (4.81)$$

or simply $\mathsf{M}^{-1}_{;\mu}=\mathsf{S}\mathsf{M}'^{-1}_{;\mu}\mathsf{S}^{T}$.

Covariant derivatives arise wherever ordinary derivatives arise, if it is desired to express the results in covariant form. For example, perturbation expansions (such as multipole expansions, etc.) typically generate derivatives of fields, and one can develop versions of covariant perturbation theory. We have relegated further discussion of covariant derivatives to Appendix D.

E. Discussion of the classical equations of motion

Equations (4.70) and (4.77) are the reduced classical equations of motion, i.e., the equations that result after all possible translational and rotational degrees of freedom have been separated. Since there are $3n-6$ shape degrees of freedom in Eq. (4.77) and one angular momentum degree of freedom in Eq. (4.70), the reduced system has overall $3n-5$ degrees of freedom. Three more (translational) degrees of freedom are contained in the center of mass motion, $\ddot{\mathbf{R}}_s=0$, and two more in the orientational motion. The two remaining orientational degrees of freedom are represented by four first-order differential equations; one of these is $d|\mathbf{L}|^2/dt=0$, and the other three are contained in $\dot{\mathsf{R}}=\Omega(t)\mathsf{R}$ (which can be regarded as three equations for the three Euler angles). The reduced system is decoupled from the translational and orientational degrees of freedom; once the reduced system is solved, so that q^{μ} and $\mathbf{L}$ become known functions of time, the orientational equations can then be solved as a time-dependent system. In the reduced system, the $3n-6$ shape degrees of freedom are coupled to the one angular momentum degree of freedom, and rotational invariance alone will not allow any further separation of these $3n-5$ degrees of freedom. In the case of molecules, however, a further adiabatic separation of the $3n-6$ shape degrees of freedom from the one angular momentum degree of freedom is possible due to the ordering of time scales which make up the Born-Oppenheimer approximation. Of course, this further separation is only approximate.

In the special case $\mathbf{L}=0$, the angular momentum sphere shrinks to a point and the angular momentum degree of freedom becomes vacuous, so that Eqs. (4.77) become autonomous in the shape coordinates. In this case, the reduced system has only $3n-6$ degrees of freedom. As noted earlier, if we have both $\mathbf{L}=0$ and $V=0$ (free particles), then the reduced motion is a geodesic on shape space.

Equation (4.77) is the generalization of the radial equation in ordinary central force motion (the two-body problem) to the case $n\geqslant 3$. Although the analogies are not perfect, it is useful to note that in the two-body problem the one-dimensional shape space has coordinate $q=r$, and the moment of inertia is mr^2. Furthermore, as on all one-dimensional manifolds, the metric is Euclidean, $g_{\mu\nu}=g_{11}=m=\text{const.}$, and antisymmetric tensors vanish, $\mathbf{B}_{\mu\nu}=0$. With this in mind, we can compare Eq. (4.77) to the two-body radial equation

$$m\ddot{r}=-\frac{d}{dr}\left[\frac{L^2}{2mr^2}+V(r)\right]. \quad (4.82)$$

We see that in the case $n\geqslant 3$ the quantity $(1/2)\mathbf{L}\cdot\mathsf{M}^{-1}\cdot\mathbf{L}$, the covariant derivative of which appears in the shape equations of motion, is the generalization of the centrifugal potential $L^2/2mr^2$ in the case $n=2$. We shall call this quantity the centrifugal potential in all cases; we note that it is otherwise the vertical component of the kinetic energy.

The term $\mathbf{L}\cdot\mathbf{B}_{\mu\nu}\dot{q}^{\nu}$ in Eq. (4.77) represents the Coriolis forces on the system, since this term is first order in the velocities. This term obviously resembles the relativisitic electromagnetic 4-force on a charged particle, $eF_{\mu\nu}\dot{x}^{\nu}$, with e replaced by $\mathbf{L}$ and $F_{\mu\nu}$ by $\mathbf{B}_{\mu\nu}$. In this analogy, the scalar charge e has become the vector $\mathbf{L}$ because ordinary electromagnetic fields are Abelian gauge fields, whereas ours here are non-Abelian. A closer analogy is given by Wong's equations (Wong, 1970), the classical equations of motion of a particle in a Yang-Mills field, in which the analog of $\mathbf{L}$ is the vector of isotopic spin. In Wong's equations, the evolution of the isotopic spin vector is governed by a separate equation, analogous to our equation for $\dot{\mathbf{L}}$. Wong's equations, however, assume a space-time background that is flat; the presence of the non-Euclidean metric in our prob-

lem makes our equations of motion more analogous to those of a particle moving in a combined gravitational and Yang-Mills field in general relativity. The resemblance of the Coriolis term in the equations of motion (4.77) to the electromagnetic force on a charged particle is reminiscent of Larmor's theorem, in which the effects of a magnetic field on a charged particle are mimicked by a rotating frame; indeed, the present formalism can be thought of as a non-Abelian generalization of Larmor's theorem.

In the case of the three-body problem, we have seen that the Coriolis tensor $\mathbf{B}_{\mu\nu}$ has the form of a monopole. As is well known, a classical charged particle moving in the field of an ordinary Dirac monopole spirals toward the monopole on a conical surface and then, in general, reflects at some minimum radius and spirals back out. But in our problem, such motion can never be seen in pure form, because there is no way to switch off the centrifugal potential. In addition, shape space is non-Euclidean, and the gauge fields are non-Abelian.

In the two-body problem, particles with $L\neq 0$ cannot reach the origin $r=0$, at least when the true potential $V(r)$ is less singular than the centrifugal potential, as we shall assume throughout the following discussion. Similar effects occur in the three-body problem, due to the fact that the centrifugal potential $(1/2)\mathbf{L}\cdot\mathsf{M}^{-1}\cdot\mathbf{L}$ is positive definite and the fact that $\mathbf{L}$ can change its direction but not its magnitude. For example, as we approach the three-body collision in shape space, all three eigenvalues of M approach zero, as shown explicitly by Eq. (3.107), and the centrifugal potential grows without bound. Therefore, by conservation of energy, there is a lower bound on how close we can come in shape space to a three-body collision when $\mathbf{L}\neq 0$. For example, in the case of free particles, it is easy to show that

$$w\geqslant\frac{L^2}{2E}, \tag{4.83}$$

where w is the three-body shape coordinate and E is the total energy of the system. These facts can be easily generalized to the case $n>3$.

When $\mathbf{L}\neq 0$, the centrifugal potential also tends to repel the system away from collinear configurations, at which one of the eigenvalues of M, say I_3, goes to zero. By analogy, if we shoot bullets at the broadside of a barn, a two-dimensional surface in three-dimensional space, then there is a set of finite measure (codimension 0) in the space of initial conditions giving trajectories that will hit the barn (we can imagine standing in one place, but varying the initial direction and speed of the bullets). But if we stand at one position q_0^μ in the shape space of the three-body problem and vary $\dot{q}_0^\mu$, trying to hit the wall of collinear configurations, a two-dimensional surface bounding the three-dimensional shape space, then we find that most trajectories do not reach the wall, but reflect before hitting it. In this game we must of course specify the initial angular momentum $\mathbf{L}_0$, which we assume is fixed at some nonzero value. Then the subset of initial conditions that do hit the wall is two-dimensional in the three-dimensional space of initial conditions (it has codimension 1). The trajectories that do hit the wall must evolve in such a way that L_3, the component of $\mathbf{L}$ in the direction of collinearity, vanishes precisely at the moment collinearity is achieved. These facts have implications for the behavior of the quantum wave function in the neighborhood of collinear configurations.

The equations of motion, Eqs. (4.70) and (4.77), can also be used to obtain the conditions for relative equilibria. A relative equilibrium is defined as a motion for which $\dot{q}^\mu=0$, so that the shape is not changing and the system is moving as if it were a rigid body. A well-known example is the equilateral triangle Lagrange solution in the three-body gravitational problem.

If $\dot{q}^\mu=0$, then by Eq. (4.77) we have

$$\tfrac{1}{2}\mathbf{L}\cdot\mathsf{M}^{-1}_{;\mu}\cdot\mathbf{L}+V_{,\mu}=0, \tag{4.84}$$

which usually cannot be satisfied unless $\mathbf{L}=$const, as we shall assume. But by Eq. (4.70) this in turn implies $\mathbf{L}\times\mathsf{M}^{-1}\mathbf{L}=0$, or

$$\mathsf{M}^{-1}\mathbf{L}=\frac{1}{I}\mathbf{L}, \tag{4.85}$$

where I is an eigenvalue of M, corresponding, say, to eigenvector $\mathbf{e}$. Thus $\mathbf{L}=L\mathbf{e}$, and Eq. (4.84) becomes

$$\tfrac{1}{2}L^2(\mathbf{e}\cdot\mathsf{M}^{-1}_{;\mu}\cdot\mathbf{e})+V_{,\mu}=0 \tag{4.86}$$

or simply

$$\frac{\partial}{\partial q^\mu}\left[\frac{L^2}{2I(q)}+V(q)\right]=0. \tag{4.87}$$

Here we have used a covariant version of "Feynman's theorem," i.e., we have written $\mathsf{M}^{-1}\mathbf{e}=(1/I)\mathbf{e}$, so that by the Leibnitz rule for covariant derivatives (see Appendix D) we have

$$\mathsf{M}^{-1}_{;\mu}\mathbf{e}+\mathsf{M}^{-1}\mathbf{e}_{;\mu}=\left(\frac{1}{I}\right)_{,\mu}\mathbf{e}+\frac{1}{I}\mathbf{e}_{;\mu}, \tag{4.88}$$

from which follows

$$\mathbf{e}\cdot\mathsf{M}^{-1}_{;\mu}\cdot\mathbf{e}=\left(\frac{1}{I}\right)_{,\mu}. \tag{4.89}$$

Equation (4.87) is the condition for a relative equilibrium. Clearly the locations of relative equilibria in shape space are parametrized by the value of L^2. The issue of the stability of the equilibria is a more complicated matter; in recent years considerable attention has been devoted to the stability and bifurcation of relative equilibria (Smale, 1971; Palmore, 1973; Marsden, 1992).

F. The classical Hamiltonian

It is now straightforward to obtain the classical Hamiltonian, except that we must again use an anholonomic basis for the orientational degrees of freedom if we wish to work with the angular momentum $\mathbf{L}$ instead of the

momenta p_i conjugate to the Euler angles θ^i. Therefore we invoke Eq. (C20) and change notation appropriately, to obtain

$$H=\boldsymbol{\omega}\cdot\mathbf{L}+p_\mu\dot{q}^\mu-L(\boldsymbol{\omega},q^\mu,\dot{q}^\mu), \tag{4.90}$$

where we have omitted the term $\mathbf{P}_s\cdot\dot{\mathbf{R}}_s$ corresponding to the translational degrees of freedom, and where we must use Eqs. (4.47) and (4.49) to eliminate $\boldsymbol{\omega}$ and $\dot{q}^\mu$ in favor of $\mathbf{L}$ and p_μ. Actually, it is easier to note that the Hamiltonian is simply the energy of the system, $K+V$; the use of anholonomic frames does not change this fact. The vertical component of the kinetic energy was given in Eq. (4.16) and is just the centrifugal potential, whereas the horizontal component (4.17) is easily expressed in terms of momenta by inverting Eq. (4.49),

$$\dot{q}^\mu=g^{\mu\nu}(p_\nu-\mathbf{L}\cdot\mathbf{A}_\nu). \tag{4.91}$$

Altogether, the classical Hamiltonian is

$$H=\tfrac{1}{2}\mathbf{L}\cdot\mathsf{M}^{-1}\cdot\mathbf{L}+\tfrac{1}{2}g^{\mu\nu}(p_\mu-\mathbf{L}\cdot\mathbf{A}_\mu)(p_\nu-\mathbf{L}\cdot\mathbf{A}_\nu)+V(q). \tag{4.92}$$

In this form, H is manifestly gauge invariant.

Another form of this Hamiltonian, in which the gauge invariance is effectively hidden, is popular in the molecular physics literature. This alternative form is obtained by using the gauge-dependent pseudo-metric $h_{\mu\nu}$ and its inverse $h^{\mu\nu}$ instead of $g_{\mu\nu}$ and $g^{\mu\nu}$, and by completing the square of the kinetic energy, regarded as a quadratic polynomial in $\mathbf{L}$. The quadratic coefficient (the matrix contracted with L_iL_j) in the kinetic energy is $\tilde{\mathsf{M}}^{-1}$, defined by Eq. (4.37). An equivalent definition of $\tilde{\mathsf{M}}$ is

$$\tilde{\mathsf{M}}=\mathsf{M}-\mathsf{M}(\mathbf{A}_\mu h^{\mu\nu}\mathbf{A}_\nu^T)\mathsf{M}=\mathsf{M}-\mathbf{a}_\mu h^{\mu\nu}\mathbf{a}_\nu^T, \tag{4.93}$$

as we show by multiplying the right-hand side of Eq. (4.93) by that of Eq. (4.37) and using Eq. (4.18). Unlike the true moment-of-inertia tensor, the modified tensor $\tilde{\mathsf{M}}$ is not gauge covariant. This tensor is prominent in the literature on molecular vibrations, as it appears explicitly in the Wilson-Howard-Watson Hamiltonian; nevertheless, we are not aware of any physical interpretation of the correction term in Eq. (4.37) or (4.93). Of course, if such an interpretation exists, it must be tied to the specific gauge conventions used. It is possible, however, to provide a geometrical interpretation of this tensor, and its lack of gauge covariance; we shall do this in Sec. V.

To incorporate the terms linear in $\mathbf{L}$ in the Hamiltonian, we use the identity

$$\tilde{\mathsf{M}}\mathbf{A}_\mu g^{\mu\nu}=\mathsf{M}\mathbf{A}_\mu h^{\mu\nu}=\mathbf{a}_\mu h^{\mu\nu}, \tag{4.94}$$

as easily follows from Eqs. (4.93) and (4.18), and we define

$$\mathbf{K}=\mathbf{a}_\mu h^{\mu\nu}p_\nu, \tag{4.95}$$

so that the cross terms are of the form $-\mathbf{L}\cdot\tilde{\mathsf{M}}^{-1}\cdot\mathbf{K}$. Under the Eckart conventions, the vector $\mathbf{K}$ is referred to as "the angular momentum of vibration" (Wilson and Howard, 1936), although since $\mathbf{K}$ is not gauge covariant, this terminology is tied to the specific gauge convention. Finally, for the constant term in the Hamiltonian we use the identity

$$g^{\mu\nu}=h^{\mu\nu}+h^{\mu\sigma}(\mathbf{a}_\sigma\cdot\tilde{\mathsf{M}}^{-1}\cdot\mathbf{a}_\tau)h^{\tau\nu}, \tag{4.96}$$

which is easily proved with Eqs. (4.37) and (4.18). Altogether, the Hamiltonian becomes

$$H=\tfrac{1}{2}(\mathbf{L}-\mathbf{K})\cdot\tilde{\mathsf{M}}^{-1}\cdot(\mathbf{L}-\mathbf{K})+\tfrac{1}{2}h^{\mu\nu}p_\mu p_\nu+V(q). \tag{4.97}$$

There are several more identities connecting M, $\tilde{\mathsf{M}}$, $g^{\mu\nu}$, and $h^{\mu\nu}$ which are useful in translating the traditional molecular physics literature into manifestly gauge-invariant form. One of these is

$$h^{\mu\nu}=g^{\mu\nu}-g^{\mu\sigma}(\mathbf{A}_\sigma\cdot\tilde{\mathsf{M}}\cdot\mathbf{A}_\tau)g^{\tau\nu}. \tag{4.98}$$

Another useful identity is

$$(\det\mathsf{M})(\det g_{\mu\nu})=(\det\tilde{\mathsf{M}})(\det h_{\mu\nu}). \tag{4.99}$$

To prove this identity, we use Eq. (4.115) and another factorization of the metric tensor,

$$G'_{ab}=\begin{pmatrix}\Lambda^T & \Lambda^T\mathbf{a}_\kappa h^{\kappa\sigma}\\ 0 & \delta^\sigma_\mu\end{pmatrix}\begin{pmatrix}\tilde{\mathsf{M}} & 0\\ 0 & h_{\sigma\tau}\end{pmatrix}\begin{pmatrix}\Lambda & 0\\ h^{\tau\lambda}\mathbf{a}_\lambda\Lambda & \delta^\tau_\nu\end{pmatrix}, \tag{4.100}$$

where the conventions regarding indices are the same as those in Eq. (4.115). It is necessary to use Eq. (4.93) in deriving Eq. (4.100). Taking determinants yields Eq. (4.99). The matrix that appears in the middle on the right-hand side of Eq. (4.100) is the metric with respect to the *vielbein* of vectors parallel and perpendicular to the gauge surface, to be discussed in Sec. V.

We return now to the Hamiltonian in the manifestly gauge-invariant form (4.92). The phase-space coordinates are $(\theta^i,\mathbf{L},q^\mu,p_\mu)$, of which q^μ,p_μ are ordinary canonical variables. But the vector $\mathbf{L}$ contains the components of the orientational momentum with respect to the anholonomic frame of left-invariant covector fields $\Lambda^{(i)}$ (the dual basis) on the rotation-group manifold, so the orientational coordinates are noncanonical and satisfy nonstandard Poisson bracket relations. According to Eqs. (C22) and (4.56), these are

$$\{\theta^i,\theta^j\}=0,\quad \{\theta^i,L_j\}=X^i_{(j)},\quad \{L_i,L_j\}=-\epsilon_{ijk}L_k. \tag{4.101}$$

Of these the final one is noteworthy because of the minus sign, which is due to the fact that the L_i are the body components of the angular momentum.

The Poisson brackets involving the space components of the angular momentum are also of interest and can be derived by using $\mathbf{L}_s=\mathsf{R}\mathbf{L}$, Eqs. (4.101) and (4.34) and the chain rule property of the Poisson bracket. The results are

$$\{L_{si},L_j\}=0,\quad \{L_{si},L_{sj}\}=\epsilon_{ijk}L_{sk}. \tag{4.102}$$

The second of these can also be derived by retracing the derivation of $\{L_i,L_j\}$, but using the right-invariant *vielbein* and the space version of the structure constants

(4.59). Of course the same result is obtained by using the original definition of the angular momentum, Eq. (3.19), and the canonical Poisson bracket in the original variables $\{\boldsymbol{\rho}_{s\alpha}\}$ (this is the standard calculation of the angular momentum Poisson bracket relations in elementary mechanics). The same Poisson brackets then hold in any other coordinate system, since the Poisson bracket does not change under coordinate transformations.

As noted previously, the space components of the angular momentum are the generators of rotations acting from the left, i.e., of the symmetry operation $\mathsf{R}\mapsto\mathsf{QR}$, where $\mathsf{Q}\in\mathrm{SO}(3)$. This symmetry operation leaves the Lagrangian invariant, so that $\mathbf{L}_s$ is conserved. The body components of angular momentum are the generators of rotations acting from the right, i.e., $\mathsf{R}\mapsto\mathsf{RQ}$. Such rotations do not leave the Lagrangian invariant, so $\mathbf{L}$ is not conserved. But since left and right rotations commute with one another, the Poisson bracket $\{L_{si},L_j\}$ vanishes.

Given the Poisson brackets (4.101), we can write down the Poisson bracket of any two functions f and g, expressed in terms of the phase-space coordinates $(\theta^i,\mathbf{L},q^\mu,p_\mu)$. It is

$$\{f,g\}=X^i_{(j)}\left(\frac{\partial f}{\partial\theta^i}\frac{\partial g}{\partial L_j}-\frac{\partial f}{\partial L_j}\frac{\partial g}{\partial\theta^i}\right)-\mathbf{L}\cdot\left(\frac{\partial f}{\partial\mathbf{L}}\times\frac{\partial g}{\partial\mathbf{L}}\right)+\left(\frac{\partial f}{\partial q^\mu}\frac{\partial g}{\partial p_\mu}-\frac{\partial f}{\partial p_\mu}\frac{\partial g}{\partial q^\mu}\right). \tag{4.103}$$

It is straightforward to use these Poisson brackets to compute the equations of motion, as in Eqs. (C27) and (C26); the results are of course the same as those we derived from the Lagrangian.

We are already using noncanonical variables to avoid the unpleasantness of Euler angles. A somewhat more convenient set of noncanonical variables is obtained if we replace the canonical but gauge-dependent shape momentum p_μ by the covariant shape velocity,

$$v_\mu=p_\mu-\mathbf{L}\cdot\mathbf{A}_\mu, \tag{4.104}$$

which is gauge invariant. Now the phase-space coordinates are $(\theta^i,\mathbf{L},q^\mu,v_\mu)$, which are noncanonical in both the orientational and shape variables. Of the Poisson brackets of these coordinates among themselves, the ones involving v_μ are the following:

$$\{\theta^i,v_\mu\}=-X^i_{(j)}A^j_\mu,\quad \{\mathbf{L},v_\mu\}=\mathbf{A}_\mu\times\mathbf{L},\qquad \{q^\mu,v_\nu\}=\delta^\mu_\nu,\quad \{v_\mu,v_\nu\}=\mathbf{L}\cdot\mathbf{B}_{\mu\nu}. \tag{4.105}$$

In these coordinates, the Hamiltonian is simply

$$H=\tfrac{1}{2}\,\mathbf{L}\cdot\mathsf{M}^{-1}\cdot\mathbf{L}+\tfrac{1}{2}\,g^{\mu\nu}v_\mu v_\nu+V(q). \tag{4.106}$$

These coordinates are closely tied to an anholonomic frame of horizontal and vertical vector fields in the fiber bundle and in a certain sense are the most "natural."

G. Transforming the Schrödinger equation

Now that we have succeeded in transforming the classical Lagrangian and Hamiltonian to shape and orientational coordinates and in eliminating those five degrees of freedom which can be eliminated, we turn to the analogous problem in quantum mechanics. We carry out the quantum transformation in two steps; in this section we transform the Schrödinger equation to shape and orientational coordinates, and in the next we separate out the orientational degrees of freedom to obtain the reduced Schrödinger equation.

We write $\Psi(\mathbf{r}_{s1},\ldots,\mathbf{r}_{sn})$ for the wave function of the n-particle system in the lab coordinates, and we assume the Schrödinger equation is

$$-\sum_{\alpha=1}^{n}\frac{\hbar^2}{2m_\alpha}\nabla^2_{s\alpha}\Psi+V(\mathbf{r}_{s1},\ldots,\mathbf{r}_{sn})\Psi=E^{\mathrm{tot}}\Psi, \tag{4.107}$$

where $\nabla_{s\alpha}=\partial/\partial\mathbf{r}_{s\alpha}$ and where V is invariant under translations and rotations. This is, of course, only a model. For example, if the system is an atom, we neglect spin-orbit and other relativistic effects; if it is a molecule or an atom-molecule system, then V is a Born-Oppenheimer potential, and we neglect surface crossing and other nonadiabatic effects, as well as the fact that the Hamiltonian should incorporate another gauge potential, the one associated with the adiabatic transport of electronic wave functions (Mead and Truhlar, 1979; Mead, 1992). The interaction between that gauge potential and the one that is the subject of this paper is a largely unexplored area.

We separate the translational degrees of freedom by writing

$$\Psi(\mathbf{r}_{s1},\ldots,\mathbf{r}_{sn})=\left(\frac{M^3}{\Pi_\alpha m_\alpha^3}\right)^{-1/4}F(\mathbf{R}_s)\Phi(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1}), \tag{4.108}$$

where the $\{\boldsymbol{\rho}_{s\alpha}\}$ are mass-weighted Jacobi coordinates and the mass factors in the transformation are chosen so that the normalization integral has the form,

$$\int|\Psi|^2d^3\mathbf{r}_{s1}\ldots d^3\mathbf{r}_{sn}=\int|F|^2d^3\mathbf{R}_s\int|\Phi|^2d^3\boldsymbol{\rho}_{s1}\ldots d^3\boldsymbol{\rho}_{s,n-1}. \tag{4.109}$$

In Eq. (4.108) the mass factor is the inverse square root of the Jacobian of the transformation, $(\mathbf{r}_{s1},\ldots,\mathbf{r}_{sn})\to(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1},\mathbf{R}_s)$, obtained from the transformation properties of the metric tensor according to a method explained momentarily. The Schrödinger equation on the (translation-reduced) configuration space is

$$-\frac{\hbar^2}{2}\sum_{\alpha=1}^{n-1}\nabla^2_{\rho s\alpha}\Phi+V(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1})\Phi=E\Phi, \tag{4.110}$$

where $\nabla_{\rho s\alpha}=\partial/\partial\boldsymbol{\rho}_{s\alpha}$ and where E is the internal energy, the translational energy having been separated out according to $E^{\mathrm{tot}}=E+E^{\mathrm{c.m.}}$.

To transform the Schrödinger equation to shape and orientational coordinates, we shall write $x^a=(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1})$ and $x'^a=(\theta^i,q^\mu)$ for the old and new coordinates, respectively, where $a=1,\ldots,3n-3$.

Quite generally, when transforming from one system of coordinates to another, the wave function may be transformed either as a scalar or as a half-density (in which case the new wave function is the square root of the Jacobian times the old wave function). We begin by transforming the wave function to the new coordinates as a scalar, writing

$$\Phi(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1})=\phi(\theta^i,q^\mu), \tag{4.111}$$

where the new symbol ϕ merely indicates the new variables upon which the wave function depends.

The Jacobian connecting the old and new coordinates is

$$J=\left|\det\frac{\partial x^a}{\partial x'^b}\right|=\left|\det\frac{\partial(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1})}{\partial(\theta^i,q^\mu)}\right|. \tag{4.112}$$

It is conveniently calculated in terms of the old and new metric tensors, G_{ab} and G'_{ab} respectively, defined in terms of the kinetic energy by

$$2K=G_{ab}\dot{x}^a\dot{x}^b=G'_{ab}\dot{x}'^a\dot{x}'^b, \tag{4.113}$$

which implies the transformation law for covariant tensors,

$$G'_{ab}=\frac{\partial x^c}{\partial x'^a}G_{cd}\frac{\partial x^d}{\partial x'^b}. \tag{4.114}$$

On taking the determinant of both sides of this equation and noting that $G_{ab}=\delta_{ab}$, we have $G=\det(G_{ab})=1$ and $G'=\det(G'_{ab})=J^2$. Therefore we may compute G' in order to find J.

But G'_{ab} is given in Eq. (4.35) (where it was called simply G_{ab}). To find its determinant, we factor the matrix according to

$$G'_{ab}=\begin{pmatrix}\Lambda^T & 0\\ \mathbf{A}_\mu & \delta^\sigma_\mu\end{pmatrix}\begin{pmatrix}\mathsf{M} & 0\\ 0 & g_{\sigma\tau}\end{pmatrix}\begin{pmatrix}\Lambda & \mathbf{A}_\nu\\ 0 & \delta^\tau_\nu\end{pmatrix}, \tag{4.115}$$

where the Greek indices combine according to the row-column pattern $(\mu\sigma)(\sigma\tau)(\tau\nu)=(\mu\nu)$. Thus we have

$$G'=(\det\Lambda)^2D, \tag{4.116}$$

where

$$D=(\det\mathsf{M})(\det g_{\mu\nu})=(\det\tilde{\mathsf{M}})(\det h_{\mu\nu}), \tag{4.117}$$

according to Eq. (4.99). The symbol D stands for "determinants." Finally, we have

$$J=|\det\Lambda|D^{1/2}. \tag{4.118}$$

The Jacobian has factored into the product of a function only of the Euler angles, $|\det\Lambda|$, and a function only of the shape coordinates, $D^{1/2}$.

The identity (4.115) is equivalent to transforming the metric tensor from the coordinate basis (θ^i,q^μ) to a frame of horizontal and vertical vector fields. These vector fields constitute an anholonomic frame on the $(3n-3)$-dimensional configuration space, i.e., the fiber bundle, and are not to be confused with the three-dimensional anholonomic frame of vector fields $X^i_{(j)}$ on the rotation group introduced earlier. As we see, the metric tensor is block diagonalized in this frame, which simply means that the horizontal vectors are orthogonal to the vertical vectors. This block diagonalization is of course the same we achieved earlier when we block diagonalized the kinetic energy in the classical Lagrangian, as in Eq. (4.21). Many of the calculations of this paper achieve their most elegant and simple form when expressed in terms of this frame of horizontal and vertical vector fields, and we shall use this frame later in a calculation of the Riemann tensor on the fiber bundle. We have also used it previously in an implicit way when we introduced the noncanonical variables $(\mathbf{L},v_\mu)$ into the classical Hamiltonian (4.106), since these variables are effectively the components of the momentum of the system with respect to the basis of forms dual to the horizontal and vertical vector fields.

We can now transform the normalization integral. We note first that the combination $|\det\Lambda|d^3\boldsymbol{\theta}$ is the (unnormalized) Haar measure on the rotation-group manifold. One way to see this is to resort to the explicit Euler-angle conventions discussed in Appendix B (the only occasion in this paper where we need explicit Euler-angle conventions), and to use Eq. (B9) to write

$$|\det\Lambda|d^3\boldsymbol{\theta}=\sin\beta\,d\alpha\,d\beta\,d\gamma, \tag{4.119}$$

which we recognize as the Haar measure in the Euler angles $\boldsymbol{\theta}=(\alpha,\beta,\gamma)$. Alternatively, we can write $\lambda^i=\Lambda^{(i)}_j d\theta^j$ for the left-invariant differential forms on the rotation-group manifold [denoted $\Lambda^{(i)}$ in Eq. (4.60)], so that the invariant volume element is

$$\lambda^1\wedge\lambda^2\wedge\lambda^3=(\det\Lambda)d\alpha\wedge d\beta\wedge d\gamma. \tag{4.120}$$

In any case, it is important to note that $|\det\Lambda|d^3\boldsymbol{\theta}$ is actually independent of Euler-angle conventions. Finally we normalize the Haar measure and define

$$d\mathsf{R}=\frac{|\det\Lambda|d^3\boldsymbol{\theta}}{8\pi^2}=\frac{\sin\beta\,d\alpha\,d\beta\,d\gamma}{8\pi^2}, \tag{4.121}$$

and we introduce a new wave function ψ by

$$\psi(\theta^i,q^\mu)=(8\pi^2)^{1/2}D^{1/4}\phi(\theta^i,q^\mu), \tag{4.122}$$

so that

$$\int|\Phi|^2d^3\boldsymbol{\rho}_{s1}\ldots d^3\boldsymbol{\rho}_{s,n-1}=\int\left(\prod_\mu dq^\mu\right)\int d\mathsf{R}\,|\psi(\theta^i,q^\mu)|^2. \tag{4.123}$$

Effectively, we have transformed the wave function as a scalar in the orientational coordinates, but as a half-density in the shape coordinates. Many authors prefer to transform the wave function as a scalar also in the shape coordinates.

Before proceeding with the transformation of the Schrödinger equation, we consider the transformation of the angular momentum operators. The angular momentum about the center of mass, referred to the space frame, is represented by the operator

$$\mathbf{L}_s=-i\hbar\sum_{\alpha=1}^{n-1}\boldsymbol{\rho}_{s\alpha}\times\frac{\partial}{\partial\boldsymbol{\rho}_{s\alpha}}. \tag{4.124}$$

As for the body angular momentum, it turns out that the definition we want is

$$\mathbf{L}=\mathsf{R}^T\mathbf{L}_s\,. \tag{4.125}$$

This is the same as the classical definition of the body angular momentum, but since the operator $\mathbf{L}_s$ does not commute with a function of θ^i such as R, this formula (and the operator ordering indicated) must be justified. To this end, let us consider a definite quantum state represented by a wave function $\Phi(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1})=\phi(\theta^i,q^\mu)$, and let us imagine a point moving in configuration space and sampling the values of $\Phi=\phi$. We know that angular momentum generates rotations which classically are motions along the fibers (i.e., they are purely vertical motions), so for the sake of the following argument we shall require that the motion of the point be purely vertical. We shall write its velocity either as $(\mathbf{v}_{s1},\ldots,\mathbf{v}_{s,n-1})$ or as $(\boldsymbol{\omega},0)$ (the latter with respect to the angular velocity and shape basis), where $\mathbf{v}_{s\alpha}=\dot{\boldsymbol{\rho}}_{s\alpha}$ as in Eq. (3.48) and where we set $\dot{q}^\mu=0$ since the motion is vertical. Then by Eq. (3.49) we have

$$\mathbf{v}_{s\alpha}=\mathsf{R}(\boldsymbol{\omega}\times\boldsymbol{\rho}_\alpha)=(\mathsf{R}\boldsymbol{\omega})\times\boldsymbol{\rho}_{s\alpha}\,. \tag{4.126}$$

Next we compute the rate of change of Φ as seen by the moving point. We have

$$\begin{aligned}\frac{d\Phi}{dt}&=\sum_{\alpha=1}^{n-1}\mathbf{v}_{s\alpha}\cdot\frac{\partial\Phi}{\partial\boldsymbol{\rho}_{s\alpha}}\\&=(\mathsf{R}\boldsymbol{\omega})\cdot\sum_{\alpha=1}^{n-1}\boldsymbol{\rho}_{s\alpha}\times\frac{\partial\Phi}{\partial\boldsymbol{\rho}_{s\alpha}}\\&=\frac{i}{\hbar}(\mathsf{R}\boldsymbol{\omega})\cdot\mathbf{L}_s\Phi=\frac{i}{\hbar}\boldsymbol{\omega}\cdot\mathbf{L}\Phi,\end{aligned} \tag{4.127}$$

where we use Eq. (4.125). On the other hand, since $\Phi=\phi$, we also have

$$\frac{d\Phi}{dt}=\frac{d\phi}{dt}=\dot{\theta}^j\frac{\partial\phi}{\partial\theta^j}=\omega^iX^j_{(i)}\frac{\partial\phi}{\partial\theta^j}, \tag{4.128}$$

which is consistent with Eq. (4.127) for all $\boldsymbol{\omega}$ if and only if

$$L_i=X^j_{(i)}p_j\,, \tag{4.129}$$

where

$$p_j=-i\hbar\,\frac{\partial}{\partial\theta^j}. \tag{4.130}$$

Of course, Eq. (4.129) is exactly the classical formula (4.48), but here the coefficients $X^j_{(i)}$, which depend on θ^i, do not commute with p_i. Altogether, we see that with the operator ordering indicated, both formulas (4.125) and (4.129) are reasonable in both the classical and the quantum domain. Finally, given Eq. (4.129), it is easy to calculate the commutator of the body components of angular momentum; the algebra is essentially the same as in the computation of the classical Poisson bracket in Eq. (4.101), and it leads to

$$[L_i,L_j]=-i\hbar\,\epsilon_{ijk}L_k\,, \tag{4.131}$$

with the same minus sign as in the classical formula.

Because of the noncommutativity of the factors in Eq. (4.129), it is not obvious that the body angular momentum is a vector of Hermitian operators. To show that it is, we consider two wave functions ψ_1 and ψ_2, and define

$$\langle\psi_1|\psi_2\rangle=\int d^3\boldsymbol{\theta}|\det\Lambda|\,\psi_1^*\psi_2\,, \tag{4.132}$$

where for simplicity we suppress the q integrations which have no effect on the following calculation. Next we consider the scalar product $\langle\psi_1|L_i\psi_2\rangle$, which we transform by integration by parts. We have

$$\begin{aligned}\langle\psi_1|L_i\psi_2\rangle&=\int d^3\boldsymbol{\theta}|\det\Lambda|\,\psi_1^*\left(-i\hbar X^j_{(i)}\frac{\partial\psi_2}{\partial\theta^j}\right)\\&=\int d^3\boldsymbol{\theta}(+i\hbar)\frac{\partial}{\partial\theta^j}(|\det\Lambda|X^j_{(i)}\psi_1^*)\psi_2\,,\end{aligned} \tag{4.133}$$

where the boundary terms can be shown to vanish. Then the Hermiticity of L_i follows from the identity,

$$\frac{\partial}{\partial\theta^j}[|\det\Lambda|X^j_{(i)}]=0, \tag{4.134}$$

so that

$$\begin{aligned}\langle\psi_1|L_i\psi_2\rangle&=\int d^3\boldsymbol{\theta}|\det\Lambda|\left(-i\hbar X^j_{(i)}\frac{\partial\psi_1}{\partial\theta^j}\right)^*\psi_2\\&=\langle L_i\psi_1|\psi_2\rangle.\end{aligned} \tag{4.135}$$

A similar calculation will show that the operator p_i defined in Eq. (4.130) is not Hermitian.

To prove the useful identity (4.134) it is permissable to drop the absolute value signs, since the sign of $\det\Lambda$ is constant over the rotation group (the invariant volume measure cannot change sign). Then we expand the derivatives to obtain

$$\frac{\partial}{\partial\theta^j}[(\det\Lambda)X^j_{(i)}]=(\det\Lambda)(X^k_{(\ell)}\Lambda^{(\ell)}_{k,j}X^j_{(i)}+X^j_{(i),j}) \tag{4.136}$$

$$=(\det\Lambda)[d\Lambda^{(\ell)}(X_{(i)},X_{(\ell)})+X^k_{(\ell)}X^j_{(i)}\Lambda^{(\ell)}_{j,k}+X^j_{(i),j}]. \tag{4.137}$$

But of the three terms on the right, the first is $-c^{\ell}_{i\ell}=-\epsilon_{\ell i\ell}=0$ and the second is $-X^k_{(\ell),k}X^j_{(i)}\Lambda^{(\ell)}_j=-X^k_{(i),k}$ which cancels the third. Thus the identity is proven.

Now we return to the Schrödinger equation (4.110) and write the kinetic energy in terms of the covariant expression for the Laplace-Beltrami operator, which has been used in calculations of this sort since at least the time of Podolsky (1928). This is

$$\begin{aligned}\sum_{\alpha=1}^{n-1}\nabla^2_{\rho s\alpha}\Phi&=\frac{1}{\sqrt{G}}\,\frac{\partial}{\partial x^a}\left(\sqrt{G}G^{ab}\frac{\partial\Phi}{\partial x^b}\right)\\&=\frac{1}{\sqrt{G'}}\,\frac{\partial}{\partial x'^a}\left(\sqrt{G'}G'^{ab}\frac{\partial\phi}{\partial x'^b}\right).\end{aligned} \tag{4.138}$$

Next we use Eqs. (4.116) and (4.122) and multiply the Schrödinger equation through by $(8\pi^2)^{1/2}D^{1/4}$ to obtain

$$-\frac{\hbar^2}{2}\frac{1}{|\det\Lambda|D^{1/4}}\frac{\partial}{\partial x'^a}\left[|\det\Lambda|D^{1/2}G'^{ab}\frac{\partial}{\partial x'^b}(D^{-1/4}\psi)\right] + V\psi = E\psi. \tag{4.139}$$

The contravariant metric tensor G'^{ab} that appears here was displayed in Eq. (4.36), where it was called simply G^{ab}.

The kinetic-energy expression in Eq. (4.139) consists of four blocks, which can be simplified by means of the identity (4.134), the definition (4.129), and the definition

$$p_\mu = -i\hbar\frac{\partial}{\partial q^\mu}. \tag{4.140}$$

In this process, due attention must be paid to the noncommutativity of the various factors; since $\mathbf{A}_\mu$, M, and $g^{\mu\nu}$ depend only on q^μ, they commute with each other and with $\mathbf{L}$, but not with p_μ. The following equations summarize the results:

$$\mathsf{RR}\ \text{block} = \tfrac{1}{2}[\mathbf{L}\cdot\mathsf{M}^{-1}\cdot\mathbf{L} + (\mathbf{L}\cdot\mathbf{A}_\mu)g^{\mu\nu}(\mathbf{L}\cdot\mathbf{A}_\nu)]\psi, \tag{4.141}$$

$$q\mathsf{R}\ \text{block} = -\tfrac{1}{2}(\mathbf{L}\cdot\mathbf{A}_\mu)g^{\mu\nu}p_\nu\psi - \frac{i\hbar}{8}\frac{D_{,\nu}}{D}(\mathbf{L}\cdot\mathbf{A}_\mu)g^{\mu\nu}\psi, \tag{4.142}$$

$$\mathsf{R}q\ \text{block} = -\tfrac{1}{2}p_\mu g^{\mu\nu}(\mathbf{L}\cdot\mathbf{A}_\nu)\psi + \frac{i\hbar}{8}\frac{D_{,\mu}}{D}(\mathbf{L}\cdot\mathbf{A}_\nu)g^{\mu\nu}\psi, \tag{4.143}$$

$$qq\ \text{block} = \tfrac{1}{2}p_\mu g^{\mu\nu}p_\nu\psi + V_2\psi, \tag{4.144}$$

where in the final expression we set

$$V_2 = \frac{\hbar^2}{2}D^{-1/4}\frac{\partial}{\partial q^\mu}\left(g^{\mu\nu}\frac{\partial D^{1/4}}{\partial q^\nu}\right). \tag{4.145}$$

Altogether, the Schrödinger equation is $H\psi = E\psi$, where

$$H = \tfrac{1}{2}\mathbf{L}\cdot\mathsf{M}^{-1}\cdot\mathbf{L} + \tfrac{1}{2}(p_\mu - \mathbf{L}\cdot\mathbf{A}_\mu)g^{\mu\nu}(p_\nu - \mathbf{L}\cdot\mathbf{A}_\nu) + V_2(q) + V(q). \tag{4.146}$$

Except for the ordering of operators and the term V_2, this Hamiltonian is the same as the classical expression (4.92).

The term V_2 arises from nonclassical commutators, as evidenced by the $\hbar^2$ coefficient. Although it is written as if it were a potential energy, it belongs physically to the horizontal kinetic energy. It is somewhat troublesome to calculate this term in practice, because (unlike the true potential V) it does not transform as a scalar under changes of coordinates on shape space. (If it did, it would be possible to compute it in one coordinate system once and for all and then to transform it as a scalar.) This term is, however, gauge invariant. A number of different ways to write V_2 are discussed by Essén (1978). Here we shall report on a new decomposition of this term, namely,

$$V_2 = \frac{\hbar^2}{2}\frac{[(\det\mathsf{M})^{1/4}]_{;\mu}{}^{;\mu}}{(\det\mathsf{M})^{1/4}} + \frac{\hbar^2}{2}g^{-1/4}\frac{\partial}{\partial q^\mu}\left(g^{\mu\nu}\frac{\partial g^{1/4}}{\partial q^\nu}\right), \tag{4.147}$$

where $g = \det g_{\mu\nu}$. The first term in this expression, involving the covariant Laplacian of $(\det\mathsf{M})^{1/4}$, is a scalar, while the second term, although not a scalar, depends only on $g_{\mu\nu}$ and is independent of M. (Both terms are gauge invariant.) Therefore the first term, at least, is easy to transform from one system of shape coordinates to another. We shall provide a proof of this decomposition in future publications. The term V_2 is considered again in Sec. V, when we discuss the Eckart conventions.

H. Reducing the Schrödinger equation

Now we reduce the Schrödinger equation, i.e., we separate out the dependence on the Euler angles. The resulting reduced Schrödinger equation involves the $3n-6$ shape degrees of freedom, represented by differential operators in the shape coordinates q^μ, plus one-body angular momentum degree of freedom, represented by finite-dimensional matrices for the body angular momentum operators. Correspondingly, the reduced wave function is a $(2\ell+1)$-component spinor, which is a function of q^μ. In addition, we shall explicitly demonstrate the gauge covariance of the reduced wave function and reduced Hamiltonian. This calculation calls on the standard theory of angular momentum in quantum mechanics, in which we think primarily in terms of active transformations and follow the conventions of Messiah (1966). Hirschfelder and Wigner (1935) treated this problem for a specific choice of gauge and shape space-coordinates.

If $\mathsf{Q}\in\mathrm{SO}(3)$, then we denote the corresponding active rotation operator acting on wave functions by $\mathcal{R}(\mathsf{Q})$, so that

$$(\mathcal{R}(\mathsf{Q})\Phi)(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1}) = \Phi(\mathsf{Q}^{-1}\boldsymbol{\rho}_{s1},\ldots,\mathsf{Q}^{-1}\boldsymbol{\rho}_{s,n-1}). \tag{4.148}$$

On transforming to shape and orientational coordinates, this becomes

$$(\mathcal{R}(\mathsf{Q})\psi)(\mathsf{R},q^\mu) = \psi(\mathsf{Q}^{-1}\mathsf{R},q^\mu), \tag{4.149}$$

since $\boldsymbol{\rho}_{s\alpha} = \mathsf{R}\boldsymbol{\rho}_\alpha$ and since $\boldsymbol{\rho}_\alpha$ does not change under active rotations of the system (the body frame is rotated along with the body).

We denote an eigenfunction of L^2 and L_{sz} corresponding to quantum numbers ℓ,m by $\Phi_{\ell m}$, $\phi_{\ell m}$, or $\psi_{\ell m}$. We assume that for fixed ℓ the wave functions corresponding to different m are related by raising and lowering operators and standard phase conventions, so that

$$(\mathcal{R}(\mathsf{Q})\psi_{\ell m})(\mathsf{R},q^\mu) = \sum_{k=-\ell}^{+\ell}\psi_{\ell k}(\mathsf{R},q^\mu)D^\ell_{km}(\mathsf{Q}), \tag{4.150}$$

where $D^\ell_{km}(\mathsf{Q})$ is the standard $(2\ell+1)\times(2\ell+1)$ irreducible matrix representative of $\mathsf{Q}\in\mathrm{SO}(3)$. Thus, by

combining Eqs. (4.149) and (4.150), we can express the $\psi_{\ell m}$ (for $m=-\ell,\ldots,+\ell$) at one point on a fiber in terms of the $\psi_{\ell m}$ at any other point. In particular, we can express the $\psi_{\ell m}$ at some orientation R in terms of the $\psi_{\ell m}$ at the identity (the reference orientation). Therefore we define

$$\chi^{\ell}_{k}(q^{\mu})=\frac{1}{\sqrt{2\ell+1}}\psi_{\ell k}(\mathsf{I},q^{\mu}), \tag{4.151}$$

so that

$$\psi_{\ell m}(\mathsf{R},q^{\mu})=\sqrt{2\ell+1}\sum_{k=-\ell}^{+\ell}\chi^{\ell}_{k}(q^{\mu})D^{\ell}_{mk}(\mathsf{R})^{*}. \tag{4.152}$$

The wave function $\chi^{\ell}_{k}(q^{\mu})$ is a $(2\ell+1)$-component spinor, which it is tempting to think of as the "wave function on shape space." But actually $\chi^{\ell}_{k}(q^{\mu})$ is only the wave function on the section $\mathcal{S}$; in truth there is no wave function on shape space, i.e., no gauge-invariant way to define such a function. Since $\chi^{\ell}_{k}(q^{\mu})$ is defined on $\mathcal{S}$, it is gauge dependent. The only exception to these statements occurs for s waves ($\ell=0$), for which the wave function χ^{ℓ} is gauge invariant and can be thought of as living on shape space.

The normalization of $\chi^{\ell}_{k}(q^{\mu})$ is obtained as follows:

$$\begin{aligned}\int\left(\prod_{\alpha}d^{3}\boldsymbol{\rho}_{s\alpha}\right)&|\Phi(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1})|^{2}\\&=\int\left(\prod dq^{\mu}\right)d\mathsf{R}\,|\psi_{\ell m}(\mathsf{R},q^{\mu})|^{2}\\&=\sum_{k=-\ell}^{+\ell}\int\left(\prod dq^{\mu}\right)|\chi^{\ell}_{k}(q^{\mu})|^{2},\end{aligned} \tag{4.153}$$

where we have used Eq. (4.152) and the orthogonality theorem,

$$\int d\mathsf{R}D^{\ell}_{km}(\mathsf{R})^{*}D^{\ell'}_{k'm'}(\mathsf{R})=\frac{\delta_{\ell\ell'}\delta_{mm'}\delta_{kk'}}{2\ell+1}. \tag{4.154}$$

Next, we need the action of the body angular momentum on χ^{ℓ}_{k}. To obtain the action of the space angular momentum on χ^{ℓ}_{k}, we denote the rotation matrix representing a rotation by angle θ about the ith coordinate axis by $\mathsf{Q}_{i}(\theta)$, and the corresponding rotation operator by $\mathcal{R}_{i}(\theta)$. Then we have

$$\begin{aligned}(L_{si}\psi_{\ell m})(\mathsf{R},q^{\mu})&=i\hbar\frac{d}{d\theta}\bigg|_{\theta=0}(\mathcal{R}_{i}(\theta)\psi_{\ell m})(\mathsf{R},q^{\mu})\\&=i\hbar\frac{d}{d\theta}\bigg|_{\theta=0}\psi_{\ell m}(\mathsf{Q}_{i}(\theta)^{-1}\mathsf{R},q^{\mu})\\&=i\hbar\frac{d}{d\theta}\bigg|_{\theta=0}\sqrt{2\ell+1}\\&\quad\times\sum_{k}\chi^{\ell}_{k}(q^{\mu})D^{\ell}_{mk}(\mathsf{Q}_{i}(\theta)^{-1}\mathsf{R})^{*}\\&=i\hbar\frac{d}{d\theta}\bigg|_{\theta=0}\sqrt{2\ell+1}\sum_{k,k'}\chi^{\ell}_{k}(q^{\mu})\\&\quad\times\times D^{\ell}_{k'm}(\mathsf{Q}_{i}(\theta))D^{\ell}_{k'k}(\mathsf{R})^{*}\\&=\sqrt{2\ell+1}\sum_{k,k'}\chi^{\ell}_{k}(q^{\mu})\\&\quad\times(\mathcal{L}_{i})_{k'm}D^{\ell}_{k'k}(\mathsf{R})^{*},\end{aligned} \tag{4.155}$$

where we use Eqs. (4.149) and (4.152) and where $\mathcal{L}_{i}$ is the standard $(2\ell+1)\times(2\ell+1)$ irreducible matrix representative of the i component of the angular momentum operator, so that $D^{\ell}(\mathsf{Q}_{i}(\theta))=\exp(-i\theta\mathcal{L}_{i}/\hbar)$. Finally, we use Eq. (4.125) and the adjoint transformation property of the angular momentum matrices,

$$R_{ji}\mathcal{L}_{j}=D^{\ell}(\mathsf{R})\mathcal{L}_{i}D^{\ell}(\mathsf{R})^{\dagger}, \tag{4.156}$$

to transform Eq. (4.155) from the space to the body angular momentum, finding

$$\begin{aligned}(L_{i}\psi_{\ell m})(\mathsf{R},q^{\mu})&=\sqrt{2\ell+1}\sum_{k,k'}\chi^{\ell}_{k'}(q^{\mu})\\&\quad\times(\mathcal{L}_{i})_{k'k}D^{\ell}_{mk}(\mathsf{R})^{*}.\end{aligned} \tag{4.157}$$

Thus, under the mapping $\psi_{\ell m}\mapsto L_{i}\psi_{\ell m}$, we have

$$\chi^{\ell}_{k}(q^{\mu})\mapsto(L_{i}\chi^{\ell}_{k})(q^{\mu})=\sum_{k'}(\mathcal{L}_{i})_{k'k}\chi^{\ell}_{k'}(q^{\mu}). \tag{4.158}$$

In other words, $\chi^{\ell}_{k}(q^{\mu})$, regarded as a column spinor, transforms by multiplication by the transpose of $\mathcal{L}_{i}$. (We could equally well regard it as a row spinor, transforming by right multiplication by $\mathcal{L}_{i}$.)

Therefore when we substitute Eq. (4.152) into the Schrödinger equation, multiply through by $D^{\ell}_{mk'}(\mathsf{R})$, and integrate over R, we find $H\chi^{\ell}=E\chi^{\ell}$, where χ^{ℓ} is the column spinor and where H is exactly as in Eq. (4.146) except that the body angular momentum operators L_{i} are reinterpreted as the transposed matrices $\mathcal{L}_{i}^{T}$. Because of the transpose, these matrices satisfy the commutation relations (4.131) (with the minus sign).

The wave function $\chi^{\ell}_{k}(q^{\mu})$ is gauge dependent, for if we write $\psi_{\ell m}$, $\psi'_{\ell m}$, χ^{ℓ}_{k}, χ'^{ℓ}_{k}, etc., for the old and new wave functions under the gauge transformation $\mathsf{R}=\mathsf{R}'\mathsf{S}^{T}$, then we have

$$\psi_{\ell m}(\mathsf{R},q^{\mu})=\psi'_{\ell m}(\mathsf{R}',q^{\mu})=\psi'_{\ell m}(\mathsf{RS},q^{\mu}), \tag{4.159}$$

where the first equality indicates what we mean by the transformed wave function. But this implies

$$\chi^{\ell}_{k}(q^{\mu})=\frac{1}{\sqrt{2\ell+1}}\psi_{\ell k}(\mathsf{I},q^{\mu})=\frac{1}{\sqrt{2\ell+1}}\psi'_{\ell k}(\mathsf{S},q^{\mu}), \tag{4.160}$$

or, by Eq. (4.152),

$$\chi^{\ell}_{k}(q^{\mu})=\sum_{k_{1}}\chi'^{\ell}_{k_{1}}(q^{\mu})D^{\ell}_{kk_{1}}(\mathsf{S})^{*}. \tag{4.161}$$

We abbreviate this by writing

$$\chi^{\ell} = D^{\ell}(\mathsf{S}^{-1})^T \chi'^{\ell}, \tag{4.162}$$

where we think of χ^{ℓ} and χ'^{ℓ} as column spinors.

The Hamiltonian (4.146), with L_i interpreted as $\mathcal{L}_i^T$, is a $(2\ell+1)\times(2\ell+1)$ matrix of operators. It is not gauge invariant, but rather has the transformation property

$$HD^{\ell}(\mathsf{S}^{-1})^T = D^{\ell}(\mathsf{S}^{-1})^T H', \tag{4.163}$$

where H' is the same as H but with $\mathbf{A}_\mu$ and M replaced by $\mathbf{A}'_\mu$ and M', the new fields under the gauge transformation specified by $\mathsf{S}(q)$ as in Eqs. (3.68) and (3.74). Therefore, if $H\chi^{\ell} = E\chi^{\ell}$, then $H'\chi'^{\ell} = E\chi'^{\ell}$, and the Schrödinger equation is gauge covariant in this sense. In this transformation we do not replace $L_i = \mathcal{L}_i^T$ by any primed versions of themselves, as we did in the classical transformation (3.67), because here the symbols $L_i = \mathcal{L}_i^T$ stand for constant matrices, nor do we introduce primed versions of the operators p_μ, which continue to represent $-i\hbar\partial/\partial q^\mu$. (We recall that in the classical Hamiltonian, the canonical momenta p_μ were gauge dependent.)

To prove Eq. (4.163), we must pull the matrix $D^{\ell}(\mathsf{S}^{-1})^T$ to the left past the matrices $L_i = \mathcal{L}_i^T$ and the operators $p_\mu = -i\hbar\partial/\partial q^\mu$, with which it does not commute. To do this, we use the relations

$$\mathcal{L}_i^T D^{\ell}(\mathsf{S}^{-1})^T = \mathsf{S}_{ij} D^{\ell}(\mathsf{S}^{-1})^T \mathcal{L}_j^T \tag{4.164}$$

and

$$D^{\ell}(\mathsf{S})^T p_\mu D^{\ell}(\mathsf{S}^{-1})^T = \boldsymbol{\gamma}_\mu \cdot \mathbf{L} + p_\mu, \tag{4.165}$$

where $\boldsymbol{\gamma}_\mu$ is defined in Eq. (3.71) and where $\mathbf{L}$ is the vector of transposed matrices $\mathcal{L}_i^T$. These imply

$$(p_\mu - \mathbf{L}\cdot\mathbf{A}_\mu) D^{\ell}(\mathsf{S}^{-1})^T = D^{\ell}(\mathsf{S}^{-1})^T (p_\mu - \mathbf{L}\cdot\mathbf{A}'_\mu) \tag{4.166}$$

and

$$(\mathbf{L}\cdot\mathsf{M}^{-1}\cdot\mathbf{L}) D^{\ell}(\mathsf{S}^{-1})^T = D^{\ell}(\mathsf{S}^{-1})^T (\mathbf{L}\cdot\mathsf{M}'^{-1}\cdot\mathbf{L}), \tag{4.167}$$

from which Eq. (4.163) follows immediately.

To prove Eq. (4.164), we note that it is simply a transposed version of the adjoint transformation law (4.156). As for Eq. (4.165), we let ξ^μ be an arbitrary vector and consider the operator $\xi^\mu\partial/\partial q^\mu$ acting on $D^{\ell}(\mathsf{S})$. We have

$$\begin{aligned}
\xi^\mu \frac{\partial D^{\ell}(\mathsf{S})}{\partial q^\mu} &= \lim_{\epsilon\to 0}\frac{1}{\epsilon}[D^{\ell}\{\mathsf{S}(q+\epsilon\xi)\} - D^{\ell}(\mathsf{S}(q))] \\
&= \lim_{\epsilon\to 0}\frac{1}{\epsilon}[D^{\ell}(\mathsf{S}+\epsilon\xi^\mu \mathsf{S}_{,\mu}) - D^{\ell}(\mathsf{S})] \\
&= \lim_{\epsilon\to 0}\frac{1}{\epsilon} D^{\ell}(\mathsf{S})[D^{\ell}(\mathsf{I}+\epsilon\xi^\mu\Gamma_\mu) - I] \\
&= -\frac{i}{\hbar} D^{\ell}(\mathsf{S})\xi^\mu \gamma_\mu^k \mathcal{L}_k .
\end{aligned} \tag{4.168}$$

In this equation, I is the 3×3 identity and I is the $(2\ell+1)\times(2\ell+1)$ identity matrix. But since ξ^μ is arbitrary, we can drop it from both sides of this equation and then take the Hermitian conjugate and then the transpose of both sides to obtain Eq. (3.165).

V. MISCELLANEOUS RESULTS

In this section we present several miscellaneous results that did not fit into the presentation as developed so far. We begin with the Bianchi identities and other field equations satisfied by the Coriolis tensor. We present a collection of identities that are important for expressing various quantities of physical interest in terms of shape and orientational coordinates and their conjugate momenta. Then we present a collection of identities involving the Jacobian of the coordinate transformation $(\boldsymbol{\rho}_{s1}, \ldots, \boldsymbol{\rho}_{s,n-1}) \to (\theta^i, q^\mu)$. Following this, we present a collection of formulas related to the horizontal and vertical projection operators. We derive a set of further identities by methods borrowed from the literature on Kaluza-Klein theories, in which the basic idea is to express trivial tensor identities valid on the (translation-reduced) configuration space in terms of fields on shape space. These identities amount to various field equations satisfied by M, $\mathbf{B}_{\mu\nu}$, and $g_{\mu\nu}$. Finally, we present some comments on the Eckart conventions and on the geometrical meaning of the modified moment-of-inertia tensor $\tilde{\mathsf{M}}$, which is ubiquitous in the literature based on the Eckart conventions.

A. Bianchi identities and other field equations satisfied by $\mathbf{B}_{\mu\nu}$

The Bianchi identity for the Riemann tensor is a standard subject, which is summarized in Appendix E. The Coriolis curvature tensor also satisfies a Bianchi identity, namely,

$$\mathbf{B}_{[\mu\nu;\sigma]} = 0, \tag{5.1}$$

where the square brackets in the subscript indicate complete antisymmetrization, as explained by Eq. (A3). This Bianchi identity is the non-Abelian analog of the Maxwell equation $\nabla\cdot\mathbf{B} = 0$, and it says, in a sense, that the Coriolis tensor has no magnetic sources, at least in regions of shape space where the tensor itself and its derivatives are defined. Of course, in the three-body problem, we know that there is a magnetic source (i.e., the Iwai monopole) at the three-body collision, but Eq. (5.1) is singular there. In the general case (arbitrary n), $\mathbf{B}_{\mu\nu}$ is defined and differentiable at all noncollinear shapes, and Eq. (5.1) is valid at such points. The identity (5.1) is proved by directly expanding out the covariant derivatives, as in Eq. (D10), whereupon all the terms involving Christoffel symbols vanish. One then uses Eq. (3.87) connecting $\mathbf{B}_{\mu\nu}$ and $\mathbf{A}_\mu$, whereupon all terms cancel. This is a standard calculation in gauge theories.

The Bianchi identity for the Coriolis tensor can be regarded as a field equation satisfied by that tensor. This is a natural point of view, in spite of the fact that the n-body problem is not a field theory, and the fields that occur in it are not dynamical variables. Because the gauge theory of the n-body problem is non-Abelian, the

field equations satisfied by $\mathbf{B}_{\mu\nu}$ are more like Yang-Mills field equations than Maxwell's equations, although by analogy we can use language borrowed from ordinary electromagnetic theory. It is in this sense that we say that $\mathbf{B}_{\mu\nu}$ has no magnetic sources (except possibly at collinear configurations).

Similarly, we might ask whether $\mathbf{B}_{\mu\nu}$ has any electric sources, i.e., whether the current $\mathbf{J}^{\mu}$ in the Yang-Mills field equation $\mathbf{B}^{\mu\nu}{}_{;\nu}=\mathbf{J}^{\mu}$ is nonzero. This question is motivated by the three-body problem, in which the analogy with the Dirac monopole makes it clear that the Coriolis field produced by the Iwai monopole has no electric sources (in the electromagnetic analogy, the field is curl-free). In fact, we have been able to show for any value of n that such "electric currents" vanish, i.e., that

$$\mathbf{B}^{\mu\nu}{}_{;\nu}=0. \tag{5.2}$$

We shall present the proof of this fact in future publications.

B. A new class of identities

In Sec. IV we succeeded in transforming the classical Hamiltonian from Jacobi coordinates $\{\boldsymbol{\rho}_{s\alpha}\}$ to shape and orientational coordinates (θ^i,q^{μ}). Properly speaking, this was not just a point transformation on configuration space, but rather a coordinate transformation on phase space involving both the coordinates and their conjugate momenta. We also introduced various noncanonical coordinate systems on phase space; these are not only more natural than canonical coordinates but also easier to use. Similarly, in transforming the quantum Hamiltonian, we introduced operators (the body angular momenta) that satisfy nontrivial commutation relations. Such operators are analogous to classical noncanonical coordinates.

It is of interest to transform other observables besides the Hamiltonian into a shape and orientational representation. Examples include the kinetic energy or angular momentum of various subsystems of the n-particle system or the various commuting observables that are used in constructing hyperspherical harmonics. Democracy transformations play an important role in this process; democratic invariants such as the Hamiltonian are easier to transform than other quantities. Although we shall not report on such calculations in this paper, we will present various identities we discovered in the process of carrying out these calculations, because we feel they are of fundamental importance in understanding the gauge theory of the n-body problem.

We begin with a simple but useful formula,

$$\sum_{\alpha=1}^{n-1}\boldsymbol{\rho}_{\alpha}\times\boldsymbol{\rho}_{\alpha;\mu}=0, \tag{5.3}$$

which involves the covariant derivatives of the vectors $\boldsymbol{\rho}_{\alpha}(q^{\mu})$ that specify the gauge. This formula is interesting because it is equivalent to the definition of the gauge potential (3.56). That is, suppose we know that we have a covariant derivative that satisfies all the properties laid out in Appendix D, but we do not know the definition of $\mathbf{A}_{\mu}$. Then the demand that Eq. (5.3) be valid is equivalent to the definition (3.56). To see this, we simply expand out the left-hand side of Eq. (5.3) to find

$$\sum_{\alpha}\boldsymbol{\rho}_{\alpha}\times\boldsymbol{\rho}_{\alpha,\mu}-\sum_{\alpha}\boldsymbol{\rho}_{\alpha}\times(\mathbf{A}_{\mu}\times\boldsymbol{\rho}_{\alpha})=\mathbf{a}_{\mu}-\mathsf{M}\mathbf{A}_{\mu}. \tag{5.4}$$

Thus the vanishing of this quantity is equivalent to the definition of $\mathbf{A}_{\mu}$. Any formula involving covariant derivatives that can be proved by expressing the covariant derivatives in terms of ordinary derivatives plus correction terms and then appealing to the definition of $\mathbf{A}_{\mu}$ can also be proved by using only Eq. (5.3). The latter approach is preferable because it involves only covariant derivatives at every step.

Equation (5.3) has some interesting consequences. Taking the covariant derivative of this equation, we have

$$\sum_{\alpha}\boldsymbol{\rho}_{\alpha;\nu}\times\boldsymbol{\rho}_{\alpha;\mu}+\sum_{\alpha}\boldsymbol{\rho}_{\alpha}\times\boldsymbol{\rho}_{\alpha;\mu\nu}, \tag{5.5}$$

which we antisymmetrize in μ,ν, using Eq. (D13), to find

$$\mathsf{M}\mathbf{B}_{\mu\nu}=2\sum_{\alpha}\boldsymbol{\rho}_{\alpha;\mu}\times\boldsymbol{\rho}_{\alpha;\nu}. \tag{5.6}$$

This is a simple identity, which proves useful in many applications.

Another consequence of Eq. (5.3) is that the antisymmetric part of the tensor $\Sigma_{\alpha}\boldsymbol{\rho}_{\alpha}\otimes\boldsymbol{\rho}_{\alpha;\mu}^{T}$ vanishes, i.e., this tensor is symmetric. We express this result in terms of the "moment tensor" K, defined by

$$\mathsf{K}=\sum_{\alpha=1}^{n-1}\boldsymbol{\rho}_{\alpha}\otimes\boldsymbol{\rho}_{\alpha}^{T}, \tag{5.7}$$

whose covariant derivative satisfies

$$\frac{1}{2}\mathsf{K}_{;\mu}=\sum_{\alpha}\boldsymbol{\rho}_{\alpha;\mu}\otimes\boldsymbol{\rho}_{\alpha}^{T}=\sum_{\alpha}\boldsymbol{\rho}_{\alpha}\otimes\boldsymbol{\rho}_{\alpha;\mu}^{T}. \tag{5.8}$$

The moment tensor is related to the moment-of-inertia tensor by

$$\mathsf{M}=(\mathrm{Tr}\mathsf{K})\mathsf{I}-\mathsf{K}. \tag{5.9}$$

Another interesting and useful identity is

$$g_{\mu\nu}=\sum_{\alpha}\boldsymbol{\rho}_{\alpha;\mu}\cdot\boldsymbol{\rho}_{\alpha;\nu}. \tag{5.10}$$

This is easily proved directly from the definition (4.18) by eliminating the ordinary derivatives in $h_{\mu\nu}$ in favor of covariant derivatives.

Further identities can be derived from Eq. (5.10). Taking the covariant derivative of this equation, we have

$$g_{\mu\nu;\sigma}=0=\sum_{\alpha}(\boldsymbol{\rho}_{\alpha;\mu}\cdot\boldsymbol{\rho}_{\alpha;\nu\sigma}+\boldsymbol{\rho}_{\alpha;\mu\sigma}\cdot\boldsymbol{\rho}_{\alpha;\nu}). \tag{5.11}$$

To analyze this, we define $T_{\mu\nu\sigma}=\Sigma_{\alpha}\boldsymbol{\rho}_{\alpha;\mu}\cdot\boldsymbol{\rho}_{\alpha;\nu\sigma}$, so that Eq. (5.11) is equivalent to

$$T_{\mu\nu\sigma}+T_{\nu\mu\sigma}=0, \tag{5.12}$$

i.e., $T_{\mu\nu\sigma}$ is antisymmetric in the first and second indices. On the other hand, we have

$$T_{\mu\nu\sigma}-T_{\mu\sigma\nu}=\sum_\alpha \boldsymbol{\rho}_{\alpha;\mu}\cdot\boldsymbol{\rho}_{\alpha;[\nu\sigma]}=\mathbf{B}_{\nu\sigma}\cdot\sum_\alpha \boldsymbol{\rho}_\alpha\times\boldsymbol{\rho}_{\alpha;\mu}=0, \tag{5.13}$$

on account of Eqs. (D13) and (5.3). Therefore $T_{\mu\nu\sigma}$ is symmetric in the second and third indices. These symmetries are consistent only if $T_{\mu\nu\sigma}$ vanishes, i.e.,

$$\sum_\alpha \boldsymbol{\rho}_{\alpha;\mu}\cdot\boldsymbol{\rho}_{\alpha;\sigma\nu}=0. \tag{5.14}$$

This is a relatively strong statement due to the large number (three) of free indices. By taking further covariant derivatives it is possible to obtain identities involving the Riemann tensor.

C. Jacobian identities

We turn now to a class of identities involving the Jacobian of the coordinate transformation, $(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1})\to(\theta^i,q^\mu)$. There are both forward and inverse Jacobians. We obtain the components of the forward Jacobian by differentiating Eq. (3.41):

$$\frac{\partial\boldsymbol{\rho}_{s\alpha}}{\partial\theta^i}=\frac{\partial\mathsf{R}}{\partial\theta^i}\boldsymbol{\rho}_\alpha, \tag{5.15}$$

$$\frac{\partial\boldsymbol{\rho}_{s\alpha}}{\partial q^\mu}=\mathsf{R}\frac{\partial\boldsymbol{\rho}_\alpha}{\partial q^\mu}. \tag{5.16}$$

Here we are thinking of the functions $\boldsymbol{\rho}_\alpha(q^\mu)$ as "known," due to some choice of gauge, although this is not a necessary point of view. Of these, Eq. (5.15) can be transformed with the help of Eq. (4.34) into

$$\frac{\partial\rho_{s\alpha j}}{\partial\theta^i}=\mathsf{R}_{jk}\epsilon_{k\ell m}\Lambda_i^{(\ell)}\rho_{\alpha m}, \tag{5.17}$$

or

$$\frac{\partial\boldsymbol{\rho}_{s\alpha}}{\partial\theta^i}=\mathsf{R}\left(\frac{\partial\boldsymbol{\omega}}{\partial\dot\theta^i}\times\boldsymbol{\rho}_\alpha\right), \tag{5.18}$$

where we use Eq. (4.51).

The components of the inverse Jacobian are $\partial\theta^i/\partial\boldsymbol{\rho}_{s\alpha}$ and $\partial q^\mu/\partial\boldsymbol{\rho}_{s\alpha}$. Since the forward and inverse Jacobians are inverse matrices, we have

$$\frac{\partial\boldsymbol{\rho}_{s\alpha}}{\partial\theta^i}\otimes\left(\frac{\partial\theta^i}{\partial\boldsymbol{\rho}_{s\beta}}\right)^T+\frac{\partial\boldsymbol{\rho}_{s\alpha}}{\partial q^\mu}\otimes\left(\frac{\partial q^\mu}{\partial\boldsymbol{\rho}_{s\beta}}\right)^T=\mathsf{I}\delta_{\alpha\beta}, \tag{5.19}$$

and

$$\sum_\alpha \frac{\partial\theta^i}{\partial\boldsymbol{\rho}_{s\alpha}}\cdot\frac{\partial\boldsymbol{\rho}_{s\alpha}}{\partial\theta^j}=\delta_{ij}, \tag{5.20}$$

$$\sum_\alpha \frac{\partial\theta^i}{\partial\boldsymbol{\rho}_{s\alpha}}\cdot\frac{\partial\boldsymbol{\rho}_{s\alpha}}{\partial q^\mu}=0, \tag{5.21}$$

$$\sum_\alpha \frac{\partial q^\mu}{\partial\boldsymbol{\rho}_{s\alpha}}\cdot\frac{\partial\boldsymbol{\rho}_{s\alpha}}{\partial\theta^i}=0, \tag{5.22}$$

$$\sum_\alpha \frac{\partial q^\mu}{\partial\boldsymbol{\rho}_{s\alpha}}\cdot\frac{\partial\boldsymbol{\rho}_{s\alpha}}{\partial q^\nu}=\delta^\mu_\nu. \tag{5.23}$$

From these we can solve for the components of the inverse Jacobian in terms of the components of the forward Jacobian.

Before doing this, however, we comment on the vectors $\boldsymbol{\rho}_\alpha(q^\mu)$, which are $3n-3$ functions of $3n-6$ variables. These functions are not invertible, and it would seem that there is no meaning to the derivatives $\partial q^\mu/\partial\boldsymbol{\rho}_\alpha$, unlike the derivatives $\partial q^\mu/\partial\boldsymbol{\rho}_{s\alpha}$, which are part of the inverse Jacobian. But, in fact, the derivatives $\partial q^\mu/\partial\boldsymbol{\rho}_\alpha$ can be given meaning, since the q^μ, being rotationally invariant, are functions of the Jacobi dot products and triple products, which can be expressed in terms either of the space or of the body components of the Jacobi vectors:

$$\boldsymbol{\rho}_{s\alpha}\cdot\boldsymbol{\rho}_{s\beta}=\boldsymbol{\rho}_\alpha\cdot\boldsymbol{\rho}_\beta, \tag{5.24}$$

$$\boldsymbol{\rho}_{s\alpha}\cdot(\boldsymbol{\rho}_{s\beta}\times\boldsymbol{\rho}_{s\gamma})=\boldsymbol{\rho}_\alpha\cdot(\boldsymbol{\rho}_\beta\times\boldsymbol{\rho}_\gamma). \tag{5.25}$$

Therefore the q^μ can be expressed as functions of the body vectors $\{\boldsymbol{\rho}_\alpha\}$, and we have

$$\frac{\partial q^\mu}{\partial\boldsymbol{\rho}_\alpha}=\mathsf{R}^T\frac{\partial q^\mu}{\partial\boldsymbol{\rho}_{s\alpha}}. \tag{5.26}$$

With this understanding, we can rewrite Eqs. (5.22) and (5.23) as

$$\sum_\alpha \frac{\partial q^\mu}{\partial\boldsymbol{\rho}_\alpha}\cdot\mathsf{R}^T\frac{\partial\boldsymbol{\rho}_{s\alpha}}{\partial\theta^i}=0, \tag{5.27}$$

$$\sum_\alpha \frac{\partial q^\mu}{\partial\boldsymbol{\rho}_\alpha}\cdot\frac{\partial\boldsymbol{\rho}_\alpha}{\partial q^\nu}=\delta^\mu_\nu, \tag{5.28}$$

where we use Eq. (5.16).

Now we can present useful forms for the elements of the inverse Jacobian. First we have the identity

$$\frac{\partial q^\mu}{\partial\boldsymbol{\rho}_\alpha}=g^{\mu\nu}\boldsymbol{\rho}_{\alpha;\nu}. \tag{5.29}$$

To prove this, it suffices to show that with this substitution Eqs. (5.27) and (5.28) are satisfied, since the inverse of a matrix is unique. As for Eq. (5.27), we have

$$\sum_\alpha g^{\mu\nu}\boldsymbol{\rho}_{\alpha;\nu}\cdot\mathsf{R}^T\frac{\partial\boldsymbol{\rho}_{s\alpha}}{\partial\theta^i}=g^{\mu\nu}\frac{\partial\boldsymbol{\omega}}{\partial\dot\theta^i}\cdot\sum_\alpha \boldsymbol{\rho}_\alpha\times\boldsymbol{\rho}_{\alpha;\nu}=0, \tag{5.30}$$

where we use Eq. (5.18) in the first equality and (5.3) in the second. As for Eq. (5.28), we have

$$\sum_\alpha g^{\mu\sigma}\boldsymbol{\rho}_{\alpha;\sigma}\cdot\boldsymbol{\rho}_{\alpha,\nu}=g^{\mu\sigma}\left(\sum_\alpha \boldsymbol{\rho}_{\alpha;\sigma}\cdot\boldsymbol{\rho}_{\alpha;\nu}+\mathbf{A}_\nu\cdot\sum_\alpha \boldsymbol{\rho}_\alpha\times\boldsymbol{\rho}_{\alpha;\sigma}\right)$$
$$=g^{\mu\sigma}g_{\sigma\nu}=\delta^\mu_\nu, \tag{5.31}$$

where we use Eqs. (5.3) and (5.10) in the second equality.

A useful form for the other part of the inverse Jacobian, $\partial\theta^i/\partial\boldsymbol{\rho}_{s\alpha}$, is obtained as follows. First we substitute Eqs. (5.18) and (5.29) into Eq. (5.19), writing the result in the form

$$\mathsf{R}\left(\frac{\partial\boldsymbol{\omega}}{\partial\dot\theta^i}\times\boldsymbol{\rho}_\alpha\right)\otimes\left(\frac{\partial\theta^i}{\partial\boldsymbol{\rho}_{s\beta}}\right)^T = \mathsf{I}\delta_{\alpha\beta}-(\mathsf{R}\boldsymbol{\rho}_{\alpha,\mu})\otimes(g^{\mu\nu}\boldsymbol{\rho}^T_{\beta;\nu}\mathsf{R}^T). \tag{5.32}$$

Next we multiply this by R^T on the left and by R on the right to clear most of the R's, and then we cross on the left with $\boldsymbol{\rho}_\alpha$ and sum on α. Swapping α,β, we have

$$\mathsf{M}\frac{\partial\boldsymbol{\omega}}{\partial\dot\theta^i}\otimes\left(\frac{\partial\theta^i}{\partial\boldsymbol{\rho}_{s\alpha}}\right)^T\mathsf{R}=\mathsf{P}_\alpha-\mathbf{a}_\mu\otimes(g^{\mu\nu}\boldsymbol{\rho}^T_{\alpha;\nu}), \tag{5.33}$$

where

$$\mathsf{P}_\alpha\leftrightarrow\boldsymbol{\rho}_\alpha. \tag{5.34}$$

Finally, multiplying by M^{-1}, we have

$$\frac{\partial\boldsymbol{\omega}}{\partial\dot\theta^i}\otimes\left(\frac{\partial\theta^i}{\partial\boldsymbol{\rho}_{s\alpha}}\right)^T\mathsf{R}=\mathsf{M}^{-1}\mathsf{P}_\alpha-\mathbf{A}_\mu\otimes(g^{\mu\nu}\boldsymbol{\rho}^T_{\alpha;\nu}) \tag{5.35}$$

or, on reverting to index notation and juggling indices,

$$\Lambda^{(i)}_k\mathsf{R}_{\ell j}\frac{\partial\theta^k}{\partial\rho_{s\alpha\ell}}=(\mathsf{M}^{-1})^{ik}\epsilon_{k\ell j}\rho_{\alpha\ell}-A^i_\mu g^{\mu\nu}\rho_{\alpha j;\nu}. \tag{5.36}$$

This is easily solved for $\partial\theta^k/\partial\rho_{s\alpha\ell}$, but is generally more useful in the form given.

D. Horizontal and vertical projectors

Equation (5.14) shows the decomposition of an arbitrary system velocity, represented in the angular velocity and shape basis, into horizontal and vertical components. One can easily construct from this equation the components of the horizontal and vertical projection operators, call them Π_h and Π_v, with respect to the same basis.

These projection operators take on interesting forms in the basis in which a system velocity $|v\rangle$ is represented by $(\mathbf{v}_1,\ldots,\mathbf{v}_{n-1})$, where $\mathbf{v}_\alpha=\mathsf{R}^T\mathbf{v}_{s\alpha}=\mathsf{R}^T\dot{\boldsymbol{\rho}}_{s\alpha}$. We shall call this the "body-frame basis." The body-frame basis is an anholonomic frame in the tangent spaces over configuration space in which the scalar product has the simple form

$$\langle v'|v\rangle=\sum_\alpha\mathbf{v}'_\alpha\cdot\mathbf{v}_\alpha. \tag{5.37}$$

A convenient basis for the three-dimensional subspace of vertical velocities consists of the vectors $|\ell_i\rangle$, defined in the body-frame basis by

$$|\ell_i\rangle=(\mathbf{e}_i\times\boldsymbol{\rho}_1,\ldots,\mathbf{e}_i\times\boldsymbol{\rho}_{n-1}), \tag{5.38}$$

where $\mathbf{e}_i$ is the ith unit vector, i.e., the vector with components $(\mathbf{e}_i)_j=\delta_{ij}$. The vectors $|\ell_i\rangle$ are the same as the vectors $X_{(i)}$ introduced in Eq. (4.60), if the latter are interpreted as vector fields on the fiber bundle rather than on the rotation-group manifold. They are, however, represented here in the body-frame basis, rather than the coordinate basis (θ^i,q^μ), as in Eq. (4.60). To establish this connection in detail, we return to Eq. (4.65) and let $\delta\phi=\delta t$, to represent a body rotation about axis $\mathbf{n}$ of unit angular velocity. This implies $\mathbf{v}_{s\alpha}=\mathbf{R}(\mathbf{n}\times\boldsymbol{\rho}_\alpha)$, or, with $\mathbf{n}=\mathbf{e}_i$, $\mathbf{v}_\alpha=\mathbf{e}_i\times\boldsymbol{\rho}_\alpha$.

The vectors $|\ell_i\rangle$ have the property that if $|v\rangle$ is a system velocity, then

$$\langle\ell_i|v\rangle=\mathbf{e}_i\cdot\sum_\alpha\boldsymbol{\rho}_\alpha\times\mathbf{v}_\alpha=L_i, \tag{5.39}$$

so that a velocity $|v\rangle$ is horizontal if and only if $\mathbf{L}=0$ (which we knew already). The vectors $|\ell_i\rangle$ are not orthonormal, but satisfy

$$\langle\ell_i|\ell_j\rangle=\sum_\alpha(\mathbf{e}_i\times\boldsymbol{\rho}_\alpha)\cdot(\mathbf{e}_j\times\boldsymbol{\rho}_\alpha)=M_{ij}. \tag{5.40}$$

Now we develop an expression for the vertical projector. We write an arbitrary system velocity in the form

$$|v\rangle=v^i|\ell_i\rangle+|v_h\rangle, \tag{5.41}$$

where $|v_h\rangle$ is the horizontal projection of $|v\rangle$. But according to Eq. (5.40), the vertical components are given by $v^i=(\mathsf{M}^{-1})^{ij}\langle\ell_j|v\rangle$, so that

$$\Pi_v=|\ell_i\rangle(\mathsf{M}^{-1})^{ij}\langle\ell_j|. \tag{5.42}$$

We note incidentally that $v^i=\omega^i$, a fact that has been expressed previously in various forms. Another notation for Π_v is the following. If $|v'\rangle=\Pi_v|v\rangle$, with $|v\rangle=(\mathbf{v}_1,\ldots,\mathbf{v}_{n-1})$ and $|v'\rangle=(\mathbf{v}'_1,\ldots,\mathbf{v}'_{n-1})$, then we write

$$\mathbf{v}'_\alpha=\sum_\beta\Pi^v_{\alpha\beta}\mathbf{v}_\beta, \tag{5.43}$$

where $\Pi^v_{\alpha\beta}$ is a set of 3×3 tensors, indexed by α,β. Then Eq. (5.42) is equivalent to

$$\Pi^v_{\alpha\beta}=\mathsf{P}^T_\alpha\mathsf{M}^{-1}\mathsf{P}_\beta, \tag{5.44}$$

where again $\mathsf{P}_\alpha\leftrightarrow\boldsymbol{\rho}_\alpha$.

It is of interest to verify the expected properties of Π_v in the form (5.44). First, Π_v is idempotent, $(\Pi_v)^2=\Pi_v$, or

$$\sum_\gamma\Pi^v_{\alpha\gamma}\Pi^v_{\gamma\beta}=\Pi^v_{\alpha\beta}, \tag{5.45}$$

as follows from Eq. (5.44) and the identity,

$$\mathsf{M}=\sum_\alpha\mathsf{P}_\alpha\mathsf{P}^T_\alpha=\sum_\alpha\mathsf{P}^T_\alpha\mathsf{P}_\alpha. \tag{5.46}$$

Next, it annihilates any horizontal vector, for if we use Eq. (5.44) in Eq. (5.43) we find

$$\mathbf{v}'_\alpha=\sum_\beta\mathsf{P}^T_\alpha\mathsf{M}^{-1}\mathsf{P}_\beta\mathbf{v}_\beta=\mathsf{P}^T_\alpha\mathsf{M}^{-1}\mathbf{L}, \tag{5.47}$$

which vanishes if $\mathbf{L}=0$. Finally, it has no effect on the vertical basis $|\ell_i\rangle$, since

$$\sum_\beta\mathsf{P}^T_\alpha\mathsf{M}^{-1}\mathsf{P}_\beta(\mathbf{e}_i\times\boldsymbol{\rho}_\beta)=-\boldsymbol{\rho}_\alpha\times(\mathsf{M}^{-1}\mathsf{M}\mathbf{e}_i)=\mathbf{e}_i\times\boldsymbol{\rho}_\alpha. \tag{5.48}$$

As for the horizontal projector Π_h, it has an interesting form in the same notation introduced in Eq. (5.43), namely,

$$\Pi^h_{\alpha\beta}=g^{\mu\nu}\boldsymbol{\rho}_{\alpha;\mu}\otimes\boldsymbol{\rho}^T_{\beta;\nu}. \tag{5.49}$$

To prove this result, we first note that Π_h is idempotent, as follows from an application of Eq. (5.10). Next, it follows from Eq. (5.3) that Π_h annihilates any vertical velocity vector, i.e., $\Pi_h|\mathscr{l}_i\rangle=0$. Finally, to show that Π_h has no effect on a horizontal velocity vector, we write an arbitrary velocity $\mathbf{v}_\alpha$ in the form

$$\mathbf{v}_\alpha=(\mathsf{M}^{-1}\mathbf{L})\times\boldsymbol{\rho}_\alpha+\boldsymbol{\rho}_{\alpha;\sigma}\dot{q}^\sigma, \tag{5.50}$$

as follows from Eqs. (3.49) and (3.57), so that if $|v'\rangle=\Pi_h|v\rangle$, then

$$\mathbf{v}'_\alpha=\sum_\beta\,\Pi^h_{\alpha\beta}\mathbf{v}_\beta=\boldsymbol{\rho}_{\alpha;\mu}\dot{q}^\mu=\mathbf{v}_\alpha-(\mathsf{M}^{-1}\mathbf{L})\times\boldsymbol{\rho}_\alpha, \tag{5.51}$$

where we use Eqs. (5.3) and (5.10) in the second equality. Therefore, if $\mathbf{L}=0$ (a horizontal vector), then $\Pi_h|v\rangle=|v\rangle$.

Since the horizontal and vertical spaces are orthogonal and complementary, we must have $\Pi_h+\Pi_v=I$, or

$$\Pi^h_{\alpha\beta}+\Pi^v_{\alpha\beta}=g^{\mu\nu}\boldsymbol{\rho}_{\alpha;\mu}\otimes\boldsymbol{\rho}^T_{\beta;\nu}+\mathsf{P}^T_\alpha\mathsf{M}^{-1}\mathsf{P}_\beta=\delta_{\alpha\beta}\mathsf{I}. \tag{5.52}$$

A direct proof of this property follows by using Eqs. (5.29) and (5.36) to transform the metric tensor $G_{ab}=\delta_{ab}$ in the coordinates $(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1})$ to the coordinates (θ^i,q^μ), whereupon it has the form indicated in Eq. (4.35). This calculation is sufficiently long that we will not repeat it here.

E. Field equations of the Kaluza-Klein type

A glance at the definitions of the fields M, $\mathbf{A}_\mu$, and $g_{\mu\nu}$, Eqs. (3.53), (3.56), and (4.18), respectively, suggests that there must be identities or field equations connecting these quantities. Indeed, a number of such identities can be constructed by methods that are well known in the literature on Kaluza-Klein theories (Cho, 1975; Coquereaux, 1988). These identities are not at all trivial in appearance or easy to verify directly from the definitions of M, $\mathbf{A}_\mu$, and $g_{\mu\nu}$. We remark that in Kaluza-Klein theories the idea is to show how complicated field equations on space-time, such as the coupled Einstein-Yang-Mills equations, are manifestations of simpler field equations on a higher-dimensional space, which is a principal fiber bundle over space-time. In our problem, the analog of space-time is shape space, but the philosophy is somewhat different; instead of taking complicated equations on a base space and simplifying them by going to a larger space, we are starting with the larger space (the translation-reduced configuration space, which has the structure of a principal fiber bundle), and reducing the dimensionality, at the expense of dealing with a more complex (or at least richer) structure to the equations of motion.

We begin with the (translation-reduced) configuration space, upon which some coordinates x^a are imposed and upon which the metric tensor, connection components, and Riemann tensor are $\tilde{g}_{ab}$, $\tilde{\Gamma}^a_{bc}$, and $\tilde{R}^a{}_{bcd}$, respectively. We use tildes to denote these fields on configuration space and to contrast them with the analogous fields $g_{\mu\nu}$, $\Gamma^\mu_{\sigma\tau}$, and $R^\mu{}_{\nu\sigma\tau}$ on shape space. Of course, configuration space is the Euclidean manifold $\mathbb{R}^{3n-3}$, so $\tilde{R}^a{}_{bcd}=0$. (We have previously written G_{ab} for what we are now calling $\tilde{g}_{ab}$.) Furthermore, if Euclidean coordinates are chosen, i.e., $x^a=(\boldsymbol{\rho}_{s1},\ldots,\boldsymbol{\rho}_{s,n-1})$, then $\tilde{g}_{ab}=\delta_{ab}$ and $\tilde{\Gamma}^a_{bc}=0$. Our strategy will be to express the vanishing of the Riemann tensor on configuration space in terms of a shape and orientational representation, whereupon a number of identities result.

We shall express tensors on configuration space, not in a coordinate basis, but rather in an anholonomic basis of horizontal and vertical vector fields. Appendix E summarizes the computation of the Riemann tensor in an anholonomic frame; we shall call on the formulas of that Appendix freely, making the notational changes μ,ν, etc., $\rightarrow a,b$, etc. We shall not place overbars on the anholonomic indices, but it is to be understood that all quantities $\tilde{g}_{ab}$, $\tilde{\Gamma}^a_{bc}$, $\tilde{R}^a{}_{bcd}$, etc., are taken with respect to the anholonomic frame. Furthermore, the comma notation applied to the quantities $\tilde{g}_{ab}$, $\tilde{\Gamma}^a_{bc}$, etc., will be interpreted as in Eq. (E10). When we break up components into vertical and horizontal parts, we shall write, for example, $a=(i,\mu)$, $b=(j,\nu)$, etc., corresponding to $3n-3=3+(3n-6)$. For example, $\tilde{g}_{\mu\nu}$ refers to the components of the metric with respect to the anholonomic horizontal basis vectors e_μ, e_ν and is conceptually distinct from $g_{\mu\nu}$, the components of the metric on shape space with respect to the coordinate basis q^μ. (As it turns out, however, $\tilde{g}_{\mu\nu}=g_{\mu\nu}$.)

We shall denote the basis vectors on configuration space by e_a or (e_i,e_μ), where e_i are the vertical vectors and e_μ the horizontal. These vectors are defined by

$$e_i=X^j_{(i)}\frac{\partial}{\partial\theta^j}, \tag{5.53}$$

$$e_\mu=\frac{\partial}{\partial q^\mu}-A^i_\mu e_i, \tag{5.54}$$

where we follow the standard practice in differential geometry of representing vector fields by the associated differential operators. (The contravariant components in coordinate basis x^a are the coefficients of the operators $\partial/\partial x^a$.) The vertical vector fields e_i are identical to the fields $|\mathscr{l}_i\rangle$ introduced earlier. The horizontal vectors e_μ are the horizontal projections of the coordinate basis vectors $\partial/\partial q^\mu$; the latter are tangent to the section $\mathcal{S}$ (since varying one of the q^μ while holding all other variables fixed, including the θ^i, means moving along the section $\mathcal{S}$) and are not generally horizontal themselves.

We denote the dual basis of forms by σ^a or (σ^i,σ^μ). These are given by

$$\sigma^i=\Lambda^{(i)}_j d\theta^j+A^i_\mu dq^\mu, \tag{5.55}$$

$$\sigma^\mu=dq^\mu, \tag{5.56}$$

so that $\sigma^a(e_b)=\delta^a_b$. The matrix transforming the coordinate basis of forms $(d\theta^i, dq^\mu)$ to the anholonomic basis (σ^i,σ^μ) is the same as that displayed in Eq. (4.115), which confirms our earlier statement that the block-diagonalized metric seen in that equation (the center matrix on the right-hand side) is the component matrix of the metric with respect to the anholonomic basis of horizontal and vertical vector fields. In present language, this means that

$$\tilde{g}_{ij}=M_{ij},\quad \tilde{g}_{\mu\nu}=g_{\mu\nu},\quad \tilde{g}_{i\nu}=\tilde{g}_{\mu j}=0,$$
$$\tilde{g}^{ij}=(\mathsf{M}^{-1})_{ij},\quad \tilde{g}^{\mu\nu}=g^{\mu\nu},\quad \tilde{g}^{i\nu}=g^{\mu j}=0. \tag{5.57}$$

The computation of the structure constants of the anholonomic frame is straightforward. First we have $[e_i,e_j]=\epsilon_{ijk}e_k$, in accordance with the calculation leading to Eq. (4.56). From this we easily find $[e_i,e_\mu]=-\epsilon_{ijk}A^j_\mu e_k$ and $[e_\mu,e_\nu]=-B^i_{\mu\nu}e_i$. Therefore the structure constants are

$$c^k_{ij}=\epsilon_{ijk},\quad c^k_{i\mu}=-c^k_{\mu i}=-\epsilon_{ijk}A^j_\mu=(\mathsf{A}_\mu)_{ki},$$
$$c^k_{\mu\nu}=-B^k_{\mu\nu},\quad c^\mu_{ab}=0. \tag{5.58}$$

Next we compute the connection components according to Eq. (E13). The following facts simplify this calculation. First, the components $\tilde{g}_{ab}$ are independent of θ^i, so $\tilde{g}_{ab,i}=0$; second, $\tilde{g}_{ab}$ is block diagonal, as indicated by Eq. (5.57); and third, $c^\mu_{ab}=0$. The connection components are

$$\tilde{\Gamma}^k_{ij}=(\mathsf{M}^{-1})_{k\ell}F_{\ell ij},\quad \tilde{\Gamma}^\mu_{ij}=-\tfrac{1}{2}g^{\mu\nu}M_{ij;\nu}=-\tfrac{1}{2}M_{ij}{}^{;\mu},$$
$$\tilde{\Gamma}^k_{i\nu}=\tfrac{1}{2}(\mathsf{M}^{-1})_{k\ell}M_{\ell i;\nu}-(\mathsf{A}_\nu)_{ki},\quad \tilde{\Gamma}^\mu_{i\nu}=-\tfrac{1}{2}M_{ik}B^{k\mu}{}_\nu,$$
$$\tilde{\Gamma}^k_{\nu j}=\tfrac{1}{2}(\mathsf{M}^{-1})_{k\ell}M_{\ell j;\nu},\quad \tilde{\Gamma}^\mu_{\nu j}=-\tfrac{1}{2}M_{jk}B^{k\mu}{}_\nu,$$
$$\tilde{\Gamma}^k_{\mu\nu}=\tfrac{1}{2}B^k_{\mu\nu},\quad \tilde{\Gamma}^\sigma_{\mu\nu}=\Gamma^\sigma_{\mu\nu}, \tag{5.59}$$

where we define

$$F_{ijk}=\tfrac{1}{2}(M_{j\ell}\epsilon_{\ell ik}+M_{k\ell}\epsilon_{\ell ij}+M_{i\ell}\epsilon_{\ell kj})=-F_{jik}. \tag{5.60}$$

Finally, we compute the components of the Riemann tensor according to Eq. (E16). We present these in their completely covariant forms, which are most symmetrical:

$$\begin{aligned}
0=\tilde{R}_{ijk\ell}&=(\mathsf{M}^{-1})_{mn}(F_{mi\ell}F_{njk}-F_{mik}F_{nj\ell})\\
&\quad-\epsilon_{mk\ell}F_{ijm}+\tfrac{1}{4}(M_{i\ell;\mu}M_{jk}{}^{;\mu}\\
&\quad-M_{ik;\mu}M_{j\ell}{}^{;\mu}),\\
0=\tilde{R}_{ij\nu k}&=F_{ijk;\nu}+\tfrac{1}{2}[(\mathsf{M}_{;\nu}\mathsf{M}^{-1})_{j\ell}F_{\ell ik}\\
&\quad-(\mathsf{M}_{;\nu}\mathsf{M}^{-1})_{i\ell}F_{\ell jk}]+\tfrac{1}{4}[M_{ik;\lambda}(\mathsf{M}\mathbf{B}^\lambda{}_\nu)_j\\
&\quad-M_{jk;\lambda}(\mathsf{M}\mathbf{B}^\lambda{}_\nu)_i],\\
0=\tilde{R}_{i\nu j\tau}&=\tfrac{1}{4}(\mathsf{M}_{;\tau}\mathsf{M}^{-1}\mathsf{M}_{;\nu})_{ij}-\tfrac{1}{2}(\mathsf{M}_{;\nu\tau})_{ij}\\
&\quad+\tfrac{1}{4}(\mathsf{M}\mathbf{B}_{\lambda\tau})_i(\mathsf{M}\mathbf{B}^\lambda{}_\nu)_j+\tfrac{1}{2}B^k_{\nu\tau}F_{ikj},\\
0=\tilde{R}_{ij\sigma\tau}&=\tfrac{1}{4}(\mathsf{M}_{;\tau}\mathsf{M}^{-1}\mathsf{M}_{;\sigma})_{ij}-\tfrac{1}{4}(\mathsf{M}_{;\sigma}\mathsf{M}^{-1}\mathsf{M}_{;\tau})_{ij}\\
&\quad+\tfrac{1}{2}\epsilon_{ij\ell}(\mathsf{M}\mathbf{B}_{\sigma\tau})_\ell+\tfrac{1}{4}[(\mathsf{M}\mathbf{B}_{\lambda\tau})_i(\mathsf{M}\mathbf{B}^\lambda{}_\sigma)_j\\
&\quad-(\mathsf{M}\mathbf{B}_{\lambda\sigma})_i(\mathsf{M}\mathbf{B}^\lambda{}_\tau)_j],
\end{aligned} \tag{5.61}$$

$$0=\tilde{R}_{i\nu\sigma\tau}=\tfrac{1}{2}(\mathsf{M}\mathbf{B}_{\sigma\tau})_{i;\nu}-\tfrac{1}{4}(\mathsf{M}_{;\sigma}\mathbf{B}_{\tau\nu})_i-\tfrac{1}{4}(\mathsf{M}_{;\tau}\mathbf{B}_{\nu\sigma})_i,$$
$$0=\tilde{R}_{\mu\nu\sigma\tau}=R_{\mu\nu\sigma\tau}-\tfrac{1}{2}\mathbf{B}_{\mu\nu}\cdot\mathsf{M}\cdot\mathbf{B}_{\sigma\tau}-\tfrac{1}{4}\mathbf{B}_{\mu\sigma}\cdot\mathsf{M}\cdot\mathbf{B}_{\nu\tau}+\tfrac{1}{4}\mathbf{B}_{\mu\tau}\cdot\mathsf{M}\cdot\mathbf{B}_{\nu\sigma}.$$

In these equations, for example, $\mathsf{M}_{;\nu}$ is the covariant derivative of the tensor M, which has components $M_{ij;\nu}$. The last of these equations allows the Riemann tensor on shape space, $R_{\mu\nu\sigma\tau}$, to be expressed in terms of the moment-of-inertia tensor and the Coriolis tensor; this is very convenient computationally. The resulting expression can easily be contracted to obtain the Ricci tensor,

$$R_{\mu\nu}=\tfrac{3}{4}\mathbf{B}_{\mu\sigma}\cdot\mathsf{M}\cdot\mathbf{B}_\nu{}^\sigma, \tag{5.62}$$

from which follows Eq. (4.44).

F. Comments on the Eckart conventions

We now present some comments on the Eckart conventions, which are a standard subject in the theory of molecular vibrations (Eckart, 1935; Wilson, Decius, and Cross, 1955; Louck and Galbraith, 1976; Biedenharn and Louck, 1981; Ezra, 1982). The new element in the following discussion is the geometrical interpretation of the Eckart frame and its properties in terms of a section of the fiber bundle.

The Eckart conventions consist of a choice of body frame and a choice of coordinate system on shape space. Eckart's original motivation for his conventions is attributed to Casimir (1931), who supposed that it should be possible to choose a frame to make the "Coriolis coupling terms," the terms linear in $\mathbf{L}$ in the Hamiltonian (4.92) or (4.97), of the same order as the terms quadratic in $\mathbf{L}$, at least when the amplitude of vibrational motion is small. These terms are not gauge invariant, but it is convenient in certain non-gauge-invariant perturbation schemes to make them as small as possible. Since these terms all involve the product $\mathbf{L}\cdot\mathbf{A}_\mu$, Casimir's condition is satisfied if the frame is chosen so that $\mathbf{A}_\mu$ vanishes at the equilibrium shape of the molecule. As we have noted previously, this condition is geometrically equivalent to the demand that the section $\mathcal{S}$ of the fiber bundle be perpendicular to the equilibrium fiber, i.e., that it be purely horizontal at the equilibrium shape. This is a local condition on the choice of body frame, and there are many gauges that satisfy it, but Eckart's (1935) actual choice of frame was, in fact, a global construction.

The conditions specifying the section $\mathcal{S}$ and hence the Eckart frame were given in Eq. (3.47); as noted, these constitute a set of linear constraints on the vectors $\boldsymbol{\rho}_{s\alpha}$, so the Eckart section is a $(3n-6)$-dimensional vector subspace of the configuration space. The Eckart section is illustrated schematically in Fig. 20. In the figure, F_0 is the equilibrium fiber, and $Q_0=\{\boldsymbol{\rho}_{\alpha 0}\}$ is an arbitrarily chosen reference orientation on that fiber. (Some authors choose the reference orientation to be the one in which the principal axis frame for the equilibrium shape coincides with the space frame, but this is not necessary.) We do not distinguish between $\boldsymbol{\rho}_{s\alpha 0}$ and $\boldsymbol{\rho}_{\alpha 0}$ since the configuration in question is a reference, for which

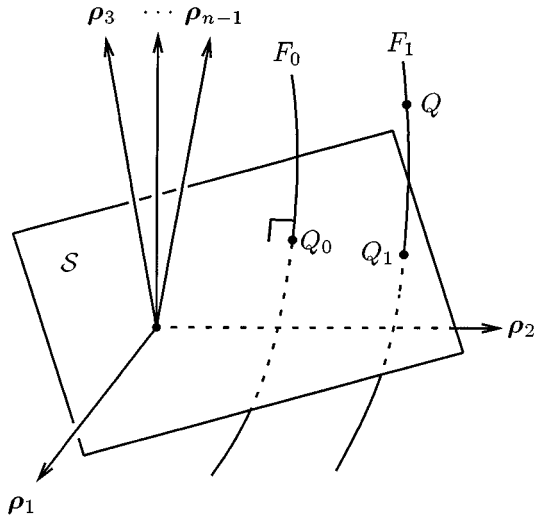

FIG. 20. The Eckart section $\mathcal{S}$, which is a $(3n-6)$-dimensional vector subspace of configuration space. The equilibrium fiber is F_0, which is orthogonal to the section at reference configuration Q_0. Fiber F_1 is another fiber, representing a shape displaced from equilibrium.

space and body frames coincide. As indicated schematically in the figure, the equilibrium fiber is orthogonal to the Eckart section $\mathcal{S}$ at the configuration Q_0; but other fibers such as F_1 are not orthogonal to the section at their point of intersection, Q_1 in the figure.

Given an arbitrary configuration $Q=\{\boldsymbol{\rho}_{s\alpha}\}$, it is of interest to know the rotation matrix R that connects it with the corresponding reference configuration, say, $Q_1=\{\boldsymbol{\rho}_{s\alpha 1}\}=\{\boldsymbol{\rho}_{\alpha 1}\}$, since this rotation in effect defines the body frame for the given configuration. Such configurations Q and Q_1 are illustrated lying on fiber F_1 in Fig. 20. Since these configurations are related by $\boldsymbol{\rho}_{s\alpha}=\mathsf{R}\boldsymbol{\rho}_{\alpha 1}$ and since $\{\boldsymbol{\rho}_{\alpha 1}\}$ satisfies Eq. (3.47), we have

$$\sum_\alpha (\mathsf{R}^T\boldsymbol{\rho}_{s\alpha})\times\boldsymbol{\rho}_{\alpha 0}=0 \tag{5.63}$$

or

$$\mathsf{F}^T\mathsf{R}=\mathsf{R}^T\mathsf{F}, \tag{5.64}$$

where

$$\mathsf{F}=\sum_\alpha \boldsymbol{\rho}_{s\alpha}\otimes\boldsymbol{\rho}_{\alpha 0}^T. \tag{5.65}$$

The columns of F have been called the "Eckart vectors" by Louck and Galbraith (1976).

The matrix F is regarded as a function of the configuration $\{\boldsymbol{\rho}_{s\alpha}\}$. It is a symmetric non-negative definite matrix at the equilibrium configuration, $\boldsymbol{\rho}_{s\alpha}=\boldsymbol{\rho}_{\alpha 0}$, at which point the rank of F is equal to the dimensionality of the equilibrium configuration itself. Thus F is a singular matrix at the equilibrium configuration only if that configuration is linear or planar. In the following discussion, we shall assume that the equilibrium configuration is three-dimensional, so that F is positive definite there; the case of planar equilibria can be handled with some simple modifications to the formalism, but the Eckart frame is not defined for collinear equilibria.

Since by our assumptions F is nonsingular at the equilibrium, by continuity it will be nonsingular in some neighborhood of the equilibrium. Then, according to the polar decomposition theorem, F (at any point in the neighborhood) can be factored uniquely into the product $\mathsf{F}=\mathsf{R}\mathsf{T}$, where T is positive definite symmetric and R is orthogonal. Since F itself is positive definite symmetric at the equilibrium and since the polar decomposition is unique, we have $\mathsf{R}=\mathsf{I}$ at the equilibrium, i.e., R is a proper orthogonal matrix at the equilibrium. Therefore, by continuity, R is a proper orthogonal matrix at all points in the neighborhood where F is nonsingular.

In fact, R is the matrix that rotates the space frame to body frame, i.e., it is the same R that appears in Eq. (5.64). This follows because T is the unique positive-definite square root of $\mathsf{F}^T\mathsf{F}$, so that $\mathsf{R}=\mathsf{F}\mathsf{T}^{-1}$. Therefore $\mathsf{T}=\mathsf{R}^T\mathsf{F}$ is symmetric and Eq. (5.64) is satisfied. The matrix R provides the usual definition of the Eckart frame.

A different definition of the "Eckart frame" has recently been given by Iwai (1987a, 1987b, 1987c, 1992) and by Tachibana and Iwai (1986). In our language, what these authors call the Eckart frame is the parallel-transported frame, which we discuss in Appendix D. This frame is not defined as a field over shape space, but only as a function of time (or other parameter) along a curve $q^\mu(t)$ in shape space. We believe, however, that this definition of the Eckart frame is at variance with the original definition of Eckart (1935), which is used throughout the literature on molecular vibrations. We believe that a correct geometrical interpretation of Eckart's original definition is given in terms of sections of the fiber bundle, as we have described above, so that the Eckart frame is defined as a field over shape space. On the other hand, the parallel-transported frame, by whatever name, is geometrically compelling and useful in practice. For example, it has been discovered and used by Jellinek and Li (1989, 1990) in their recent work on rotations of atomic clusters.

We turn now to Eckart's definition of shape coordinates. The geometry underlying this definition is very simple. Since Eckart's section $\mathcal{S}$ is a $(3n-6)$-dimensional vector subspace of configuration space, which itself is a Euclidean space, it is possible to choose $3n-6$ Euclidean coordinates q^μ on the section, with an origin conveniently selected so that $q^\mu=0$ at the equilibrium. These coordinates can then be interpreted as shape coordinates, due to the one-to-one mapping between points of shape space and points of the section, although as discussed earlier the metric $g_{\mu\nu}$ on shape space is not the same as the metric $h_{\mu\nu}$ on the section. In fact, in Euclidean section coordinates, we have $h_{\mu\nu}=h^{\mu\nu}=\delta_{\mu\nu}$, a condition that simplifies somewhat the molecular Hamiltonian in the form (4.97). Of course, such Euclidean section coordinates are not unique, but are subject to orthogonal transformations in the $3n-6$ variables q^μ; by some choice of such a transformation,

the quadratic term in the expansion of the potential energy about the equilibrium position can be diagonalized, so that

$$V(q)=V(0)+\frac{1}{2}\sum_{\mu}\ \omega_{\mu}^{2}(q^{\mu})^{2}+O((q^{\mu})^{3}). \tag{5.66}$$

When this is done, the q^{μ} are normal-mode coordinates for small-amplitude vibrations, and the ω_{μ} are the frequencies. In many common molecules, these frequencies are degenerate.

In such (Eckart) coordinates, the equation of the section has the form

$$\boldsymbol{\rho}_{s\alpha}=\boldsymbol{\rho}_{\alpha}(q^{\mu})=\boldsymbol{\rho}_{\alpha 0}+\mathbf{F}_{\alpha\mu}q^{\mu}, \tag{5.67}$$

where the coefficients $\mathbf{F}_{\alpha\mu}=\partial\boldsymbol{\rho}_{\alpha}/\partial q^{\mu}$ are constants. Thus, in Eckart coordinates, there is a linear relationship between the lab coordinates of reference configurations and the shape coordinates, although this is not true for other configurations (since the construction of R as a function of $\{\boldsymbol{\rho}_{s\alpha}\}$, given above, involves nonlinearities). The relation (5.67) causes the field $\mathbf{a}_{\mu}$ to be linear in q^{μ} and the moment of inertia tensor M to be quadratic in q^{μ}; these facts simplify a number of computations. Given a model for the equilibrium shape of a molecule and a knowledge of the potential energy in a neighborhood of the equilibrium, it is straightforward to compute the constants $\mathbf{F}_{\alpha\mu}$; methods for doing this are described by Wilson, Decius, and Cross (1955).

Although the Eckart frame and coordinates are, in principle, not restricted to small-amplitude vibrations, it seems that they lose many of their advantages when amplitudes are not small (De Celles and Darling, 1969). This fact diminishes somewhat the interest in an examination of the global properties of the Eckart frame and coordinates, about which much could be said. When the molecular potential energy is stiff only in certain directions in shape space, but nearly flat in others, as often happens, a modification of the Eckart conventions due to Sayvetz is often used (Sayvetz, 1939; Ezra, 1982).

We now discuss the effect of the Eckart conventions on the form of the Hamiltonian. We speak first of the classical Hamiltonian. We have previously derived a manifestly gauge-invariant version of this Hamiltonian, Eq. (4.92), which by rearranging terms we converted into an alternate form (4.97). This rearrangement was valid in any gauge and coordinates, although there is some simplification in the Eckart gauge and coordinates due to the relation $h_{\mu\nu}=h^{\mu\nu}=\delta_{\mu\nu}$.

We have also derived an expression for the quantum Hamiltonian, (4.146), which is valid in any gauge and any coordinates on shape space. However, if we attempt to rearrange this definition in a manner similar to the classical rearrangement leading to Eq. (4.97), we find that there are several new terms that arise due to nonclassical commutators. But if Eckart gauge and coordinates are used, many of these extra terms disappear, and we are left with

$$H=\tfrac{1}{2}(\mathbf{L}-\mathbf{K})\cdot\tilde{\mathsf{M}}^{-1}\cdot(\mathbf{L}-\mathbf{K})+\tfrac{1}{2}p_{\mu}p_{\mu}+V_{2}(q)+V(q). \tag{5.68}$$

In this expression, $\tilde{\mathsf{M}}$ is defined exactly as in the classical formulas, Eq. (4.37) or (4.93), and the definition of the quantum operator **K** also follows the classical formula (4.95), with $h_{\mu\nu}=\delta_{\mu\nu}$. Because of the special features of the Eckart conventions, the terms in Eq. (4.95) commute, and ordering is not an issue.

Finally, the gauge-invariant V_2 term in Eq. (5.68) is defined, as before, by Eq. (4.145), but is here to be specialized to the Eckart coordinates. In a nontrivial calculation by Watson (1968), this term was shown to undergo a remarkable simplification in the Eckart coordinates and gauge, with the final result being

$$V_{2}=-\frac{\hbar^{2}}{8}\mathrm{Tr}\tilde{\mathsf{M}}^{-1}. \tag{5.69}$$

Watson's result is much simpler than his derivation, which suggests that a simpler derivation must exist. A different derivation of Eq. (5.69) has been given by Louck (1976), but it is also nontrivial.

Using geometric reasoning, we have been able to find a simpler derivation of Watson's result. We shall report on the details of this calculation in future publications, and only comment here on the basic ideas. Although, as noted earlier, V_2 does not transform as a scalar under general changes of coordinates on shape space, nevertheless it is easy to see that it does transform as a scalar under linear (possibly inhomogeneous) changes of coordinates. For example, if one restricts consideration to gauge surfaces that are vector subspaces of configuration space upon which linear coordinates are used (we call these "linear conventions"), then V_2 can be viewed as a scalar on this surface. Furthermore, the surface itself is specified by any three linearly independent vectors orthogonal to the surface (or the forms that annihilate the surface). Therefore the value of V_2 must be expressible in terms of the fiber determining a point on the surface, and the orthogonal vectors. Following these ideas leads to a considerable simplification of Watson's derivation. It turns out that not all linear conventions lead to as great a simplification as in Watson's expression; the Eckart linear conventions are special and lead to even greater simplification.

G. Geometrical meaning of the tensor $\tilde{M}$

We shall now provide a geometrical interpretation of the tensor $\tilde{\mathsf{M}}$, which is defined by Eq. (4.37) or (4.93). We feel this is important, in view of the frequency with which this tensor occurs in the molecular physics literature, in spite of its lack of gauge covariance. Although most applications of $\tilde{\mathsf{M}}$ employ the Eckart conventions, in the following we shall make no assumptions about gauge or shape coordinates. In the following we sometimes drop the Dirac brackets when writing vectors, without distinction; for example, vectors e_i and $|e_i\rangle$ are the same.

The basic result is

$$\tilde{M}_{ij}=\langle f_i|f_j\rangle, \tag{5.70}$$

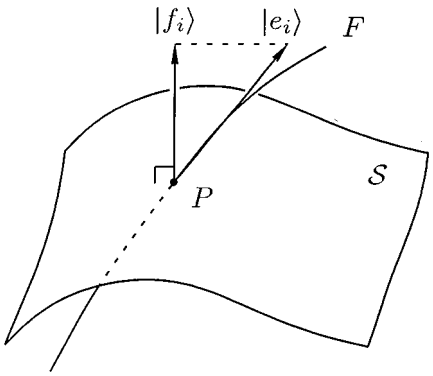

FIG. 21. Illustration of vectors $|e_i\rangle$ and $|f_i\rangle$. The fiber shown passes through the gauge surface $\mathcal{S}$ at configuration P and is not orthogonal to the surface. Vectors $|e_i\rangle$ span the space of vertical vectors, which are tangent to the fiber. Vectors $|f_i\rangle$ are the projections of $|e_i\rangle$ onto the normal to the surface. The tensor $\tilde{\mathsf{M}}$ contains the scalar products $\langle f_i|f_j\rangle$.

in which f_i, $i=1,2,3$, are the vectors obtained by projecting the vectors e_i, defined in Eq. (5.53), onto the three-dimensional space perpendicular to the gauge surface $\mathcal{S}$. Since the gauge surface in general is not perpendicular to the fibers, the space perpendicular to the gauge surface is not the same as the space of vertical vectors (which the e_i span). The general situation is illustrated in Fig. 21, in which the fiber F passing through a point P on the gauge surface $\mathcal{S}$ is not orthogonal to the surface. Obviously the space perpendicular to the gauge surface has no gauge-invariant meaning, which explains the lack of gauge covariance of $\tilde{\mathsf{M}}$.

To prove Eq. (5.70), we first introduce projectors $\Pi_\parallel$ and $\Pi_\perp$ parallel and perpendicular to the gauge surface, respectively. We obtain an expression for $\Pi_\parallel$ as follows. First we note that the vectors f_μ, defined by

$$f_\mu=\frac{\partial}{\partial q^\mu}=e_\mu+A^i_\mu e_i, \tag{5.71}$$

are parallel to the gauge surface. On computing the scalar products of these vectors and using $\langle e_i|e_j\rangle=M_{ij}$, $\langle e_i|e_\mu\rangle=0$, and $\langle e_\mu|e_\nu\rangle=g_{\mu\nu}$, we find

$$\langle f_\mu|f_\nu\rangle=g_{\mu\nu}+A^i_\mu M_{ij}A^j_\nu=h_{\mu\nu}, \tag{5.72}$$

in accordance with Eq. (4.18). Therefore if we decompose an arbitary velocity vector $|v\rangle$ into its components perpendicular and parallel to the gauge surface,

$$|v\rangle=|v_\perp\rangle+v^\mu|f_\mu\rangle, \tag{5.73}$$

then we find $v^\mu=h^{\mu\nu}\langle f_\nu|v\rangle$ or

$$\Pi_\parallel=|f_\mu\rangle h^{\mu\nu}\langle f_\nu|. \tag{5.74}$$

The perpendicular projector is then defined by $\Pi_\perp=1-\Pi_\parallel$.

Next, defining $|f_i\rangle$ as the perpendicular projections of $|e_i\rangle$, we have

$$|f_i\rangle=\Pi_\perp|e_i\rangle=|e_i\rangle-|f_\mu\rangle h^{\mu\nu}a_{i\nu}, \tag{5.75}$$

where we use Eqs. (5.74) and the scalar product,

$$\langle f_\mu|e_i\rangle=a_{i\mu}, \tag{5.76}$$

as follows from Eq. (5.71). Finally, we have

$$\langle f_i|f_j\rangle=\langle e_i|\Pi_\perp\Pi_\perp|e_j\rangle=M_{ij}-a_{i\mu}h^{\mu\nu}a_{j\nu}=\tilde{M}_{ij}, \tag{5.77}$$

where we use Eq. (4.93) and the fact that $\Pi_\perp$ is idempotent. This proves Eq. (5.70).

VI. CONCLUSIONS

We have attempted to do several things in this review. First, since most of the fundamental developments in the gauge theory of deformable, rotating systems have been carried out by mathematicians and particle physicists, that is, people who have not worked on applied problems in the relevant areas, we felt it was important to master the applied literature and to assess the impact of the new ideas. This literature is vast, of course, so we narrowed our focus to the atomic and molecular fields, with lesser emphasis on nuclear physics. We mostly neglected classical fields such as celestial mechanics. Within this body of literature we found that the geometrical and specifically gauge-theoretical point of view is indeed new and that it provides a new perspective from which to judge both old and new problems within the theory, as well as the historically accepted solutions to old problems. For example, we found that the standard Wilson-Howard-Watson Hamiltonian of molecular physics is written in a form that almost maximally disguises the geometrical meaning of the various contributions to the energy, mainly because of the gauge-specific features of the Eckart conventions. For another example, we found that the old question of whether it is possible to transform away the Coriolis coupling terms in the Hamiltonian reduces to the question of the vanishing of the curvature form (which does not vanish, so it is impossible to transform away the Coriolis coupling). We also found that the geometrical perspective simplifies some of the standard theory. For example, the derivation of Watson's expression for the extra term in the quantum Hamiltonian, what we call V_2 in Eq. (4.147), is notoriously difficult, and we were able to simplify it.

Second, we attempted to assimilate the more mathematical developments in this field from a physicist's perspective and to express them in a physicist's language. For example, while it is true that the reduction theory of Marsden, Weinstein, and others is quite general, it nevertheless expresses the reduced Hamiltonian in terms of such concepts as pullbacks, quotient spaces, etc., whereas coordinate-based expressions would also be useful for applications. In the case of the n-body problem, we believe the reduced Hamiltonian in the coordinate form shown by Eq. (4.92) or the reduced equations of motion in the form of Eq. (4.77) are new. These are of course straightforward but necessary developments.

Third, the gauge-theoretical notation and point of view suggest a number of issues, which we tried to address. For example, we found that simply the use of covariant derivatives led to a number of identities satisfied

by the various fields on shape space, among which are Eqs. (5.3), (5.6), (5.10), (5.14), and (5.29). We believe all these identities are new; in most cases, we have found their proper geometrical interpretation (not given in this review). Also, the Kaluza-Klein identities are fairly obvious from a gauge-theoretical point of view, and we have found them useful for various purposes (especially the one giving the Riemann tensor on shape space in terms of other fields).

Fourth, we found and worked on a number of new questions relating to n-body dynamics. These problems are only mentioned in passing in this review, but this review forms the background necessary to develop their solutions. The following is a list of some of these questions, which we shall discuss more fully in future publications. First, as mentioned above, we have developed a simplified derivation of Watson's expression for V_2 and a generalization of such terms. Second, we have found a new form for the kinetic-energy operator for the four-body problem [partially anticipated by Zickendraht (1969)], in which shape space is fibrated by the democracy group. Thus, shape space itself becomes a principal fiber bundle (apart from exceptional points), for which, as it turns out, the curvature vanishes and the base space is Euclidean. This work was part of a larger study of gauge fields introduced by particle democracy. Third, we have shown that the Coriolis tensor satisfies a set of Yang-Mills field equations with no sources, except for singularities of the monopole type. This question was naturally motivated by Iwai's discovery that the Coriolis field has a monopole form for the three-body problem. Fourth, we have found the explicit relation between Smith's hyperspherical harmonics and the standard spherical harmonics for charged-particle motion in a monopole field (they are essentially identical). Fifth, we have studied symmetries of the metric in the n-body problem; this project was motivated by the observation that in the three-body problem the metric has a higher symmetry group than the democracy group [SO(3) instead of SO(2)]. We showed that no higher symmetry exists for $n>3$. As a part of this work, we have investigated the possibility of diagonalizing the metric for $n=4$. Sixth, we have investigated the interaction between the adiabatic gauge potential of Mead and Truhlar and Berry and the Coriolis gauge potential of this paper. This same subject has recently been investigated by Tachibana (private communication).

Finally, we should like to raise some other possibilities. Since all physical results must be gauge invariant, it should be possible to develop gauge-invariant perturbation theory. This would certainly be a new perspective on problems of rovibrational coupling. The gauge-theoretical point of view is also relevant to reaction-path theory and would be a new perspective there as well. Problems in molecular physics involving internal rotors or other subsystems with well separated time scales lead to new kinds of adiabatic processes, which should properly be described in terms of appropriate gauge groups. We hope to develop some of these ideas in the future.

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APPENDIX A: CONVENTIONS AND NOTATION

In this paper, 3-vectors are represented in boldface, e.g., $\mathbf{r}_{s\alpha}$, $\mathbf{L}$, or $\boldsymbol{\omega}$, although for vectors of other dimensionality the practice varies. A boldfaced symbol does not stand for the vector in an abstract or geometrical sense, but rather for the collection of components of the abstract vector with respect to some frame. Vectors referred to the space or inertial frame are indicated with a subscript s, as in $\mathbf{r}_{s\alpha}$ or $\mathbf{L}_s$; the absence of a subscript s indicates the body frame, as in $\mathbf{r}_\alpha$ or $\mathbf{L}$. Components themselves are indicated in italics, e.g., L_i or L_{si}.

We represent 3×3 matrices or tensors in sans serif, e.g., M or I= identity, and their components in italics, e.g., M_{ij}. Where the distinction is relevant, such tensors have a subscript s when referred to the space frame and are written without this subscript when referred to the body frame. The practice varies for matrices or tensors of other sizes, which are sometimes represented in terms of their components, e.g., G_{ab}, $g_{\mu\nu}$, or $D_{\alpha\beta}$, and sometimes in sans serif, e.g., D.

We denote the complete contraction of two 3-vectors with a 3×3 matrix, either with dots or with a transpose notation for vectors. For example, $\mathbf{L}\cdot\mathsf{M}^{-1}\cdot\mathbf{L}$ is the same as $\mathbf{L}^T\mathsf{M}^{-1}\mathbf{L}$.

The juxtaposition of two 3-vectors is dyadic notation for a 3×3 tensor; for example, $\mathbf{A}_\mu\mathbf{A}_\nu^T$ is the tensor with i,j components $A_\mu^i A_\nu^j$. Sometimes we insert a tensor product symbol $\otimes$ to make this more clear, as in $\boldsymbol{\rho}_\alpha\otimes\boldsymbol{\rho}_{\alpha;\mu}^T$.

Greek indices α, β, etc., at the beginning of the alphabet refer to masses or reduced masses and run from 1 to n (for vectors like $\mathbf{r}_{s\alpha}$) or from 1 to $n-1$ (for vectors like $\boldsymbol{\rho}_{s\alpha}$); there is no summation implied on these mass indices. For all other types of indices, a repeated index is

summed over, although sometimes an explicit summation sign is provided for clarity.

Greek indices μ, ν, etc., in the middle of the alphabet refer to shape coordinates and run from 1 to $3n-6$. These indices are always positioned as superscripts or subscripts to indicate contravariant or covariant transformation laws, respectively, under changes of shape coordinates, and indices are raised and lowered with the shape-space metric $g_{\mu\nu}$.

Latin indices i, j, etc., in the middle of the alphabet run from 1 to 3, and refer to the components of Cartesian vectors in three-dimensional space, such as $r_{\alpha i}$. The superscript or subscript position of such indices is not significant, since only orthogonal transformations on $\mathbb{R}^3$ are of interest. The same Latin indices are used for the components of vectors and tensors involving angular quantities, such as $\boldsymbol{\omega}$, $\mathbf{L}$, M, or $\mathbf{A}_\mu$. In such cases the basis with respect to which the components are referred is really a basis in the Lie algebra of the rotation group SO(3) or its dual, rather than a Cartesian basis in the single-particle configuration space $\mathbb{R}^3$. This distinction is not large from a notational standpoint, but for angular vectors and tensors we do, in fact, usually place indices in contravariant or covariant positions to indicate the distinction between the Lie algebra and its dual, treating the moment-of-inertia tensor as a metric. However, since we consider only orthogonal transformations on such indices, the superscript or subscript position of the indices can be safely ignored.

Latin indices a, b, etc., at the beginning of the alphabet run from 1 to $3n-3$ and are used to index coordinates on the (translation-reduced) configuration space. The contravariant or covariant position of such indices is always respected, and indices are raised and lowered with the metric G_{ab}.

In this paper, we generally view rotation operators, in a coordinatefree sense, in an active manner, as for example the operator that maps the reference orientation of a system of particles into some actual orientation. In the process, we imagine an old frame (such as the space frame) being actively rotated into a new frame (such as the body frame). When we represent the rotation operator by a matrix, we use the matrix elements of the operator with respect to the old frame. This convention gives formulas such as Eq. (3.39), in which the body components of a vector are mapped by the rotation matrix into the space components (in the opposite order suggested by the action of the operators). By this convention two successive rotations, number 1 first and number 2 second, produce the rotation matrix $\mathsf{R}_2\mathsf{R}_1$. Similar conventions apply when we perform a gauge transformation, in which an old body frame is mapped by some rotation operator into a new body frame; thus, in Eq. (3.42), the matrix S contains the components of the rotation operator with respect to the old body frame.

We use comma notation for derivatives, e.g.,

$$\mathbf{A}_{\mu,\nu}=\frac{\partial \mathbf{A}_\mu}{\partial q^\nu}, \tag{A1}$$

and semicolons for covariant derivatives, as illustrated in Eq. (4.78) and as discussed in Appendix D. The comma notation is generalized in the case of anholonomic frames, as explained in Appendix E.

We use square brackets in subscripts to indicate complete antisymmetrization. For example, if $T_{\mu\nu}$ is a (hypothetical) second-rank tensor, then

$$T_{[\mu\nu]}=T_{\mu\nu}-T_{\nu\mu}. \tag{A2}$$

Similarly, if $T_{\mu\nu\sigma}$ is a third-rank tensor, then $T_{[\mu\nu\sigma]}$ is the tensor obtained by summing over all 3! permutations of indices, weighting by the parity of the permutations. Thus, in the common case in which $T_{\mu\nu\sigma}$ is antisymmetric in two indices, say, μ,ν, the equation $T_{[\mu\nu\sigma]}=0$ is equivalent to

$$T_{\mu\nu\sigma}+T_{\nu\sigma\mu}+T_{\sigma\mu\nu}=0. \tag{A3}$$

APPENDIX B: FORMULAS AND NOTATION REGARDING THE ROTATION GROUP SO(3)

The Lie algebra of SO(3) consists of 3×3 antisymmetric matrices, which can be placed in one-to-one correspondence with 3-vectors. If $\mathbf{V}$ is any such vector (in boldface), the associated matrix V (in sans serif) is defined by

$$\mathsf{V}\mathbf{k}=\mathbf{V}\times\mathbf{k}, \tag{B1}$$

for an arbitrary vector $\mathbf{k}$. Equivalently, we have

$$V_i=-\tfrac{1}{2}\epsilon_{ijk}\mathsf{V}_{jk}, \quad \mathsf{V}_{ij}=-\epsilon_{ijk}V_k \tag{B2}$$

or

$$\mathbf{V}=\begin{pmatrix} V_1\\ V_2\\ V_3\end{pmatrix}, \quad \mathsf{V}=\begin{pmatrix} 0 & -V_3 & V_2\\ V_3 & 0 & -V_1\\ -V_2 & V_1 & 0\end{pmatrix}. \tag{B3}$$

We denote this association by writing

$$\mathbf{V}\leftrightarrow\mathsf{V}. \tag{B4}$$

This association transforms under rotations according to

$$\mathsf{Q}\mathbf{V}\leftrightarrow\mathsf{Q}\mathsf{V}\mathsf{Q}^T, \tag{B5}$$

where Q is any proper rotation matrix. Another useful property is that if we have two antisymmetric matrices V and W corresponding to vectors $\mathbf{V}$ and $\mathbf{W}$, respectively, then

$$[\mathsf{V},\mathsf{W}]\leftrightarrow\mathbf{V}\times\mathbf{W}. \tag{B6}$$

In this paper we avoid the explicit use of Euler angles as much as possible, but if an explicit convention is called for, we write

$$\mathsf{R}=\mathsf{R}_z(\alpha)\mathsf{R}_y(\beta)\mathsf{R}_z(\gamma), \tag{B7}$$

where the Euler angles are (α,β,γ), where all rotations are interpreted in an active sense, and where the subscripts indicate an axis, e.g., $\mathsf{R}_z(\alpha)$ is a rotation about the z axis by an angle of α. With these conventions, the relation between the body components of the angular velocity and the Euler angles themselves is given by

$$\begin{pmatrix}\omega_1\\ \omega_2\\ \omega_3\end{pmatrix}=\begin{pmatrix}-\sin\beta\cos\gamma & \sin\gamma & 0\\ \sin\beta\sin\gamma & \cos\gamma & 0\\ \cos\beta & 0 & 1\end{pmatrix}\begin{pmatrix}\dot\alpha\\ \dot\beta\\ \dot\gamma\end{pmatrix}. \tag{B8}$$

The components of the matrix shown are the quantities $\Lambda^{(i)}{}_j$ defined in Eq. (4.33), with i labeling the rows, j the columns. We note that

$$\det\Lambda=-\sin\beta, \tag{B9}$$

which gives us a quantity closely related to the Haar measure on the group.

APPENDIX C: LAGRANGIAN AND HAMILTONIAN MECHANICS IN ANHOLONOMIC FRAMES

Consider a configuration space of dimensionality n, on which coordinates x^μ are imposed. Let $L(x^\mu,\dot x^\mu)$ be a Lagrangian.

The velocity $\dot x^\mu$ is a contravariant vector, defined at each point along a trajectory. We suppose we are given a set of n contravariant vector fields $(X^\mu_{(1)},\ldots,X^\mu_{(n)})$, which are linearly independent at each point in some region of interest. These vector fields constitute a *vielbein* or *anholonomic frame*. The parentheses around the lower index of $X^\mu_{(\alpha)}$ are a reminder that this index labels the vector fields and is not a component index. The upper index is the usual contravariant index. Since the members of the *vielbein* are linearly independent, an arbitrary contravariant vector, such as $\dot x^\mu$, can be represented as a linear combination of them,

$$\dot x^\mu=v^\alpha X^\mu_{(\alpha)}, \tag{C1}$$

where the v^α are the expansion coefficients and where the fields $X^\mu_{(\alpha)}$ are evaluated at the point where $\dot x^\mu$ is measured. The v^α are the components of the velocity with respect to the *vielbein*, i.e., they are the anholonomic components of the velocity.

We solve Eq. (C1) for v^α,

$$v^\alpha=\Lambda^{(\alpha)}_\mu\dot x^\mu, \tag{C2}$$

where $\Lambda^{(\alpha)}_\mu$ forms a matrix in $(\alpha\mu)$ that is inverse to $X^\mu_{(\alpha)}$

$$\Lambda^{(\alpha)}_\mu X^\mu_{(\beta)}=\delta^\alpha_\beta,\quad X^\mu_{(\alpha)}\Lambda^{(\alpha)}_\nu=\delta^\mu_\nu. \tag{C3}$$

We regard $\Lambda^{(\alpha)}_\mu$ as constituting a set of n linearly independent covariant vector (covector) fields, $(\Lambda^{(1)}_\mu,\ldots,\Lambda^{(n)}_\mu)$, in terms of which an arbitrary covector can be expanded. These fields constitute the *dual basis* (dual to the *vielbein*). For example, the canonical momentum $p_\mu=\partial L/\partial\dot x^\mu$ is a covector, and we write

$$p_\mu=\pi_\alpha\Lambda^{(\alpha)}_\mu, \tag{C4}$$

where the expansion coefficients π_α are regarded as the anholonomic components of the momentum or components with respect to the dual basis.

Under a coordinate transformation, the velocity $\dot x^\mu$ transforms as a contravariant vector,

$$\dot x^\mu=\frac{\partial x^\mu}{\partial x'^\nu}\dot x'^\nu, \tag{C5}$$

as do the elements of the *vielbein*,

$$X^\mu_{(\alpha)}=\frac{\partial x^\mu}{\partial x'^\nu}X'^\nu_{(\alpha)}. \tag{C6}$$

These are consistent with Eq. (C1) only if the v^α do not change. This is correct: the components v^α are associated with the *vielbein* itself, not with any coordinate system.

On the other hand, there may exist a coordinate system, say x'^μ, for which $X'^\mu_{(\alpha)}=\delta^\mu_\alpha$, so that $v^\alpha=\dot x'^\alpha$. In this case, the *vielbein* is said to be a *coordinate basis*. In a given coordinate system it may not be obvious whether a given *vielbein* is a coordinate basis, i.e., whether a coordinate transformation $x^\mu\to x'^\mu$ exists such that $X'^\mu_{(\alpha)}=\delta^\mu_\alpha$. According to a basic theorem of differential geometry, however, the *vielbein* is a coordinate basis if and only if the Lie brackets among themselves of the vector fields constituting the vielbein vanish, i.e.,

$$[X_{(\alpha)},X_{(\beta)}]=0, \tag{C7}$$

for $\alpha,\beta=1,\ldots,n$. The Lie bracket of any two contravariant vector fields X^μ and Y^μ is another such vector field, defined by

$$[X,Y]^\mu=X^\nu\frac{\partial Y^\mu}{\partial x^\nu}-Y^\nu\frac{\partial X^\mu}{\partial x^\nu}. \tag{C8}$$

Whether or not the Lie brackets among themselves of the members of the *vielbein* vanish, they are certainly contravariant vector fields and as such can be represented as linear combinations of the members of the *vielbein*. That is, we can write

$$[X_{(\alpha)},X_{(\beta)}]=c^\gamma_{\alpha\beta}X_{(\gamma)}. \tag{C9}$$

The expansion coefficients $c^\gamma_{\alpha\beta}$ are the *structure constants* associated with the *vielbein*. They are not really constants and in general are functions of position x^μ.

Certain differential geometric notation is useful for subsequent developments. We let X^μ and Y^μ be contravariant vector fields, A_μ be a covariant vector field, and $B_{\mu\nu}$ be a covariant tensor field. We regard A_μ as an operator that acts on contravariant vector fields, and $B_{\mu\nu}$ as an operator that acts on pairs of such vector fields, defined by

$$A(X)=A_\mu X^\mu,\quad B(X,Y)=B_{\mu\nu}X^\mu Y^\nu. \tag{C10}$$

In particular, for the members of a *vielbein* and its dual basis, we have

$$\Lambda^{(\alpha)}(X_{(\beta)})=\delta^\alpha_\beta. \tag{C11}$$

We also write dA for the exterior derivative of A_μ, a second-rank, antisymmetric, covariant tensor defined by

$$(dA)_{\mu\nu}=\frac{\partial A_\nu}{\partial x^\mu}-\frac{\partial A_\mu}{\partial x^\nu}. \tag{C12}$$

The d in dA does not indicate anything infinitesimal.

With this notation, we have the following useful identity concerning a *vielbein* and its dual basis:

$$d\Lambda^{(\alpha)}(X_{(\beta)},X_{(\gamma)})=-\Lambda^{(\alpha)}([X_{(\beta)},X_{(\gamma)}])=-c^{\alpha}_{\beta\gamma}. \tag{C13}$$

The proof is straightforward; we write out the left-hand side in components and use the derivatives of Eqs. (C3) to shift derivatives from the $\Lambda^{(\alpha)}$ to the $X_{(\alpha)}$:

$$\begin{aligned} d\Lambda^{(\alpha)}(X_{(\beta)},X_{(\gamma)}) &= (\Lambda^{(\alpha)}_{\nu,\mu}-\Lambda^{(\alpha)}_{\mu,\nu})X^{\mu}_{(\beta)}X^{\nu}_{(\gamma)} \\ &= -\Lambda^{(\alpha)}_{\nu}X^{\mu}_{(\beta)}X^{\nu}_{(\gamma),\mu} \\ &\quad +\Lambda^{(\alpha)}_{\mu}X^{\mu}_{(\beta),\nu}X^{\nu}_{(\gamma)} \\ &= -\Lambda^{(\alpha)}([X_{(\beta)},X_{(\gamma)}]) \\ &= -c^{\sigma}_{\beta\gamma}\Lambda^{(\alpha)}(X_{(\sigma)})=-c^{\alpha}_{\beta\gamma}. \end{aligned} \tag{C14}$$

We now transform the Lagrangian from the coordinate-based velocity components $\dot{x}^{\mu}$ to the *vielbein* components v^{α},

$$L(x^{\mu},\dot{x}^{\mu})=\overline{L}(x^{\mu},v^{\alpha}), \tag{C15}$$

where we put an overbar on $\overline{L}$ to indicate the new independent variables. Our object is to express the Euler-Lagrange equations purely in terms of the *vielbein* quantities v^{α}, π_{α}, without reference to the coordinate-based quantities $\dot{x}^{\mu}$, p_{μ}. First we note that

$$p_{\mu}=\frac{\partial L}{\partial\dot{x}^{\mu}}=\frac{\partial\overline{L}}{\partial v^{\alpha}}\frac{\partial v^{\alpha}}{\partial\dot{x}^{\mu}}=\Lambda^{(\alpha)}_{\mu}\frac{\partial\overline{L}}{\partial v^{\alpha}}. \tag{C16}$$

But by Eq. (C4), this implies

$$\pi_{\alpha}=\frac{\partial\overline{L}}{\partial v^{\alpha}}. \tag{C17}$$

Next, to obtain the Euler-Lagrange equations in *vielbein* form, we differentiate Eq. (C4) and use the usual Euler-Lagrange equations,

$$\begin{aligned} \dot{p}_{\mu} &= \dot{\pi}_{\alpha}\Lambda^{(\alpha)}_{\mu}+\pi_{\alpha}\Lambda^{(\alpha)}_{\mu,\nu}\dot{x}^{\nu} \\ &= \frac{\partial L}{\partial x^{\mu}}=\frac{\partial\overline{L}}{\partial x^{\mu}}+\frac{\partial\overline{L}}{\partial v^{\alpha}}\frac{\partial v^{\alpha}}{\partial x^{\mu}}=\frac{\partial\overline{L}}{\partial x^{\mu}}+\pi_{\alpha}\Lambda^{(\alpha)}_{\nu,\mu}\dot{x}^{\nu}. \end{aligned} \tag{C18}$$

In this we use Eq. (C1) to eliminate $\dot{x}^{\nu}$ in favor of v^{β}, we multiply through by $X^{\mu}_{(\gamma)}$ to solve for $\dot{\pi}_{\alpha}$, and we use Eqs. (C12) and (C13) to write the result in terms of the structure constants. Finally, juggling indices, we have

$$\dot{\pi}_{\alpha}=X^{\mu}_{(\alpha)}\frac{\partial\overline{L}}{\partial x^{\mu}}-c^{\gamma}_{\alpha\beta}v^{\beta}\pi_{\gamma}. \tag{C19}$$

These, combined with Eq. (C17), are the anholonomic versions of the Euler-Lagrange equations. The first term on the right-hand side of Eq. (C19) is just the covector $\partial\overline{L}/\partial x^{\mu}$, expressed in terms of the dual basis, but the second term, containing the structure constants, has no analog in a coordinate basis.

Now we convert Hamiltonian mechanics to an anholonomic basis. We first express the definition of the Hamiltonian in terms of the *vielbein* quantities v^{α}, π_{α},

$$H=p_{\mu}\dot{x}^{\mu}-L(x^{\mu},\dot{x}^{\mu})=\pi_{\alpha}v^{\alpha}-\overline{L}(x^{\mu},v^{\alpha}), \tag{C20}$$

and then we think of the Hamiltonian as a function of (x^{μ},π_{α}) instead of the usual (x^{μ},p_{μ}). The Hamiltonian is the same as the usual one, but is expressed in terms of the noncanonical variables (x^{μ},π_{α}). Therefore Hamilton's equations in the usual sense cannot be used.

Instead, we must work with Poisson brackets. The Poisson bracket is the usual one,

$$\{f,g\}=\frac{\partial f}{\partial x^{\mu}}\frac{\partial g}{\partial p_{\mu}}-\frac{\partial f}{\partial p_{\mu}}\frac{\partial g}{\partial x^{\mu}}, \tag{C21}$$

but we must express everything in terms of (x^{μ},π_{α}). For example, for the Poisson brackets of the coordinates among themselves, we find

$$\{x^{\mu},x^{\nu}\}=0,\quad \{x^{\mu},\pi_{\alpha}\}=X^{\mu}_{(\alpha)},\quad \{\pi_{\alpha},\pi_{\beta}\}=-c^{\gamma}_{\alpha\beta}\pi_{\gamma}, \tag{C22}$$

where the final bracket requires a short calculation. Given these, the Poisson bracket of any two functions can be expressed purely in terms of the coordinates (x^{μ},π_{α}). We simply use the chain rule property of Poisson brackets, so that

$$\begin{aligned} \{f,g\} &= \frac{\partial f}{\partial x^{\mu}}\{x^{\mu},x^{\nu}\}\frac{\partial g}{\partial x^{\nu}}+\frac{\partial f}{\partial x^{\mu}}\{x^{\mu},\pi_{\alpha}\}\frac{\partial g}{\partial\pi_{\alpha}} \\ &\quad +\frac{\partial f}{\partial\pi_{\alpha}}\{\pi_{\alpha},x^{\mu}\}\frac{\partial g}{\partial x^{\mu}}+\frac{\partial f}{\partial\pi_{\alpha}}\{\pi_{\alpha},\pi_{\beta}\}\frac{\partial g}{\partial\pi_{\beta}} \end{aligned} \tag{C23}$$

or

$$\{f,g\}=X^{\mu}_{(\alpha)}\left(\frac{\partial f}{\partial x^{\mu}}\frac{\partial g}{\partial\pi_{\alpha}}-\frac{\partial f}{\partial\pi_{\alpha}}\frac{\partial g}{\partial x^{\mu}}\right)-c^{\gamma}_{\alpha\beta}\pi_{\gamma}\frac{\partial f}{\partial\pi_{\alpha}}\frac{\partial g}{\partial\pi_{\beta}}. \tag{C24}$$

In particular, we can put Hamilton's equations into Poisson bracket form, $\dot{x}^{\mu}=\{x^{\mu},H\}$, $\dot{\pi}_{\alpha}=\{\pi_{\alpha},H\}$, or

$$\dot{x}^{\mu}=X^{\mu}_{(\alpha)}\frac{\partial H}{\partial\pi_{\alpha}}, \tag{C25}$$

$$\dot{\pi}_{\alpha}=-X^{\mu}_{(\alpha)}\frac{\partial H}{\partial x^{\mu}}-c^{\gamma}_{\alpha\beta}\pi_{\gamma}\frac{\partial H}{\partial\pi_{\beta}}. \tag{C26}$$

The first of these can be transformed to the *vielbein* basis, whereupon it becomes

$$v^{\alpha}=\frac{\partial H}{\partial\pi_{\alpha}}. \tag{C27}$$

APPENDIX D: COVARIANT DERIVATIVES

In this Appendix we explain the geometrical meaning of covariant derivatives of tensors with R indices, and then we give rules for forming covariant derivatives in general. We assume a familiarity with covariant derivatives in the differential geometry of Riemannian manifolds, and we only emphasize the properties that are new from the standpoint of this background.

Covariant derivatives of tensors or tensor fields with R indices are illustrated in Eqs. (4.70) and (4.78). The

geometrical meaning of such covariant derivatives is based on the notion of a *parallel-transported* body frame, which can be explained as follows. Suppose we have a motion $q^\mu(t)$ taking place in shape space with $\mathbf{L}=0$, and suppose body frames are defined as a field over shape space in the usual manner. Then by Eq. (3.58) we have $\boldsymbol{\omega}=-\mathbf{A}_\mu\dot{q}^\mu$. But since $\boldsymbol{\omega}$ is not gauge invariant, we ask whether it can be transformed away by a redefinition of body frames. We make this redefinition, not as a field over shape space, but only as a function of time along the given orbit $q^\mu(t)$. Therefore the orthogonal matrix S which maps the old body frame to the new one is a function only of t, not (as elsewhere in the paper) of q^μ. Instead of Eq. (3.72) we have $\Omega=\mathsf{S}\Omega'\mathsf{S}^T+\mathsf{S}\dot{\mathsf{S}}^T$, or, since $\Omega=-\mathsf{A}_\mu\dot{q}^\mu$ and $\Omega'=0$, we obtain $\dot{\mathsf{S}}=(\mathsf{A}_\mu\dot{q}^\mu)\mathsf{S}$. The solution is a path-ordered exponential,

$$\mathsf{S}(t)=\left[P\exp\int_{q_0}^{q(t)}\mathsf{A}_\mu dq^\mu\right]\mathsf{S}_0. \tag{D1}$$

Although this equation does define the required S as a function of t along the given orbit, it cannot be used to define S as a field over shape space [say, by regarding the end point $q(t)$ as a variable, with curves joining it to some fixed initial point q_0], because the path-ordered exponential is path dependent. The new body frame, related to the old one along the curve by $\mathsf{S}(t)$, is the parallel-transported body frame. We may wish to choose $\mathsf{S}_0=\mathsf{I}$, so that the parallel-transported frame and the original frame are identical at the initial point.

As explained below, Eq. (4.71), the ordinary time derivative of a vector such as $\mathbf{L}$, is not gauge covariant, because $L(t_0+dt)$ and $L(t_0)$ are referred to two different body frames at points q_0^μ and $q_0^\mu+dq^\mu$. But if we refer the angular momentum at time t_0+dt to the body frame that is parallel transported from q^μ to $q^\mu+dq^\mu$, then the limit gives a gauge-covariant result. That is, we solve Eq. (D1) over an infinitesimal segment with $\mathsf{S}_0=\mathsf{S}(t_0)=\mathsf{I}$ at q_0^μ, so that

$$\mathsf{S}(t_0+dt)=\mathsf{I}+\mathsf{A}_\mu dq^\mu. \tag{D2}$$

Then, using a prime to denote components with respect to the new (parallel-transported) frame, as in Eq. (3.67), we have

$$\begin{aligned}\mathbf{L}'(t+dt)&=\mathsf{S}(t+dt)^T\mathbf{L}(t+dt)\\&=\mathbf{L}(t)+dt\left(\frac{d\mathbf{L}}{dt}-\mathsf{A}_\mu\mathbf{L}\right).\end{aligned} \tag{D3}$$

Finally, the covariant time derivative is defined by

$$\frac{D\mathbf{L}}{Dt}=\frac{\mathbf{L}'(t+dt)-\mathbf{L}(t)}{dt}=\frac{d\mathbf{L}}{dt}-\mathbf{A}_\mu\times\mathbf{L}. \tag{D4}$$

Similarly, we can modify the directional derivative of a tensor field over shape space, such as in Eq. (4.79), by evaluating the field at the displaced point with respect to the parallel-transported frame. This produces a directional covariant derivative; for example, Eq. (4.79) becomes

$$\lim_{\epsilon\to0}\frac{1}{\epsilon}[\mathsf{M}'^{-1}(q^\mu+\epsilon\xi^\mu)-\mathsf{M}^{-1}(q^\mu)]=\xi^\mu\mathsf{M}^{-1}_{;\mu}, \tag{D5}$$

where again the prime indicates components with respect to the parallel-transported frame.

These considerations suffice to define the covariant derivative in general and lead to the following rules. First, if a tensor field over shape space has only q indices (no R indices), then the covariant derivative is formed in the usual way in Riemannian geometry, with one correction term involving the Christoffel symbols for each q index. If a tensor field over shape space has only R indices (no q indices), then the covariant derivative is equal to the ordinary derivative plus one correction term, involving A_μ or $\mathbf{A}_\mu$, for each R index. An example will show the pattern. If F_{ijk} is a (hypothetical) third-rank true R tensor over shape space, then

$$F_{ijk;\mu}=F_{ijk,\mu}-\mathsf{A}_{\mu i\ell}F_{\ell jk}-\mathsf{A}_{\mu j\ell}F_{i\ell k}-\mathsf{A}_{\mu k\ell}F_{ij\ell}, \tag{D6}$$

where $\mathsf{A}_{\mu ij}$ are the components of the antisymmetric matrix A_μ. It does not matter whether the R indices are upper or lower (contravariant or covariant), since our gauge transformations are always represented by orthogonal transformations.

For example, the covariant derivative of an object with no indices (a true scalar) has no correction terms and is identical to the ordinary derivative. Thus, the gradient of the potential seen in the equations of motion (4.77) is a covariant derivative, $V_{,\mu}=V_{;\mu}$. Next, in the case of a vector field over shape space, say $\mathbf{X}=\mathbf{X}(q)$, we have $X_{i;\mu}=X_{i,\mu}-\mathsf{A}_{\mu ij}X_j$ or

$$\mathbf{X}_{;\mu}=\mathbf{X}_{,\mu}-\mathbf{A}_\mu\times\mathbf{X}. \tag{D7}$$

In the case of a second-rank tensor field, say, $\mathsf{F}=\mathsf{F}(q)$, we have

$$\mathsf{F}_{ij;\mu}=\mathsf{F}_{ij,\mu}-\mathsf{A}_{\mu ik}\mathsf{F}_{kj}-\mathsf{A}_{\mu jk}\mathsf{F}_{ik}, \tag{D8}$$

or

$$\mathsf{F}_{;\mu}=\mathsf{F}_{,\mu}-[\mathsf{A}_\mu,\mathsf{F}]. \tag{D9}$$

We discovered a special case of this formula, with $\mathsf{F}=\mathsf{M}^{-1}$, in deriving the equations of motion, but the same formula applies to any second-rank tensor field (the symmetry of M^{-1} does not matter).

If a tensor field has both R indices and q indices, then the covariant derivative has one correction term with A_μ for each R index and one with $\Gamma^\mu_{\sigma\tau}$ for each q index. For example, the covariant derivative of the Coriolis tensor is

$$\mathbf{B}_{\mu\nu;\sigma}=\mathbf{B}_{\mu\nu,\sigma}-\mathbf{A}_\sigma\times\mathbf{B}_{\mu\nu}-\Gamma^\tau_{\sigma\mu}\mathbf{B}_{\tau\nu}-\Gamma^\tau_{\sigma\nu}\mathbf{B}_{\mu\tau}. \tag{D10}$$

If a tensor is defined not as a field over shape space, but only as a function of time along an orbit $q^\mu(t)$, then the covariant time derivative D/Dt is equal to the ordinary time derivative plus one correction term in A_μ for each R index and one in $\Gamma^\mu_{\sigma\tau}$ for each q index, in which the lower index on A_μ or one of the lower indices on $\Gamma^\mu_{\sigma\tau}$ is contracted with $\dot{q}^\mu$. These rules are illustrated by Eqs. (4.70) and (4.72).

The covariant derivative of a tensor product or contraction obeys the Leibnitz rule. For example,

$$(\mathsf{M}_{ij}B^{j}_{\mu\nu})_{;\sigma}=\mathsf{M}_{ij;\sigma}B^{j}_{\mu\nu}+\mathsf{M}_{ij}B^{j}_{\mu\nu;\sigma}. \tag{D11}$$

In particular, since the covariant derivative of the metric tensor $g_{\mu\nu}$ vanishes, the formation of covariant derivatives commutes with the raising and lowering of indices.

Further rules are the following. The covariant derivative of the identity tensor vanishes, $\mathsf{I}_{;\mu}=0$, as does the covariant derivative of the Levi-Civita tensor, $\epsilon_{ijk;\mu}=0$. The covariant derivative commutes with the operator $\leftrightarrow$, so that if $\mathsf{V}\leftrightarrow\mathbf{V}$, then

$$\mathsf{V}_{;\mu}\leftrightarrow\mathbf{V}_{;\mu}. \tag{D12}$$

Multiple covariant derivatives do not commute, but their commutator involves the Coriolis curvature tensor or the Riemann curvature tensor. For example, let $\mathbf{X}$ be a vector field (one R index), T be a second-rank tensor field (two R indices), and $\mathbf{Y}_{\mu}$ a tensor with one R index and one covariant q index. Then we have

$$\mathbf{X}_{;[\mu\nu]}=\mathbf{B}_{\mu\nu}\times\mathbf{X}, \tag{D13}$$

$$\mathsf{T}_{;[\mu\nu]}=[\mathsf{B}_{\mu\nu},\mathsf{T}], \tag{D14}$$

$$\mathbf{Y}_{\mu;[\nu\sigma]}=\mathbf{B}_{\nu\sigma}\times\mathbf{Y}_{\mu}+R^{\tau}{}_{\mu\nu\sigma}\mathbf{Y}_{\tau}, \tag{D15}$$

where the $R^{\tau}{}_{\mu\nu\sigma}$ is the Riemann tensor, defined in Eq. (E1).

APPENDIX E: THE RIEMANN TENSOR

In this appendix we summarize our conventions for the Riemann tensor and we present the principal equations satisfied by it. We do this first in a coordinate basis and then in an anholonomic basis. In all of this we follow the conventions of Misner, Thorne, and Wheeler (1973), although in this paper we are interested in metrics that are positive definite, and those authors are interested in the indefinite metric of relativity theory.

We begin with some Riemannian manifold with metric $g_{\mu\nu}$ upon which coordinates x^{μ} are imposed. In the applications of interest to this paper, the manifold could be either the (translation-reduced) configuration space or shape space. The Christoffel symbols are defined as in Eq. (4.73); in terms of them, the Riemann tensor is defined by

$$R^{\mu}{}_{\nu\sigma\tau}=\Gamma^{\mu}_{\tau\nu,\sigma}-\Gamma^{\mu}_{\sigma\nu,\tau}+\Gamma^{\mu}_{\sigma\kappa}\Gamma^{\kappa}_{\tau\nu}-\Gamma^{\mu}_{\tau\kappa}\Gamma^{\kappa}_{\sigma\nu}. \tag{E1}$$

The Riemann tensor satisfies the symmetry relations

$$R_{\mu\nu\sigma\tau}=R_{\sigma\tau\mu\nu}, \tag{E2}$$

$$R_{\mu\nu\sigma\tau}=-R_{\nu\mu\sigma\tau}=-R_{\mu\nu\tau\sigma}=+R_{\nu\mu\tau\sigma}, \tag{E3}$$

$$R_{\mu[\nu\sigma\tau]}=0. \tag{E4}$$

Finally, it satisfies the Bianchi identity,

$$R_{\mu\nu[\sigma\tau;\kappa]}=0. \tag{E5}$$

The Ricci tensor is defined by

$$R_{\mu\nu}=R^{\sigma}{}_{\mu\sigma\nu}=R_{\nu\mu}, \tag{E6}$$

and the curvature scalar by

$$R=R^{\mu}{}_{\mu}. \tag{E7}$$

All of the above formulas refer to the coordinate basis x^{μ}. We also need equivalents of these formulas in an anholonomic basis. We let the anholonomic basis of vector fields be $e_{\bar{\mu}}$ with coordinate basis components $e^{\nu}_{\bar{\mu}}$, where anholonomic indices are indicated by an overbar (the analog of the parenthesized indices used elsewhere in the paper). Thus the structure constants are defined by

$$[e_{\bar{\mu}},e_{\bar{\nu}}]=c^{\bar{\tau}}_{\bar{\mu}\bar{\nu}}e_{\bar{\tau}}. \tag{E8}$$

The dual basis of covectors or forms is $\sigma^{\bar{\mu}}$ with coordinate basis components $\sigma^{\bar{\mu}}_{\nu}$ so that

$$\sigma^{\bar{\mu}}(e_{\bar{\nu}})=\delta^{\mu}_{\nu}. \tag{E9}$$

We extend the comma notation to anholonomic indices to indicate the action of the basis vectors, regarded as differential operators. For example, we set

$$S_{,\bar{\mu}}=e_{\bar{\mu}}S=e^{\nu}_{\bar{\mu}}\frac{\partial S}{\partial x^{\nu}}. \tag{E10}$$

The components of the connection (anholonomic equivalents of the Christoffel symbols) are defined by

$$\nabla_{\bar{\mu}}e_{\bar{\nu}}=\Gamma^{\bar{\tau}}_{\bar{\nu}\bar{\mu}}e_{\bar{\tau}}, \tag{E11}$$

where ∇_X is the directional covariant derivative along vector field X, and where $\nabla_{\bar{\mu}}$ is the directional covariant derivative along basis vector $e_{\bar{\mu}}$. An equivalent formula is

$$\nabla_{\bar{\mu}}\sigma^{\bar{\tau}}=-\Gamma^{\bar{\tau}}_{\bar{\nu}\bar{\mu}}\sigma^{\bar{\nu}}. \tag{E12}$$

From these one can express the components of the connection in terms of the anholonomic components of the metric and the structure constants; the result is

$$\Gamma^{\bar{\tau}}_{\bar{\nu}\bar{\mu}}=\tfrac{1}{2}g^{\bar{\tau}\bar{\kappa}}(g_{\bar{\kappa}\bar{\nu},\bar{\mu}}+g_{\bar{\kappa}\bar{\mu},\bar{\nu}}-g_{\bar{\mu}\bar{\nu},\bar{\kappa}}+g_{\bar{\nu}\bar{\lambda}}c^{\bar{\lambda}}_{\bar{\kappa}\bar{\mu}}+g_{\bar{\mu}\bar{\lambda}}c^{\bar{\lambda}}_{\bar{\kappa}\bar{\nu}}+g_{\bar{\kappa}\bar{\lambda}}c^{\bar{\lambda}}_{\bar{\mu}\bar{\nu}}). \tag{E13}$$

We note that in an anholonomic basis Γ is not necessarily symmetric in the lower two indices.

The covariant components of vectors and covectors are given by

$$X^{\bar{\mu}}{}_{;\bar{\nu}}=X^{\bar{\mu}}{}_{,\bar{\nu}}+\Gamma^{\bar{\mu}}_{\bar{\tau}\bar{\nu}}X^{\bar{\tau}}, \tag{E14}$$

$$A_{\bar{\mu};\bar{\nu}}=A_{\bar{\mu},\bar{\nu}}-\Gamma^{\bar{\tau}}_{\bar{\mu}\bar{\nu}}A_{\bar{\tau}}, \tag{E15}$$

which make the rules for tensors of other ranks clear. These are the same formulas as in a coordinate basis, except for the care which must be exercised in the positioning of the lower two indices of Γ.

Finally, the Riemann tensor itself is given by

$$R^{\bar{\mu}}{}_{\bar{\nu}\bar{\sigma}\bar{\tau}}=\Gamma^{\bar{\mu}}_{\bar{\nu}\bar{\tau},\bar{\sigma}}-\Gamma^{\bar{\mu}}_{\bar{\nu}\bar{\sigma},\bar{\tau}}+\Gamma^{\bar{\mu}}_{\bar{\kappa}\bar{\sigma}}\Gamma^{\bar{\kappa}}_{\bar{\nu}\bar{\tau}}-\Gamma^{\bar{\mu}}_{\bar{\kappa}\bar{\tau}}\Gamma^{\bar{\kappa}}_{\bar{\nu}\bar{\sigma}}-c^{\bar{\kappa}}_{\bar{\sigma}\bar{\tau}}\Gamma^{\bar{\mu}}_{\bar{\nu}\bar{\kappa}}, \tag{E16}$$

which differs from the coordinate basis formula (E1) by the presence of the final term and the care that must be exercised in the positioning of the lower two indices of Γ.

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