Body frames and frame singularities for three-atom systems

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The subject of body frames and their singularities for three-particle systems is important not only for large-amplitude rovibrational coupling in molecular spectroscopy, but also for reactive scattering calculations. This paper presents a geometrical analysis of the meaning of body frame conventions and their singularities in three-particle systems. Special attention is devoted to the principal axis frame, a certain version of the Eckart frame, and the topological inevitability of frame singularities. The emphasis is on a geometrical picture, which is intended as a preliminary study for the more difficult case of four-particle systems, where one must work in higher-dimensional spaces. The analysis makes extensive use of kinematic rotations. [S1050-2947(98)06811-5]

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I. INTRODUCTION

This paper is a part of a study of body frame singularities in the quantum dynamics of n-particle systems. As is well known, it is necessary to establish a convention for a body frame before transforming the Hamiltonian for an n-particle system to Euler angles and internal coordinates since the Euler angles are only defined relative to a body frame. After this transformation, the wave function on the internal space becomes a $(2J+1)$-component "spinor," where J is the angular momentum of the system. The process of transforming Hamiltonians in this manner is an old subject [1–3], which has recently been reviewed by us from a gauge-theoretical standpoint [4]. A body frame can be specified in practice by giving the positions of all the particles relative to the body frame as a function of the shape or internal coordinates.

Body frame singularities, the topic of this paper, occur when the positions of the particles in the body frame are nondifferentiable functions of the shape. To be more precise, we will measure the "distance" between two configurations by the mass-weighted, kinetic-energy metric, where it is understood that one or the other of the two configurations is rotated to minimize this distance. This definition of distance coincides with the measure of distance given by the metric tensor on the internal space, as explained in Ref. [4]. Then we will say that the frame is singular when the derivatives of the particle positions in the body frame with respect to distance, as the shape is changed in some continuous manner, is infinite. This definition has the advantage that it is independent of the choice of internal coordinates.

Body frame singularities are important because the wave function on the internal space is singular at the same places in the internal space as the frame singularities. The singularity in the wave function is of the same kind as in the frame; the derivatives of the wave function with respect to (mass-weighted) distance become infinite. Typically one finds that the wave function oscillates infinitely rapidly (that is, over arbitrarily small increments in shape) as some limiting manifold in the internal space is approached. The locations of these singularities in the wave function depend on the convention for the body frame, but they are independent of the potential. Thus the singularities in question occur in the exact solution of the Schrödinger equation as well as in the exact eigenfunctions of the kinetic-energy operator (whose angular parts are the hyperspherical harmonics [5]).

Frame singularities are not the only kind of singularities one will encounter in the internal dynamics of an n-particle system. Recently Pack [16] has given a careful analysis of singularities in three-body scattering calculations, including frame singularities as well as other kinds (those of the centrifugal potential and those due to a choice of coordinate system on the internal space). The work presented in this paper is different in spirit from Pack's and complementary to it. For example, Pack considers the problem of basis set contractions and how these interact with singularities in the Hamiltonian, while this paper deals only with the frame singularities themselves. On the other hand, this paper emphasizes a geometrical picture of frames that we believe is almost entirely new and is especially important for understanding the case $n\geqslant 4$. Another important issue discussed by Pack is the inevitability of frame singularities, regardless of the convention chosen for body frame; in this paper we provide a different perspective on this question, by relating frame singularities in the three-body problem to the well known string singularities that occur in the vector potential for the field of a magnetic monopole.

One of the results of this paper is to show how a version of the Eckart frame gets rid of some of the singularities present in the principal axis frame and in fact produces a configuration of singularities that is minimal, in the sense that no other frame has singularities on a smaller subset of the internal space. We would not want the reader to think, however, that we are necessarily advocating the Eckart frame for any particular approach to practical calculations. In particular, the centrifugal potential energy, which is singular in any frame at the collinear configurations, acquires some unattractive features in the Eckart frame as compared to the principal axis frame, such as off-diagonal terms and an oscillatory dependence on the kinematic angle. These issues have been carefully discussed by Pack [16]. On the other

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hand, it is our point of view that not enough is presently known about the variety of possible techniques that can be applied to three- and more-body problems (direct numerical integration, grid methods, hyperspherical harmonics, wave packets, semiclassical methods, basis set contractions, variational methods, time-dependent methods, etc.) to say that this or that frame will never be important in applications. This is especially true for the case $n \geqslant 4$, about which very little is currently known.

For example, in spite of some considerable work on four-body Hamiltonians [6–9], it appears to us that it has been only recently that a careful and fully accurate description has been given of the ranges of internal coordinates in the internal space [10–13]. Most of these studies of four-body systems have employed the principal axis frame, perhaps because this frame is naturally suggested by the singular-value decomposition of the 3×3 matrix of Jacobi vectors that naturally occurs in such problems. However, in spite of some work explicitly advocating the principal axis frame [14], it does not appear to us that anyone has studied (for $n \geqslant 4$) how the multiple branches of the principal axis frame are connected together, how a single branch may be selected in practice, or where the branch cuts must be placed in the internal space. Nor for that matter has there been any study (again for $n \geqslant 4$) of how the multiple branches and branch cuts of the principal axis frame may be eliminated by means of a frame transformation or what minimum configuration of singularities is possible with an arbitrary frame transformation.

Our purpose is to provide a framework within which general questions regarding body frames and their singularities can be addressed. In the case of the four-body problem, we have succeeded in answering the questions just listed, using a geometrical analysis of curves and surfaces in configuration space and in the internal (or shape) space. However, the four-body problem involves spaces of relatively high dimensionality (for example, the internal or shape space is six dimensional), so there is great advantage in applying our geometrical methods first to the three-body case, in order to fix ideas and form analogies that are useful in understanding the four-body case. In this way, we were led to the geometrical analysis of frames and frame singularities for the three-body problem that is presented in this paper. The reader must understand that many of the features of the three-body problem that are pointed out in this paper are intended not only to provide insight into the three-body problem itself, but also for comparison with the four-body problem. Our work on the four-body problem, which takes advantage of these analogies, is presented in the preceding paper [15].

Section II contains the principal results of this paper. We begin by presenting a geometrical picture of configuration space in the three-body problem and the surfaces that are generated by the action of external rotations and kinematic rotations. Next we discuss the internal or shape space, coordinates on it, and the action of kinematic rotations. Then we discuss the principal axis frame, its multiple branches, and how these are connected together under continuous deformations of shape. We show that there is an intimate connection between kinematic rotations and the principal axis frame and use this to develop the connectivity properties of the latter. Next we present a geometrical picture of the transformation to a version of the Eckart frame, which has been considered previously by Pack [16] and ourselves [4], and we show how this frame eliminates some or all (depending on the number of spatial dimensions) of the singularities present in the principal axis frame. Finally, we discuss parametric forms of the principal axis and Eckart frames and discuss the remaining singularities of the latter. In Sec. III we present some comments and conclusions, including a discussion of the relation between frame singularities and monopole strings, which leads to one way of viewing the topological inevitability of frame singularities.

II. FRAMES IN THE THREE-BODY PROBLEM

In this section we develop a geometrical picture of spaces and frames in the three-body problem, paying special attention to the principal axis frame, its multiple branches and singularities, and its relation to kinematic rotations and to the Eckart frame and its relation to the principal axis frame. We also discuss the inevitable singularities that exist in any choice of frame. Throughout the following discussion we will be thinking primarily of the three-body problem in three-dimensional space, although many of the results will obviously apply to the general n-body problem in three-dimensional space. In places we will make this explicit. At the end of this section we will make some comments on the three-body problem in a plane, which is slightly different from the three-body problem in space.

A. Configuration space and the action of external and kinematic rotations

We begin by establishing some notation for the three-body problem. We write $\mathbf{r}_{s\alpha}$, $\alpha=1,2$, or $\{\mathbf{r}_{s\alpha}\}=(\mathbf{r}_{s1},\mathbf{r}_{s2})$ for the two mass-weighted Jacobi vectors describing the configuration of the three-particle system, referred to the space or inertial frame. We use an s subscript on vectors or tensors referred to the space frame. We define the Jacobi vectors in terms of the laboratory positions of the three particles by requiring that $\mathbf{r}_{s1}$ lie on the line joining particles 1 and 2 and that $\mathbf{r}_{s2}$ lie on the line joining the center of mass of particles 1 and 2 with particle 3. This is the most convenient choice for configurations in the channel $12+3$. The other two standard choices of Jacobi coordinates are related to this one by means of discrete kinematic rotations in the usual way; alternatively, Radau or other choices of coordinates may be made, corresponding to continuous interpolations between the usual discrete kinematic rotations. Formulas relating interatomic distances and bond angles to Jacobi or Radau vectors and further details on coordinates can be found in Ref. [17]. The specific choice of Jacobi coordinates is important when one wishes to connect the values of these coordinates with some physical configuration of the three particles, as seen in the laboratory frame. Otherwise, this choice has little effect on the discussion or conclusions of this paper; the main effect is to cause a rotation about the w_3 axis (defined momentarily) of the physical interpretations that are attached to the points of the internal space.

The configuration space of the three-body system is the space upon which the Jacobi vectors (that is, their six components) are coordinates; this space is $\mathbb{R}^6$. To be more precise, this is the configuration space after the elimination of the center of mass coordinates, which will not be important in the following discussion. We will write Q, Q', etc., for points of this space, so that Q stands for some pair of vectors $(\mathbf{r}_{s1},\mathbf{r}_{s2})$.

A given configuration of the three-atom system may be subjected to a rigid rotation, specified by a proper orthogonal matrix $\mathsf{R}\in SO(3)$. This rotation acts on the Jacobi vectors according to

$$\mathbf{r}'_{s\alpha}=\mathsf{R}\mathbf{r}_{s\alpha}, \quad \alpha=1,2,, \tag{2.1}$$

which we view in the active sense, so that $Q=\{\mathbf{r}_{s\alpha}\}$ is the old configuration and $Q'=\{\mathbf{r}'_{s\alpha}\}$ is the new one. We will sometimes abbreviate this by writing $Q'=RQ$. The notational distinction between R (in italics) and R (in sans serif) is that R represents an element of SO(3), regarded as an abstract group (equivalently, R stands for some choice of Euler angles), while R stands for the corresponding 3×3 matrix. The equation $Q'=RQ$ could be interpreted in terms of matrix multiplication (involving 6×6 matrices), but we prefer to view it in a geometrical sense, in which the point Q is moved by a rotation R to a new point Q', whose Jacobi vectors are given by Eq. (2.1). That is, we think of R as an operator that maps configuration space into itself.

Two configurations will be considered to have the same shape if and only if they are related by a proper rotation as in Eq. (2.1); configurations of the same shape differ only in their orientation. We will sometimes refer to Eq. (2.1) as an *external* rotation, to contrast it with the kinematic rotations introduced momentarily.

If we take a specific configuration Q and act on it by all possible rotations according to Eq. (2.1), then this point sweeps out a surface in configuration space. This surface is the *orbit* of Q under the action of the rotation group, in the mathematical sense of the word ''orbit'' (not to be confused with orbits in the sense of classical mechanics).

This paper makes a modest use of mathematical terminology that may be unfamiliar to some readers. This terminology is explained briefly as it is introduced. A more thorough explanation is provided in Appendixes A and B of Ref. [15].

There are three types of orbits, depending on the configuration Q. First, if Q is a noncollinear configuration, then the orbit of Q can be regarded as a copy of the rotation group manifold SO(3). A more proper way of saying this is to say that the orbit of Q and SO(3) are *diffeomorphic*; this means (roughly) that the two manifolds have the same dimensionality and the same topology and are related by some smooth, one-to-one mapping. To fully appreciate this statement, it helps to have an image of the topology of SO(3), which is explained in Appendix B of Ref. [15]. Next, if Q is a collinear configuration, the orbit is diffeomorphic to the ordinary two-sphere S^2 because rotations about the axis of collinearity have no effect and only the direction of collinearity can be changed. In this case the orbit is two dimensional. Finally, the three-body collision is the one configuration for which the orbit is just a point since rotations have no effect on this configuration. The latter two classes of orbits form a set of measure zero in configuration space; if we exclude them, the rest of the six-dimensional configuration space is decomposed or *foliated* into a three-parameter family of three-dimensional copies of SO(3). The usual Euler angles are coordinates *along* the rotation orbits and the usual internal coordinates are parameters or coordinates *of* the rotation orbits. The noncollinear orbits are also called *fibers*, the standard terminology for them in fiber bundle theory, as explained in Ref. [4]; the space consisting of these fibers (configuration space minus the collinear configurations and the three-body collision) is the *fiber bundle*.

Kinematic rotations play an important role in the theory of the principal axis frame. They are defined by

$$\mathbf{r}'_{s\alpha}=\sum_{\beta=1}^{2} K_{\alpha\beta}(\phi)\mathbf{r}_{s\beta}, \tag{2.2}$$

where the matrix K (with components $K_{\alpha\beta}$) belongs to SO(2),

$$\mathsf{K}=\begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}. \tag{2.3}$$

The group of kinematic rotations, or the *kinematic group* for short, is SO(2) for the three-body problem. Sometimes we will abbreviate Eq. (2.2) by writing $Q'=KQ$ or $Q'(\phi)=K(\phi)Q$. Again, in the abbreviated notation, K is an element of the abstract group SO(2) and K is the corresponding matrix seen in Eq. (2.3). If Q is a specific point of configuration space, then the set of configurations swept out according to Eq. (2.2) as ϕ ranges from 0 to 2π is the orbit of Q under the action of the kinematic group; we will call these *kinematic orbits* and if necessary to avoid confusion we will refer to the earlier orbits generated by Eq. (2.1) as *rotation orbits*. Except when Q is the three-body collision, the kinematic orbits are copies of (diffeomorphic to) the kinematic group SO(2), that is, they are the circles S^1; in this case, they are also fibers or, as we will say, *kinematic fibers*.

One can say that the period of the kinematic fibers in configuration space is 2π with respect to the angle ϕ. That is, except when Q is the three-body collision, the point $Q'(\phi)$, defined by Eq. (2.2), leaves the initial point Q as ϕ pulls away from zero and does not return again until $\phi=2\pi$.

The geometry of the rotation and kinematic group actions is illustrated in Fig. 1. Configuration space is the Euclidean space $\mathbb{R}^6$, which is illustrated schematically by the set of coordinate axes. A configuration Q, assumed to be noncollinear, is acted upon by external rotations according to Eq. (2.1) and sweeps out the rotation orbit or fiber F_R. This is a three-dimensional surface diffeomorphic to the rotation group SO(3), although represented in the figure by a line. The configuration Q' has the same shape as Q, but a different orientation. Under the action (2.2) of the kinematic group, the point Q sweeps out the (one-dimensional) kinematic orbit or fiber F_K, which is a circle diffeomorphic to SO(2). As ϕ pulls away from zero and Q moves down the kinematic orbit to Q'', the shape changes, in general, so that for small angles ϕ the point Q'' lies on a different rotation fiber (F''_R in the figure) than Q.

The curve F_K illustrated in Fig. 1 does not lie inside the three-dimensional surface F_R, that is, as ϕ pulls away from zero, the curve F_K moves in a direction that is not tangential to the surface F_R. Since F_R is three dimensional, there are three directions in the six-dimensional configuration space

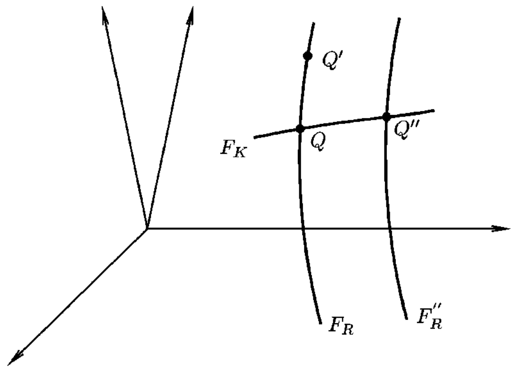

FIG. 1. A noncollinear configuration Q is acted upon by external rotation, and sweeps out the three-dimensional rotation fiber F_R. Q' is another configuration of the same shape as Q. Q is also acted upon by kinematic rotations and sweeps out the one-dimensional kinematic fiber F_K. Kinematic rotations change the shape, in general, so Q'' lies on a different rotation fiber F_R''.

that are tangential to F_R and therefore three other directions that are independent of these. In fact, one can show that as long as the configuration Q is not an oblate symmetric top (on the w_3 axis in the internal space, as explained below), the directions generated by small external rotations and small kinematic rotations are linearly independent. We are already assuming that Q is noncollinear; therefore, to make Fig. 1 accurate, we must assume that Q is also not a symmetric top. Since in the three-body problem all collinear configurations are prolate symmetric tops and conversely, we can summarize these conditions by saying that Q in Fig. 1 is an asymmetric top. The case in which Q is an oblate symmetric top will be dealt with later.

B. Shape space and kinematic orbits in the three-body problem

We turn now to the internal space or *shape space* for the three-body problem. Topologically speaking, this space is one-half of $\mathbb{R}^3$. This fact is most easily seen in the coordinates (w_1, w_2, w_3), defined by

$$w_1 = |\mathbf{r}_{s1}|^2 - |\mathbf{r}_{s2}|^2 = \rho^2 \cos 2\Theta \ \cos 2\Phi,$$

$$w_2 = 2\mathbf{r}_{s1}\cdot\mathbf{r}_{s2} = \rho^2 \cos 2\Theta \ \sin 2\Phi,$$

$$w_3 = 2|\mathbf{r}_{s1}\times\mathbf{r}_{s2}| = \rho^2 \sin 2\Theta. \tag{2.4}$$

Here ρ is the hyperradius and (Θ,Φ) are Smith's hyperspherical angles [18]. The coordinates (w_1, w_2, w_3) are closely related to the coordinates (ξ,η,ζ) defined in Ref. [17]. To Eq. (2.4) we add the definition

$$w = (w_1^2 + w_2^2 + w_3^2)^{1/2} = |\mathbf{r}_{s1}|^2 + |\mathbf{r}_{s2}|^2 = \rho^2. \tag{2.5}$$

The ranges of the coordinates are $-\infty < w_1, w_2 < +\infty$ and $0 \leqslant w_3 < +\infty$, so the physically meaningful region is $w_3 \geqslant 0$. The w_1-w_2 plane contains the collinear configurations, the w_3 axis contains the symmetric oblate tops, and the origin of the w coordinates is the three-body collision. The coordinate w_3 is proportional to the unsigned area spanned by the two Jacobi vectors. The three-body shape space and the coordinates on it are illustrated in Fig. 2. The region

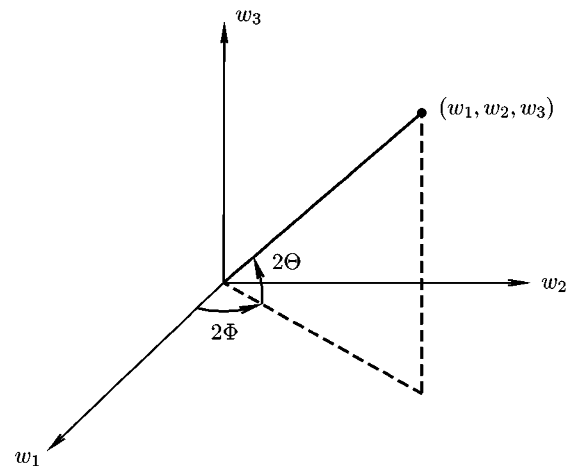

FIG. 2. Shape space in the three-body problem is the region $w_3 \geqslant 0$ in the (w_1, w_2, w_3) coordinates. Smith's hyperspherical angles Θ and Φ are illustrated.

$w_3 > 0$, $(w_1^2 + w_2^2)^{1/2} > 0$, that is, the region avoiding the $w_1 - w_2$ plane and the w_3 axis, is the region containing the asymmetric tops, where the moment of inertia tensor is nondegenerate; it is the region where the principal axis frame is defined and unique apart from a choice in the signs (the senses) of the principal axes. We will call this the *asymmetric top region.*

We will use the symbol q to stand for a point of shape space, which corresponds to some set of coordinates (w_1, w_2, w_3). It will often be understood that a point q of shape space stands for the shape contained in a point Q of configuration space, that is, that q is a label of the rotation fiber upon which Q lies.

In addition to its action (2.2) on configuration space, the kinematic group has an action on shape space, which follows simply by combining Eqs. (2.2) and (2.4). The shape coordinate w_3 is invariant under kinematic rotations, $w_3' = w_3$, while w_1 and w_2 transform according to

$$\begin{pmatrix} w_1' \\ w_2' \end{pmatrix} = \begin{pmatrix} \cos 2\phi & -\sin 2\phi \\ \sin 2\phi & \cos 2\phi \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}, \tag{2.6}$$

which is a rotation by 2ϕ about the w_3 axis. We will abbreviate this action by writing $q' = Kq$ or $q'(\phi) = K(\phi)q$. The angle 2ϕ in Eq. (2.6) is the increment in the hyperspherical angle 2Φ or can be identified with it if the initial point q lies in the plane $w_2 = 0$ with $w_1 > 0$. The curve traced out by q' as K ranges over the kinematic group is the orbit of q under the kinematic action (2.6); this curve is just a circle centered on the w_3 axis, as illustrated in Fig. 3. This circle has a period of π in the angle ϕ because ϕ is doubled in Eq. (2.6).

There are really two kinematic actions, one on configuration space [Eq. (2.2)] and one on shape space [Eq. (2.6)]. We regard the angle ϕ initially as a coordinate on the kinematic group manifold SO(2), ranging from 0 to 2π to cover all group elements; however, according to the two actions (2.2) and (2.6), ϕ can be transferred and regarded as a coordinate on the kinetic orbits in either configuration space or shape space. The external rotation group SO(3) only has one interesting action, that on configuration space [Eq. (2.1)], because points of shape space are invariant under external rotations.

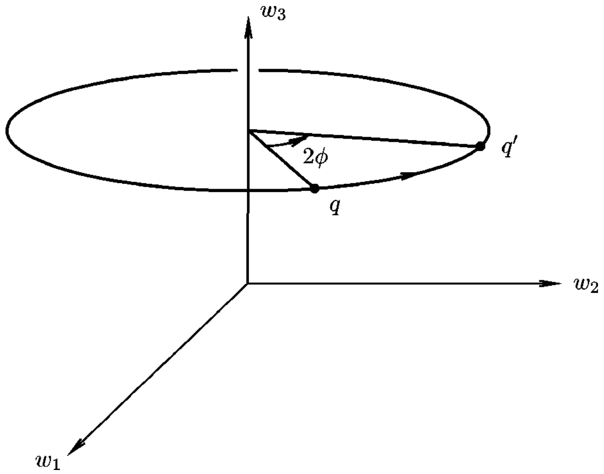

FIG. 3. The action of the kinematic group on a point q of the three-body shape space is to move this point in a circle about the w_3 axis with period $\phi=\pi$. The point q' is a typical point on this circle, the kinematic orbit of the initial point q.

C. Principal axis frame

We now consider the principal axis body frame for the three-body problem, which as mentioned above is defined and unique (modulo the senses of the axes) over the asymmetric top region. We will consider only principal axis frames in which the three bodies lie in the $x-y$ plane. Then there are eight distinct principal axis frames, that is, eight different ways of aligning a right-handed frame on the principal axes, as illustrated in Fig. 4. These frames are related to one another by a certain eight-element group of rotations, constructed from products and powers of the rotations $R_z(\pi/2)$ and $R_x(\pi)$; the notation indicates rotations about the z and x axes, respectively, by the angles given.

There is no compelling physics to dictate that any one of these frames is privileged; any one is as good as another.

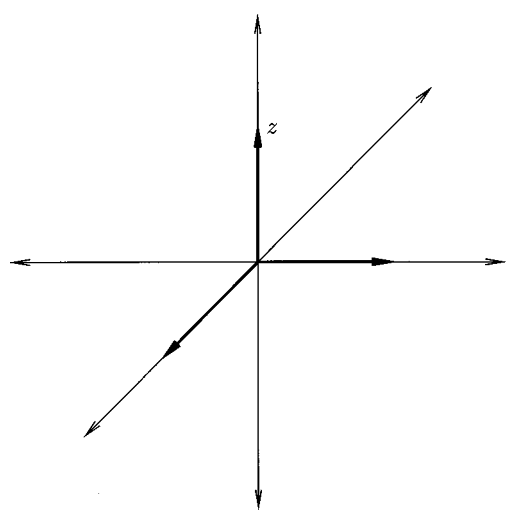

FIG. 4. The moment of inertia tensor for an asymmetric top determines three mutually orthogonal, unoriented axes (unlabeled in the figure). Assuming that the z axis is orthogonal to the plane containing the three bodies, there are two choices for the orientation of the z axis and for each of these, four choices for the orientation of the x and y axes. Altogether, there are eight choices of body frame, of which one is illustrated.

These frames can be regarded as eight branches of a multivalued function, defined over the asymmetric top region of shape space; as the shape changes, that is, as a point q moves around in the asymmetric top region, these eight branches continuously change, thereby sweeping out eight surfaces in ''frame space.'' It turns out that these eight surfaces are connected together in pairs, that is, they form four connected pieces that are disconnected from one another. Thus, by moving around in shape space, continuously tracking branches of the principal axis frame, we can continuously move from one branch to a second and back again, but not to any of the other branches.

To visualize this process, we must first realize that frame space is nothing but configuration space, upon which $(\mathbf{r}_{s1},\mathbf{r}_{s2})$ are coordinates. A choice of body frame for a particular shape is a convention for an origin in the corresponding rotation fiber, that is, the origin is an orientation for the given shape that is considered to be a reference. Once the reference is chosen for a given shape, Euler angles for all other orientations of the same shape are determined by the rotation that maps the reference into some actual orientation. We simply declare that in the reference orientation, the body frame is the same as the space frame and that as the body is rotated away from the reference into some other orientation, the body frame is rotated along with it. For example, in Fig. 1, if we consider Q to be a reference orientation for its shape, then the Euler angles of configuration Q' are those of the rotation that map Q onto Q' according to Eq. (2.1).

Geometrically speaking, this means that a choice of a body frame for a particular shape is equivalent to the choice of a point on the fiber for that shape. By extension, a choice of a (single-valued) body frame over a region of shape space is equivalent to a choice of a surface in configuration space that intersects each rotation fiber in that region in one point. This surface should be smooth, but otherwise can be quite arbitrary. This is the reason for the large number of choices of body frame. In fiber bundle terminology, explained in Ref. [4], this surface is called a *section*. The section is a three-dimensional surface in configuration space (for the n-body problem its dimensionality is $3n-6$, the same as shape space).

The principal axis frame is multivalued and therefore corresponds to eight different sections (or surfaces) in configuration space, defined over the asymmetric top region of shape space. These surfaces intersect each rotation fiber in eight points. The eight points or reference orientations on a given rotation fiber are related to one another by the eight-element group of frame rotations introduced above. Two of these surfaces are illustrated in Fig. 5. The points Q and Q' in the figure, on the same rotation fiber F_R, are two principal axis reference orientations for a given shape; Q and Q' are related by one of the eight discrete frame rotations, according to Eq. (2.1).

Next we consider what happens when we continuously track one of the branches of the principal axis frame as a point of shape space follows a closed circuit, returning to the original shape, assuming the circuit is confined to the asymmetric top region. After such a circuit, does the principal axis frame return to the original branch or does it return on another branch? A simple topological argument shows that the final branch must be the same as the initial branch on any

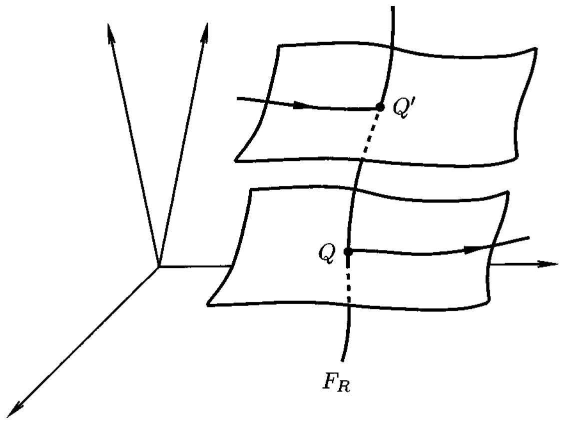

FIG. 5. The principal axis frame in the three-body problem has eight branches, of which two are illustrated in the figure. If we leave on one branch at Q, following a circuit in shape space and continuously tracking the principal axis frame, we may return at Q' on another branch, depending on the circuit in shape space.

closed circuit in the asymmetric top region that can be continuously contracted to a point, since the answer (which branch we return on) must be a continuous function of the loop and a continuous function that can take on only discrete values must be constant. More generally, continuity implies that any two circuits that can be continuously deformed into one another will return on the same final branch. The only way the final branch can change as the loop is deformed is if the loop crosses a singularity, which here means the w_3 axis. For example, as illustrated in Fig. 6, the circuits A and B cannot be deformed continuously into one another without crossing the w_3 axis and need not return on the same branch of the principal axis frame.

Since loops that do not circle the w_3 axis do not change branches on return, let us consider a loop that does circle the w_3 axis, say, once in the positive direction. Since all such loops return on the same branch, we might as well choose a nice one, such as the kinematic orbit illustrated in Fig. 3. We

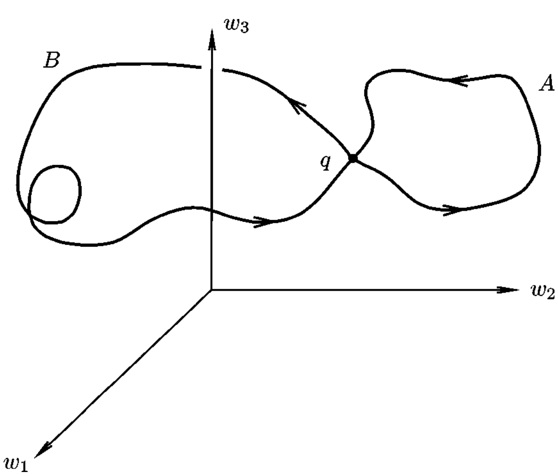

FIG. 6. Circuits in shape space that can be continuously deformed into one another (which belong to the same homotopy class) give rise to the same final branch when the principal axis frame is continuously tracked around them. Circuit A, which is contractible, returns on the original branch, whereas circuit B, which loops the w_3 axis, returns on a different branch.

wish to track the principal axis frame continuously, starting from some configuration Q in the rotation fiber over q, as ϕ goes from 0 to π. A certain general property connecting the principal axis frame and kinematic rotations allows us to determine easily the branch we return on.

D. Principal axis frame and kinematic rotations

The property in question is valid for any number of particles (not only three), so let us speak temporarily of an n-particle system. First we introduce the $3\times(n-1)$ matrix F_s with components $F_{si\alpha}$, defined by

$$F_{si\alpha}=r_{s\alpha i}, \tag{2.7}$$

where $i=1,2,3$ stands for x,y,z, where $\alpha=1,\ldots,n-1$ labels the Jacobi vectors, and again the s subscript means the space frame. Next we define the 3×3 matrix T_s with components T_{sij},

$$\mathsf{T}_s=\mathsf{F}_s\mathsf{F}_s^t, \quad T_{sij}=\sum_\alpha r_{s\alpha i}r_{s\alpha j}, \tag{2.8}$$

where the t superscript is the matrix transpose. We call T_s the *moment tensor*; it is related to the usual moment of inertia tensor M_s by

$$\mathsf{M}_s=(\mathrm{tr}\mathsf{T}_s)\mathsf{I}-\mathsf{T}_s, \tag{2.9}$$

where tr is the trace. Because of Eq. (2.9), the eigenvalues of M_s (the principal moments of inertia, call them μ_1,μ_2,μ_3) are related to the eigenvalues of T_s (call them $\lambda_1,\lambda_2,\lambda_3$) by

$$\mu_1=\lambda_2+\lambda_3, \quad \mu_2=\lambda_1+\lambda_3, \quad \mu_3=\lambda_1+\lambda_2. \tag{2.10}$$

Finally, we define the $(n-1)\times(n-1)$ matrix J, which we call the *Jacobi dot product tensor*, by

$$\mathsf{J}=\mathsf{F}_s^t\mathsf{F}_s, \quad J_{\alpha\beta}=\mathbf{r}_{s\alpha}\cdot\mathbf{r}_{s\beta}. \tag{2.11}$$

There is no s subscript on J because it is independent of frame. It is proved in Ref. [10] that the non-negative definite matrices T_s and J have the same positive eigenvalues (the positive λ's). In that reference it is also proved that if two configurations Q and Q' have the same J tensor, then either Q and Q' have the same shape or their shapes are related by a spatial inversion. Thus the Jacobi dot product tensor identifies the shape of a configuration modulo chirality (uniquely, for planar shapes, such as occur in the three-body problem).

It follows immediately from the definitions and Eqs. (2.1) and (2.2) that the matrix J (that is, all of its components) is invariant under external rotations and that T_s and M_s (all of their components) are invariant under kinematic rotations. Thus, in Fig. 1, configurations Q and Q' have the same J matrices and Q and Q'' have the same T_s and M_s matrices. The eigenvalues of these matrices (the λ's or the μ's) are invariant under both external and kinematic rotations.

This has an important geometrical interpretation. We return to the three-body problem $n=3$ for purposes of illustration. Consider a configuration Q lying on one branch of the principal axis frame, such as illustrated in Fig. 5, and consider the kinematic orbit of Q generated according to Eq. (2.2). The section (the surface representing the principal axis frame) is three dimensional, but the orbit is a one-dimensional curve. Does this curve lie in the principal axis section? Indeed it does, for as we have seen, the moment of inertia tensor M_s is invariant under the kinematic action, so if it is a diagonal matrix at Q, it will be the same diagonal matrix at all configurations reachable from Q by kinematic rotations. This means that if we wish to continuously track the principal axis frame as a point of shape space follows the kinematic action (2.6), illustrated in Fig. 3, then we simply follow the kinematic orbit in configuration space specified by Eq. (2.2).

It was mentioned above that the kinematic orbit pulls away from the rotation fiber (F_R, in Fig. 5) as ϕ pulls away from zero, that is, the kinematic orbit is not tangent to the rotation fiber at Q, and that the kinematic orbit does not return to Q until $\phi=2\pi$. These facts do not, however, preclude the possibility that the kinematic orbit might return to the original rotation fiber F_R at some other point than the initial point, say, Q', before $\phi=2\pi$. If it does, then Q and Q' will be related by some spatial rotation and we will have found some kinematic rotation that has the same effect on Q as some (external) spatial rotation, say, $KQ=RQ$. In fact, such a kinematic rotation exists, for if we substitute $\phi=\pi$ into Eq. (2.2), we find $K(\pi)\{\mathbf{r}_{s\alpha}\}=\{-\mathbf{r}_{s\alpha}\}$, that is, $K(\pi)$ causes a spatial inversion. However, this has the same effect as the external rotation $R_z(\pi)$, since the inversion takes place in the $x-y$ plane. In other words, we have

$$K(\pi)Q=R_z(\pi)Q \tag{2.12}$$

in the three-body problem.

After $\phi=\pi$, the kinematic orbit pulls away from the original rotation fiber F_R again and does not return until $\phi=2\pi$. Thus we can visualize the kinematic orbit in configuration space as ϕ varies from 0 to 2π and its relation to a typical rotation fiber, as illustrated in Fig. 7. The sequence of rotation fibers we pass through when ϕ goes from π to 2π is the same as from 0 to π, which explains the double angle 2ϕ in the kinematic action on shape space [Eq. (2.6)] and the π periodicity (instead of 2π) of the kinematic orbits in shape space. Actually, Fig. 7 is slightly misleading in one sense, for it seems to suggest that the kinematic fiber climbs a ''spiral staircase'' as ϕ goes from 0 to π and then climbs down again as ϕ goes from π to 2π; in a sense what one is climbing is the angle of rotation about the z axis, which increases from 0 to π on the first half and continues to increase from π to 2π on the second half. It would be better to think of the spiral staircase as continuing to climb but returning to where it started because z rotations inside the rotation fiber are themselves periodic, constituting a circle. Alternatively, we might say that the kinetic orbit continually goes down the spiral staircase; it appears impossible to say which at this point, because $R_z(\pi)$ and $R_z(-\pi)$ are the same rotation. (Later we will see that there is a difference.)

Now we can see why there is a change in the branch of the principal axis frame when we go once around the w_3 axis in shape space in the positive sense, following a kinematic orbit. When the kinematic orbit in shape space returns to the initial shape, the kinematic orbit in configuration space must necessarily have returned to the same shape too, but this is only defined modulo some external rotation. In fact, the spatial rotation corresponding to this circuit in shape space is $R_z(\pi)$, which connects two branches of the principal axis frame. If we go around the w_3 axis twice in shape space, the rotation generated in configuration space is $\mathsf{R}_z(\pi)^2=\mathsf{I}$, so we are back on the original branch again. This proves that the eight branches of the principal axis frame are connected in pairs, in fact, pairs related to one another by $R_z(\pi)$. The four pairs of branches are disconnected because it is not possible to get from one pair to another by kinematic rotations and because all other closed circuits on shape space (which do not cross the w_3 axis) can be continuously deformed into a closed circuit along a kinematic orbit, circling the w_3 axis some number of times. In other words, the issue of the connectivity of the branches is determined by kinematic orbits alone.

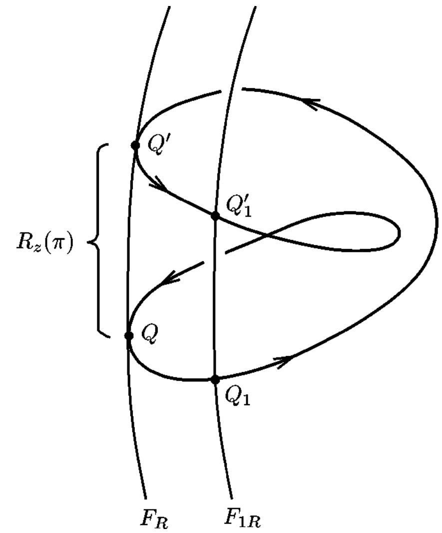

FIG. 7. A kinematic orbit in configuration space leaves a rotation fiber F_R at point Q ($\phi=0$), returns to the same fiber at a rotated point Q' ($\phi=\pi$), and then returns to the initial point Q ($\phi=2\pi$). The sequence of rotation fibers passed through is the same from $\phi=0$ to π as from $\phi=\pi$ to 2π. For example, Q_1 and Q_1' lie on the same rotation fiber F_{1R}. Configurations Q and Q' (or Q_1 and Q_1') are connected by the external rotation $\mathsf{R}_z(\pi)$.

Thus there are two branches of the principal axis frame that can be reached from some initial frame by continuous deformation. We can create a single-valued principal axis frame if we introduce a branch cut, across which the principal axis frame jumps discontinuously by $R_z(\pi)$. For example, let us take the region $w_1,w_3>0$ of the w_1-w_3 plane, that is, the surface $\Phi=0$, as an initial surface for kinematic fibers, so that the kinematic angle ϕ along the kinematic fibers and the Smith hyperspherical coordinate Φ are the same and let us place the branch cut at angle $\phi=\pi/2$, that is, along the negative w_1 axis, so that the frame is continuous everywhere except at $\phi=k\pi+\pi/2$, where k is an integer. The branch cut is a two-dimensional surface in shape space that emanates from the w_3 axis.

E. Transforming to the Eckart frame

We will now change from the principal axis to the Eckart frame, which will give us a single-valued frame over all of shape space, eliminate the branch cuts, and eliminate the singularities on the w_3 axis. In practice there are two complementary methods of specifying a body frame or, equivalently, of specifying a section of the rotation fiber bundle in configuration space. These are the parametric and constraint methods, the same methods used to specify any surface in any space (of any dimensionality). We will speak for the moment in terms of the general n-body problem. Then the rotation section is a surface of dimensionality $3n-6$ in the $(3n-3)$-dimensional configuration space; its codimension is 3.

In the parametric method, we express the surface in terms of $3n-6$ parameters q^μ, $\mu=1,\ldots,3n-6$, which identify points on the surface. Since a single-valued section will intersect each rotation fiber at one point, the parameters q^μ identify which fiber we are on, which is the same as the shape q. Thus, the parameters q^μ can also be considered to be shape coordinates. In the parametric method, we express the configuration coordinates (the space Jacobi vectors) as functions of the parameters q^μ,

$$\mathbf{r}_{s\alpha}=\mathbf{r}_\alpha(q^\mu), \tag{2.13}$$

where $\mathbf{r}_\alpha$ (without the s subscript) are the functions in question. Equation (2.13) is not true everywhere in configuration space, only on points $Q=\{\mathbf{r}_{s\alpha}\}$ that lie on the section. Since the space frame and body frame coincide at such points, the space components of the Jacobi vectors are equal to the body components on the section; this explains the notation, in which $\mathbf{r}_\alpha$ (without the s subscript) are the body components of the Jacobi vectors.

In the constraint method, the section is specified by three functions of the form

$$C_i(\mathbf{r}_{s1},\ldots,\mathbf{r}_{s,n-1})=0 \tag{2.14}$$

for $i=1,2,3$, which constrain the space components of the Jacobi vectors (three functions because the section has codimension 3). For example, the principal axis frame is specified by the constraints

$$T_{sij}=\sum_\alpha r_{s\alpha i}r_{s\alpha j}=0 \quad \text{for} \quad i\neq j, \tag{2.15}$$

which says that the off-diagonal elements of the space components of the moment tensor vanish, that is, that this tensor is diagonal. A diagonal moment tensor implies a diagonal moment of inertia tensor, so at points of configuration space satisfying Eq. (2.15), the space frame is identical to one of the principal axis frames. Notice that Eq. (2.15) specifies a set of three quadratic relations among the space components of the Jacobi vectors, so the principal axis section in configuration space can be thought of as a higher-dimensional analog of the usual ellipsoids or hyperboloids in three-dimensional space.

Another example of the constraint form of the section is given by the usual condition [3,19] for the Eckart frame,

$$\sum_\alpha \mathbf{r}_{s\alpha}\times\mathbf{r}_{se\alpha}=0, \tag{2.16}$$

where $\mathbf{r}_{se\alpha}$ (with the e subscript) are the space-component Jacobi vectors for an ''equilibrium'' configuration (specifying both shape and orientation). We put this word in quotes, because the usual purpose of the Eckart frame is to give a convenient description of small vibrations, so that $\{\mathbf{r}_{se\alpha}\}$ would be a genuine equilibrium configuration, a minimum of the potential energy. In the present discussion, however, we will choose $\{\mathbf{r}_{se\alpha}\}$ according to other criteria, based on the moment of inertia tensor. In any case, the quantities $\{\mathbf{r}_{se\alpha}\}$ in Eq. (2.16) are constants, so that equation is a linear constraint among the space components of the Jacobi vectors $\{\mathbf{r}_{s\alpha}\}$. Thus the Eckart section is a hyperplane, that is, a vector subspace of configuration space of dimensionality $3n-6$ (three dimensional, in the three-body problem).

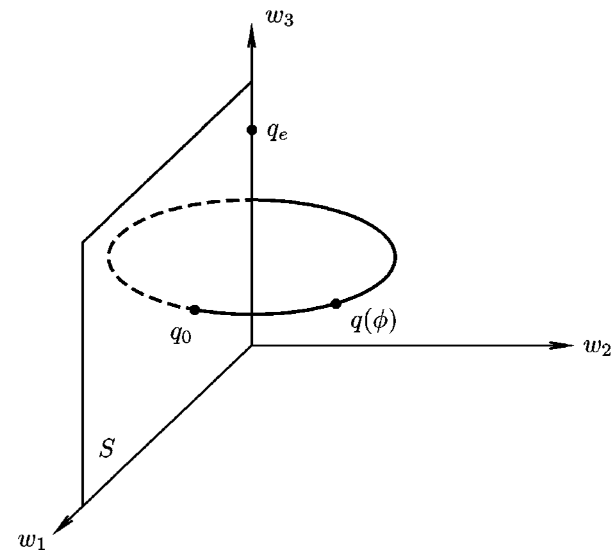

FIG. 8. The region S of the w_1-w_3 plane where $w_1,w_3>0$ is convenient as a section of the kinetic fiber bundle. An initial point q_0 on the section is acted upon by kinematic rotations and sweeps out a kinematic orbit upon which $q(\phi)$ is a typical point. The point q_e, an oblate symmetric top, is an ''equilibrium'' shape for the Eckart frame.

The equilibrium configuration we will use is a symmetric, oblate top with hyperradius $\rho_e\neq 0$, so the shape lies on the w_3 axis at coordinate $w_3=\rho_e^2$. The precise value of ρ_e is not important. At such configurations, $w_1=w_2=0$, so according to Eq. (2.4), the two Jacobi vectors are equal in magnitude and orthogonal. We orient this configuration so that the two Jacobi vectors are aligned on the x and y axes,

$$\mathbf{r}_{se1}=k\hat{\mathbf{x}}, \quad \mathbf{r}_{se2}=k\hat{\mathbf{y}}, \tag{2.17}$$

where k is the magnitude of either Jacobi vector (in fact, $k=\rho_e/\sqrt{2}$) and $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are unit vectors along the (space) x and y axes. We will also write $Q_e=\{\mathbf{r}_{se\alpha}\}$ for this equilibrium configuration and q_e for the corresponding shape (see Fig. 8).

Next we consider kinematic rotations acting on Q_e, according to Eq. (2.2). We find

$$\begin{pmatrix}\mathbf{r}'_{se1}\\ \mathbf{r}'_{se2}\end{pmatrix}=\begin{pmatrix}\cos\phi & -\sin\phi\\ \sin\phi & \cos\phi\end{pmatrix}\begin{pmatrix}k\hat{\mathbf{x}}\\ k\hat{\mathbf{y}}\end{pmatrix}=k\begin{pmatrix}\cos\phi\,\hat{\mathbf{x}}-\sin\phi\,\hat{\mathbf{y}}\\ \sin\phi\,\hat{\mathbf{x}}+\cos\phi\,\hat{\mathbf{y}}\end{pmatrix}, \tag{2.18}$$

where the notation treats vectors as elements of a matrix just as we would treat scalars. We abbreviate this equation by writing $Q_e' = K(\phi) Q_e$. Obviously, the configuration Q_e is not invariant under kinematic rotations. On the other hand, the kinematic action in shape space does nothing to q_e because q_e lies on the w_3 axis. Since the shape does not change, this means that the kinematic action (2.18) on the corresponding configuration Q_e must be equivalent to a spatial rotation, not only for the angle $\phi = \pi$ as we had earlier for general configurations Q [see Eq. (2.12)], but for any angle ϕ. This is a special property of the oblate symmetric top configurations and it means that the kinematic orbit actually does lie inside the three-dimensional rotation fiber, in contradiction with the implication of Fig. 1 (which only applied to asymmetric tops). Therefore, we must have $K(\phi) Q_e = R Q_e$ for some R. What rotation is it? The answer is $R_z(-\phi)$, as we show directly by applying Eq. (2.1). For example, for the $\alpha = 1$ Jacobi vector we have

$$\mathbf{r}'_{se1} = \mathsf{R}_z(-\phi) \mathbf{r}_{se1} = \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} k \\ 0 \\ 0 \end{pmatrix}$$

$$= k \begin{pmatrix} \cos\phi \\ -\sin\phi \\ 0 \end{pmatrix} = k(\cos\phi\, \hat{\mathbf{x}} - \sin\phi\, \hat{\mathbf{y}}), \tag{2.19}$$

which agrees with the first row of Eq. (2.18). Similarly, for the $\alpha = 2$ Jacobi vector we find

$$\mathbf{r}'_{se2} = \mathsf{R}_z(-\phi) \mathbf{r}_{se2} = k(\sin\phi\, \hat{\mathbf{x}} + \cos\phi\, \hat{\mathbf{y}}). \tag{2.20}$$

We can summarize these by writing

$$K(\phi) Q_e = R_z(-\phi) Q_e. \tag{2.21}$$

Next we consider points of shape space that lie on the initial value surface for the variable ϕ, as defined above. This is the quadrant of the $w_1 - w_3$ plane where $w_1, w_3 > 0$ and it has the property that it intersects each kinematic fiber at precisely one point. Thus this surface is similar in function to the section of the rotation fiber bundle in configuration space and can be regarded as a section of the kinematic fiber bundle. We will call it the *kinematic section*. This section is illustrated in Fig. 8. We restrict the section to the region $w_1 > 0$ because if we included $w_1 < 0$, the section would intersect each kinematic fiber at two points.

The kinematic section allows us to parametrize a point q of shape space by its kinematic angle ϕ, defined relative to the section, plus two more quantities that are kinematic invariants and label the kinematic fiber upon which q lies. There are many obvious choices for kinematic invariants: One is (λ_1, λ_2), the eigenvalues of the J tensor, and another is (w_1, w_3), the coordinates in the kinematic section where the kinematic orbit passing through q intersects the section. We must be careful in interpreting w_1 as a kinematic invariant; according to Eq. (2.6) this quantity is not a kinematic invariant, but in that equation, w_1 is the coordinate of the point q itself, whereas in the present discussion it is the coordinate of the point where the kinematic fiber passing through q intersects the section. Of course, w_3 is a kinematic invariant by any interpretation.

The J tensor is diagonal on the kinematic section since the off-diagonal element $\mathbf{r}_{s1} \cdot \mathbf{r}_{s2}$ vanishes when $w_2 = 0$. Thus, on the kinematic section, J can be expressed in terms of its eigenvalues

$$\mathsf{J} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}, \tag{2.22}$$

where $\lambda_1 = |\mathbf{r}_{s1}|^2$ and $\lambda_2 = |\mathbf{r}_{s2}|^2$. Furthermore, since $w_1, w_3 > 0$ on the section, Eq. (2.4) implies $\lambda_1 > \lambda_2 > 0$. The J tensor is not constant (nor does it remain diagonal) as we move around the kinematic orbits, but it becomes diagonal again when $\phi = \pi/2$, on the $w_1 < 0$ side of the $w_1 - w_3$ plane, where the ordering of the diagonal elements is reversed.

Let us define a body frame over the kinematic section. We pick a shape q_0 on the kinematic section, as illustrated in Fig. 8. The 0 subscript indicates that this point is an initial point of a kinematic orbit; we will also write $Q_0 = \{\mathbf{r}_{s0\alpha}\}$ for a corresponding point in configuration space. By Eq. (2.4) the two Jacobi vectors are orthogonal at shape q_0, so we can orient the configuration to place the longer Jacobi vector $\mathbf{r}_{s01}$ on the space x axis and the shorter one $\mathbf{r}_{s02}$ on the space y axis. That is, we choose the reference orientation Q_0 so that

$$\mathbf{r}_{s01} = a_1 \hat{\mathbf{x}}, \quad \mathbf{r}_{s02} = a_2 \hat{\mathbf{y}}, \tag{2.23}$$

where $a_i = \sqrt{\lambda_i} > 0$, $i = 1,2$, and where $a_1 > a_2$. This frame is obviously a principal axis frame since the moment tensor is diagonal, but it is also an Eckart frame relative to the equilibrium Q_e defined by Eq. (2.17). This follows immediately from the definition of the Eckart frame, Eq. (2.16).

Next we extend the definition of this body frame to cover all asymmetric tops by moving down kinematic orbits in shape space. Let us write $q(\phi) = K(\phi) q_0$, so that $q(\phi)$ is the ϕ-dependent point of shape space on the kinematic orbit passing through q_0 on the section, as illustrated in Fig. 8. We wish to define a point Q of configuration space corresponding to shape q, which will sweep out the external rotation section. We could do this by demanding that Q follow kinematic orbits in configuration space, that is, by writing $Q = K(\phi) Q_0$, but, as we have seen, this will just give the principal axis frame. The principal axis frame would produce a net rotation of $R_z(\pi)$ along the initial rotation fiber after $\phi = \pi$, as we have seen, and would not be single valued.

Let us therefore compensate for this spatial rotation by setting

$$Q(\phi) = R_z(\phi) K(\phi) Q_0, \tag{2.24}$$

which causes us to rotate down rotation fibers by an angle that is equal to the kinematic angle ϕ, as we move from one rotation fiber to another. [This equation does not imply the multiplication of the matrices R_z and K, which would not make sense anyway since one is 3×3 and the other is 2×2, but rather the successive application of the rotation and kinematic actions to Q_0 according to Eqs. (2.1) and (2.2).] At the value $\phi = \pi$, where there is a discontinuity or change in branch of the principal axis frame, Eq. (2.24) gives $KQ_0 = R_z(\pi) Q_0$ or $Q = Q_0$ since $\mathsf{R}_z(\pi)^2 = \mathsf{I}$. In other words, the section and corresponding frame specified by Eq. (2.24) are single valued. Equation (2.24) is strange in appearance because it sets a kinematic angle equal to an external rotation angle and in general these two angles have very different physical interpretations. However, it is precisely this shifting from kinematic to external rotations that eliminates many of the singularities in the principal axis frame.

Equation (2.24) defines an Eckart frame relative to the equilibrium Q_e, not just over the kinematic section but everywhere in shape space, as we will now show. We do this by expressing certain relations in terms of Jacobi vectors, writing $Q_e=\{\mathbf{r}_{se\alpha}\}$, $Q_0=\{\mathbf{r}_{s0\alpha}\}$, and $Q=\{\mathbf{r}_{s\alpha}\}$. We begin with Eq. (2.21), which we write in the form

$$R_z(\phi)K(\phi)Q_e=Q_e, \tag{2.25}$$

which follows since $R_z(-\phi)=R_z(\phi)^{-1}$. The rotation and kinematic actions commute (since they act on different indices) and can be taken in either order. Converting Eq. (2.25) to Jacobi vectors, we find

$$\mathbf{r}_{se\alpha}=\sum_\beta K_{\alpha\beta}(\phi)\mathsf{R}_z(\phi)\mathbf{r}_{se\beta}. \tag{2.26}$$

Similarly, converting Eq. (2.24) to Jacobi vectors, we have

$$\mathbf{r}_{s\alpha}(\phi)=\sum_\beta K_{\alpha\beta}(\phi)\mathsf{R}_z(\phi)\mathbf{r}_{s0\beta}. \tag{2.27}$$

Now, to show that the section swept out by $Q(\phi)$ is an Eckart section with equilibrium Q_e, we must show that Eq. (2.16) is satisfied with $\mathbf{r}_{s\alpha}$ identified with $\mathbf{r}_{s\alpha}(\phi)$. By substituting Eqs. (2.27) and (2.26), we have

$$\sum_\alpha \mathbf{r}_{s\alpha}\times\mathbf{r}_{se\alpha}=\sum_{\alpha,\beta,\gamma} K_{\alpha\beta}K_{\alpha\gamma}(\mathsf{R}\mathbf{r}_{s0\beta})\times(\mathsf{R}\mathbf{r}_{se\gamma})$$

$$=\sum_\alpha (\mathsf{R}\mathbf{r}_{s0\alpha})\times(\mathsf{R}\mathbf{r}_{se\alpha}), \tag{2.28}$$

where R stands for $\mathsf{R}_z(\phi)$ and K for $K(\phi)$ and we have used the orthogonality of the K matrices in the last step. Next we use the identity $(\mathsf{R}\mathbf{a})\times(\mathsf{R}\mathbf{b})=\mathsf{R}(\mathbf{a}\times\mathbf{b})$, valid for any proper rotation R and any pair of vectors $\mathbf{a},\mathbf{b}$ to write

$$\sum_\alpha \mathbf{r}_{s\alpha}\times\mathbf{r}_{se\alpha}=\mathsf{R}\left(\sum_\alpha \mathbf{r}_{s0\alpha}\times\mathbf{r}_{se\alpha}\right)=0, \tag{2.29}$$

where the last step follows because we have already shown that the point $Q_0=\{\mathbf{r}_{s0\alpha}\}$ is an Eckart frame. Thus $Q=\{\mathbf{r}_{s\alpha}\}$ does lie on the Eckart section.

F. Parametric forms and remaining singularities

It is interesting to write out Eq. (2.24) explicitly in terms of Jacobi vectors. Since we have now determined that Q lies on the Eckart section, let us change notation and write Q^E for it. Likewise, the intermediate point in Eq. (2.24) (after the action of K but before the action of R) lies on the principal axis section; therefore, let us write

$$Q^{PA}=K(\phi)Q_0, \quad Q^E=R_z(\phi)Q^{PA}. \tag{2.30}$$

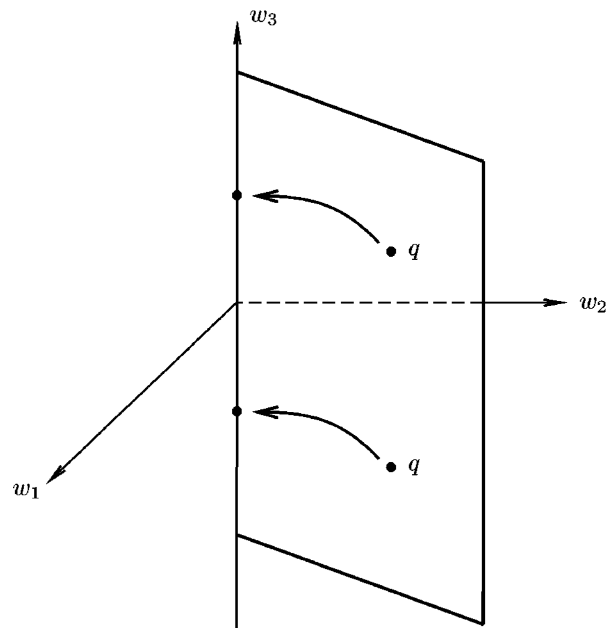

FIG. 9. The principal axis frame has singularities as we approach the w_3 axis along a plane of constant ϕ, either for $w_3>0$ or for $w_3<0$, where the latter is meaningful only for the planar three-body problem. The Eckart frame, however, is singular only on the negative w_3 axis.

Furthermore, let us write $Q^{PA}=\{\mathbf{r}_{s\alpha}^{PA}\}$ and $Q^E=\{\mathbf{r}_{s\alpha}^E\}$. Configuration Q_0 is given in Jacobi vector form by Eq. (2.23); when we apply $K(\phi)$ to this, following Eq. (2.18), we find

$$\mathbf{r}_{s1}^{PA}=a_1\cos\phi\hat{\mathbf{x}}-a_2\sin\phi\hat{\mathbf{y}},$$

$$\mathbf{r}_{s2}^{PA}=a_1\sin\phi\hat{\mathbf{x}}+a_2\cos\phi\hat{\mathbf{y}}. \tag{2.31}$$

Then, when we apply $R_z(\phi)$ to this, following Eq. (2.19), we find

$$\mathbf{r}_{s1}^E=(a_1\cos^2\phi+a_2\sin^2\phi)\hat{\mathbf{x}}+(a_1-a_2)\sin\phi\cos\phi\hat{\mathbf{y}},$$

$$\mathbf{r}_{s2}^E=(a_1-a_2)\sin\phi\cos\phi\hat{\mathbf{x}}+(a_1\sin^2\phi+a_2\cos^2\phi)\hat{\mathbf{y}}. \tag{2.32}$$

An interesting aspect about these two results is that they give us the equations of the principal axis and Eckart sections explicitly in the parametric form (2.13), in which (a_1,a_2,ϕ) can be regarded as the shape coordinates q^μ; previously we had expressions for these sections only in constraint form, Eqs. (2.15) and (2.16), respectively. These shape coordinates are neatly divided into the kinematic invariants (a_1,a_2), plus the kinematic angle ϕ.

The singularity of the principal axis frame on the w_3 axis (the oblate symmetric tops) is easily seen from Eq. (2.31). Suppose we approach the positive w_3 axis along a plane of constant ϕ, as illustrated in Fig. 9. Then the two eigenvalues λ_1,λ_2 approach a common positive value, as do their square roots a_1,a_2. Let $a_1,a_2\to a>0$. Then the limit of the principal axis frame is

$$\mathbf{r}_{s1}^{PA}=a(\cos\,\phi\hat{\mathbf{x}}-\sin\,\phi\hat{\mathbf{y}}),$$
$$\mathbf{r}_{s2}^{PA}=a(\sin\,\phi\hat{\mathbf{x}}+\cos\,\phi\hat{\mathbf{y}}),\tag{2.33}$$

which clearly depends on ϕ. Thus the limit of the principal axis frame at the symmetric oblate shapes depends on the direction of approach and the frame is not continuous there. To put this another way, if we go around the w_3 axis in a very small circle (a kinematic orbit), then the principal axis frame changes by an amount that is order unity under a small change of shape. Thus the derivatives of the principal axis frame become infinite as we approach the w_3 axis.

On the other hand, the Eckart frame approaches a well defined value on the w_3 axis, namely,

$$\mathbf{r}_{s1}^{E}=a\hat{\mathbf{x}},\quad \mathbf{r}_{s2}^{E}=a\hat{\mathbf{y}}.\tag{2.34}$$

Thus the Eckart frame eliminates not only the multiple branches and branch cuts of the principal axis frame, but also the singularities at the oblate symmetric top configurations.

At this point it is of interest to consider the three-body problem in a plane, which in some ways bears a stronger analogy to the four-body problem in space than does the three-body problem in space. For the planar three-body problem, the configuration space is $\mathbb{R}^4$ and the generic rotation orbits are one-dimensional circles diffeomorphic to SO(2) instead of SO(3). Coordinates (w_1,w_2,w_3) are still useful coordinates on shape space, but the definition of w_3 in Eq. (2.4) is replaced by

$$w_3=\hat{\mathbf{z}}\cdot(\mathbf{r}_{s1}\times\mathbf{r}_{s2}),\tag{2.35}$$

corresponding to the fact that negative w_3 values are now meaningful (w_3 is now the signed area of the triangle formed by the Jacobi vectors). Thus shape space is now all of $\mathbb{R}^3$. The collinear configurations on the w_1-w_2 plane are not singular in any important sense for the planar three-body problem because the dimensionality of the rotation orbits does not change there (unlike the three-body problem in space). It thus makes sense to extend the kinematic section through the w_1 axis, to include the quadrant $w_1>0$, $w_3<0$ in the w_1-w_3 plane, so that now the kinematic section is the entire region $w_1>0$. Kinematic invariants can still be taken to be (w_1,w_3) on the kinematic section, the eigenvalues (λ_1,λ_2), or, what is more useful, their square roots (a_1,a_2). However, the eigenvalue λ_2 and hence a_2 approach zero as we approach the w_1 axis from above, so there is the question of the sign of a_2 as we pass into the region $w_3<0$. In fact, an analytic continuation indicates that a_2 should be interpreted as the negative square root of λ_2 in the region $w_3<0$. Thus (a_1,a_2) can be taken as coordinates on the kinematic section, satisfying the condition

$$a_1>|a_2|\geqslant 0,\tag{2.36}$$

with negative values of a_2 indicating shapes of negative area.

For the planar three-body problem, it makes sense to examine the behavior of the principal axis and Eckart frames as we approach the negative w_3 axis, containing symmetric oblate tops of negative area. Again we have λ_1 and λ_2 approaching a common value as we approach the w_3 axis, but as for their square roots, it is a_1 and $-a_2$ that approach a common positive value, say a. As for the principal axis frame, it has singularities on the negative w_3 axis much like those on the positive w_3 axis. The Eckart frame, on the other hand, which is nonsingular on the positive w_3 axis, turns out to have singularities on the negative w_3 axis. The asymmetry between positive and negative w_3 arises because the quantity a_2 is negative when $w_3<0$; thus as we approach the negative w_3 axis along a plane of constant ϕ, as illustrated in Fig. 9, we have $a_1,-a_2\rightarrow a>0$. Thus Eq. (2.32) becomes,

$$\mathbf{r}_{s1}^{E}=a(\cos 2\phi\hat{\mathbf{x}}+\sin 2\phi\hat{\mathbf{y}}),$$
$$\mathbf{r}_{s2}^{E}=a(\sin 2\phi\hat{\mathbf{x}}-\cos 2\phi\hat{\mathbf{y}}),\tag{2.37}$$

which clearly depends upon the direction of approach. Thus the Eckart frame for the planar three-body problem has fewer singularities than the principal axis frame, but singularities have not been eliminated entirely.

In the planar three-body problem, both frames examined so far have singularities. Is it possible to find a frame that is free of singularities everywhere? The answer is yes for the three-body problem in space; the Eckart frame does this. However, for the three-body problem in a plane, the answer is no. It is possible to move the singularities from the negative w_3 axis to some other location, but they cannot be eliminated. For example, if instead of Eq. (2.24) we write

$$Q'^{E}(\phi)=R_z(-\phi)K(\phi)Q_0,\tag{2.38}$$

that is, if we compensate for the rotation along the rotation fibers in the opposite direction from that in Eq. (2.24), then we obtain a frame that is well behaved on the negative w_3 axis, but singular on the positive w_3 axis. This is like rotating down the ''spiral staircase,'' as suggested by the fact that $R_z(\pi)=R_z(-\pi)$. The result is another version of the Eckart frame, as indicated by the notation Q'^{E}. If we write Eq. (2.38) in terms of Jacobi coordinates, we find

$$\mathbf{r}_{s1}'^{E}=(a_1\cos^2\phi-a_2\sin^2\phi)\hat{\mathbf{x}}-(a_1+a_2)\sin\,\phi\,\cos\,\phi\hat{\mathbf{y}},$$
$$\mathbf{r}_{s2}'^{E}=(a_1+a_2)\sin\,\phi\,\cos\,\phi\hat{\mathbf{x}}+(-a_1\sin^2\phi+a_2\cos^2\,\phi)\hat{\mathbf{y}}.\tag{2.39}$$

On the positive w_3 axis, where $a_1,a_2\rightarrow a>0$, this frame becomes

$$\mathbf{r}_{s1}'^{E}=a(\cos 2\phi\hat{\mathbf{x}}-\sin 2\phi\hat{\mathbf{y}}),$$
$$\mathbf{r}_{s2}'^{E}=a(\sin 2\phi\hat{\mathbf{x}}+\cos 2\phi\hat{\mathbf{y}}),\tag{2.40}$$

which is ϕ dependent and therefore singular. However, on the negative w_3 axis, where $a_1,-a_2\rightarrow a>0$, the frame becomes

$$\mathbf{r}_{s1}'^{E}=a\hat{\mathbf{x}},\quad \mathbf{r}_{s2}'^{E}=-a\hat{\mathbf{y}}.\tag{2.41}$$

The frame (2.39) is an Eckart frame, but with an equilibrium shape located on the negative w_3 axis, call it q_e'. The corresponding orientation is

$$\mathbf{r}_{se1}'=k\hat{\mathbf{x}},\quad \mathbf{r}_{se2}'=-k\hat{\mathbf{y}}.\tag{2.42}$$

This concludes our discussion of the principal axis and Eckart frames.

III. COMMENTS AND CONCLUSIONS

Finally, we will make some comments about monopole string singularities and frame singularities in the three-body problem, which provide a rather different perspective on the whole question of frame singularities. We present this subject only in outline form since most of it has already been discussed elsewhere [4]. The relation between frame singularities and monopole singularities is important because it shows that all choices of body frame in the three-body problem lead to singularities somewhere and it shows that the singularities of the Eckart frame are of a minimal kind. A standard introduction to the theory of monopoles is given by Sakurai [21].

A magnetic monopole is a hypothetical particle with a magnetic field $\mathbf{B}(\mathbf{r})=g\mathbf{r}/r^3$, where g is the magnetic charge and $\mathbf{r}$ is the position vector in ordinary space. Since $\nabla\cdot\mathbf{B}=4\pi g\,\delta(\mathbf{r})$, there should exist a vector potential $\mathbf{A}$ such that $\mathbf{B}=\nabla\times\mathbf{A}$ in regions that do not include the origin $\mathbf{r}=\mathbf{0}$. Of course, we expect $\mathbf{A}$ to become singular as $\mathbf{r}\to\mathbf{0}$, where the singularity of $\mathbf{B}$ lies. Also, we know that the vector potential is not unique; once one vector potential $\mathbf{A}$ has been found, we can generate another by the rule $\mathbf{A}'=\mathbf{A}+\nabla f$, where f is an arbitrary scalar function.

In fact, it is not hard to find a vector potential by uncurling $\mathbf{B}$ in spherical coordinates (the result is presented by Sakurai [21]). However, one will find that this vector potential has singularities not only at $\mathbf{r}=\mathbf{0}$ as expected, but also on a line emanating from $\mathbf{r}=\mathbf{0}$. This line is the *string* of the monopole. One will find that by doing gauge transformations, the string can be moved around, for example, to point in this or that direction, but that it apparently cannot be eliminated. The question then arises, Does there exist a gauge transformation that will eliminate the string singularity, that is, can one find a vector potential $\mathbf{A}$ that is nonsingular everywhere outside of $\mathbf{r}=\mathbf{0}$? The answer is no, as can be proved by Stokes' theorem. We simply integrate $\mathbf{B}$ over a sphere centered on the origin, with a small hole cut out of it. In the limit that the size of the hole goes to zero, the integral approaches $4\pi g$. However, by Stokes's theorem, the integral must also be equal to the line integral of $\mathbf{A}$ around the small hole, which must approach zero if $\mathbf{A}$ is continuous. Therefore, $\mathbf{A}$ cannot be continuous everywhere on the sphere; it must have at least one point where it is discontinuous. This is the string.

There is also a ''Coriolis'' vector potential in the Hamiltonian for the three-body problem [4], which physically describes Coriolis forces, and it turns out that changes of body frame affect this potential in exactly the same way as changes of gauge affect a magnetic vector potential. It also turns out that the curl of this Coriolis vector potential is a monopole field in shape space, as discovered by Iwai [23]. Therefore, frame singularities in the three-body problem are isomorphic to monopole string singularities. In particular, they can be moved around by frame transformations, but they can never be completely eliminated. These frame singularities occur at the same places in shape space as the singularities of the Coriolis coupling terms in the Hamiltonian.

For example, the principal axis frame puts the string singularity on the entire w_3 axis. Since this includes both positive and negative sides, one might say that there are two strings; this is not the minimal configuration. However, by transforming to an Eckart frame, we can remove the string singularity from either the positive or negative w_3 axis, thereby leaving only one string. This is the minimal configuration. By further changes of frame, the string can be moved to other locations. For example, a common choice of body frame in practice, useful for describing the asymptotic state of $AB+C$ systems in an entrance or exit channel, is one in which the longer Jacobi vector is placed on the body z axis and the shorter one in the $x-y$ plane. Then it turns out that this frame causes the string singularity to lie on the negative w_1 axis. If the roles of the longer and shorter Jacobi vectors are reversed, then the string lies on the positive w_1 axis. These two frames and the singularities they cause in the internal Hamiltonian have been given a clear description by Pack [16]. Other choices are possible (the string can be moved to point in an arbitrary direction; it can even be curved).

The monopole analogy leads to useful insights in the three-body problem; for example, we have shown elsewhere [20] that Smith's hyperspherical harmonics for the planar three-body problem are identical to spherical harmonics for the motion of a charged particle in a monopole field. We believe that these monopole analogies will lead to further insights into the problems of basis set contraction in the three-body problem. We will report on these ideas elsewhere.

In conclusion, we have presented a geometrical analysis of frame singularities in the three-body problem. This has led to insight into the problem of locating, moving, or removing frame singularities in the three-body problem. It also has provided the necessary background for understanding the problem of frame singularities in the four-body problem. Finally, we have commented on the relationship between frame singularities in the three-body problem and the string singularities of magnetic monopoles, which is useful for constructing a proof of the impossibility of eliminating all frame singularities, as well as for providing insights into hyperspherical harmonics and other matters. In particular, we believe that hyperspherical harmonics [22], or better their generalizations as solutions of the kinetic-energy operator on the manifolds explored here and with the various choices for coordinates and frames discussed here, will serve as well behaved basis sets for problems involving reactivity and large-amplitude vibrations. Use of their discrete analogs will admit localized representations and will accelerate convergence by eliminating dynamically unimportant regions of phase space. We plan to report on these applications in the future.

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