# Internal spaces, kinematic rotations, and body frames for four-atom systems

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Four-atom systems may soon be subject to state-to-state reactive scattering calculations and understanding body frames and their singularities will be an important part of this effort. This paper examines body frames in four-atom systems, building on a geometrical analysis of the nine-dimensional configuration space and the six-dimensional internal space. Kinematic rotations are an important tool in this analysis. A central role is played by the ''kinetic cube,'' the space of all asymmetric top shapes related by kinematic rotations. The singularities, multiple branches, and connectivity of the principal axis frame are examined in detail and related to the topology of the kinetic cube. The principal axis frame has singularities on all symmetric top shapes, both oblate and prolate, of both chiralities. A version of the Eckart frame, however, has singularities only on prolate symmetric top shapes of one chirality. Frame singularities are inevitable in the four-body problem and no other frame has a smaller singular set than the Eckart frame. [S1050-2947(98)07211-4]

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## I. INTRODUCTION

This paper is the second in a series concerning body frames and their singularities in the quantum dynamics of $n$-particle systems. The first of these papers [1], concerning body frames in the three-body problem, is necessary background for the present paper, which focuses on the four-body problem. The meaning of frame singularities, their effect on internal wave functions, their topological inevitability, and the latitude one has in moving them around in the internal space are all exemplified by the three-body case and are discussed in Ref. [1]. Many of the facts presented in Ref. [1] on body frames in the three-body problem are familiar to practitioners in the field, although our geometrical perspective is almost completely different. In the four-body problem, however, the whole complex of issues surrounding frames and their singularities is much less well explored.

Recently, serious consideration has been given to the possibility of four-atom, state-to-state reactive scattering calculations [2,3]. Even three-atom scattering calculations are highly nontrivial and the step up to the four-body case is a long one. Bound-state calculations are easier, mainly because bound-state wave functions occupy a smaller portion of the configuration space than scattering wave functions. However, whenever any wave function in the four-body problem, whether bound or unbound, occupies a sufficiently large portion of the configuration space, it will be necessary to deal with frame singularities. For example, we will show in this paper that in the four-body problem with its six-dimensional internal space all definitions of body frames possess singularities on the three-dimensional manifold of collinear shapes, as well as on a four-dimensional surface that emanates from this manifold. The latter surface can be moved around by changing to a different body frame, but it cannot be eliminated. If a wave function is restricted to a sufficiently small region of the internal space, it may be possible to avoid the surfaces on which the frames are singular (or to choose a frame that places the singular surface outside the physically interesting region), but any internal wave function that crosses the singular surface will itself become singular on the surface.

The practical importance of the frame singularities will become apparent as soon as anyone computes an actual internal wave function with $J \neq 0$ for a four-atom system that occupies a sufficiently large portion of the internal space. That the frame singularities have not been noted previously in four-atom systems is due to several circumstances. First, if $J=0$, then frame singularities do not cause singularities in the internal wave function. Of course, the condition $J=0$ is more common in the literature than in the real world. Next, small-amplitude vibrations about a noncollinear equilibrium in many cases do not explore enough of the configuration space to run into frame singularities and the same is true for some types of large amplitude motion. As for collinear equilibria, in the four-body problem there are always frame singularities in the neighborhood of such shapes. These singularities can be avoided by modifying the usual formalism of frames and Euler angles, as in the (now) standard analysis of Watson [4]. However, as we show below, the surface of frame singularities in the four-body problem extends from the collinear manifold out to infinity and so always exists in regions where the standard collinear analysis is not useful. As explained in Ref. [1], the situation in the three-body problem is different and not as serious, because frame singularities need not occur at collinear shapes, nor is there any singular manifold extending out from the collinear shapes (only the three-body collision is attached to the manifold of frame singularities and that manifold, the ''string,'' can be placed in the nonphysical region).

Although there are many ways to define a body frame, in the case of the four-body problem the principal axis frame has been a popular choice in many works going back over the last 30 years [3,5–9,14]. This is presumably because the principal axis frame emerges naturally out of the singular value decomposition of the matrix of space-referred Jacobi vectors (which is $\mathsf{F}_s$ in the notation explained below; the decomposition is $\mathsf{F}_s = \mathsf{R}\Lambda\mathsf{K}^t$, where $\mathsf{R}$ is the external rotation defining the Euler angles in the principal axis frame, $\Lambda$ is the diagonal matrix of singular values, and $\mathsf{K}$ is a kinematic rotation). Partly for this reason, this paper devotes special attention to the principal axis frame. However, the principal axis frame is multiple valued or if forced to be single valued it has branch cuts and associated discontinuities. Moreover, its singular surface is not of the minimal size that can be achieved with other frames. Clearly, it is important that the question of frames and their singularities be addressed from a general standpoint, not just in the case of the principal axis frame.

The singular value decomposition just alluded to is part of what might be called the analytical or coordinate-based perspective on the $n$-body problem. This is a perspective in which the properties of the internal wave equation or wave function are transcribed into some coordinate system and expressed in terms of equations involving numbers, variables, matrices, etc. In Ref. [1] and this paper we are emphasizing a different perspective, the geometrical one. In the geometrical perspective, we view the properties of frames, wave functions, etc., in terms of curves and surfaces in the internal space. Both perspectives are important, but the geometrical one grows in significance as the dimensionalities of the spaces involved gets larger. In particular, the four-body problem involves spaces of relatively high dimensionality, where a geometrical approach is most helpful. For example, the space of asymmetric top shapes in the four-body problem that are related by kinematic rotations is the space we call the kinetic cube; it is a three-dimensional manifold with a nontrivial topology, which we discuss quite carefully below. For another example, in previous work by some of the present authors [10], it has been shown that the exit channels in four-body collinear scattering reactions can be arranged on a certain two-dimensional sphere ($S^2$), whose significance in the internal space is discussed below.

In the course of writing this paper we discovered that to fully explore body frames in the four-body problem it was necessary to delve deeper into the structure of the internal space than has been done before and especially to make extensive use of kinematic rotations. Although kinematic rotations have been used for many years, it would seem that in many people's minds they are restricted to the discrete set of transformations that map one exit channel into another (or one choice of Jacobi vectors to another). In this work, however, we have been more interested in the continuous group of kinematic rotations and its geometrical relation to the internal space. We feel we have revealed some of the mysteries of the kinematic rotations, but that other applications remain to be developed, such as to models of polyatomic dynamics in which motions are constrained to consist of pure kinematic rotations. For example, in some cases reaction paths in pseudorotational motions are approximately of this kind. Certainly kinematic rotations provide a relatively different perspective on such problems and allow one to visualize and formulate questions in a different way.

This paper involves mathematical methods of a more geometrical character than those used in Ref. [1] on the three-body problem, as is appropriate for the higher-dimensional spaces involved in the four-body problem. Such mathematical methods have not been frequently applied in molecular physics, although their use in other areas of physics and applied mathematics is common. We have tried to make this paper self-contained by providing two mathematical appendixes. Some familiarity with the elements of abstract group theory is assumed (notions such as cosets and conjugate subgroups) as well as some basic facts about the continuous groups SO(2) and SO(3) (such as the fact that they are manifolds of dimensionality one and three respectively).

Finally, we mention that we consider only the case $n=4$ in this paper, not $n\geqslant 5$. This is because there is already plenty to say about four-body problems and also because (for scattering problems, at least) practical, numerical calculations for the case $n\geqslant 5$ are a much more remote possibility than the case $n=4$.

The organization of this paper is as follows. Section II is a short section discussing the configuration space for the four-body problem and the groups (external and kinematic rotations) that act on it. Section III is another short section discussing the internal or shape space for the four-body problem and useful coordinate systems defined on it. Section IV discusses the action of kinematic rotations on the four-body shape space and analyzes in detail the three cases of asymmetric, symmetric, and spherical tops. Special attention is given to the kinematic orbits in the case of the asymmetric tops (the kinetic cube). This space is shown to be either the space of cosets of SO(3) with respect to the subgroup (the viergruppe) of diagonal, proper orthogonal matrices or of SU(2) with respect to the eight-element quaternion subgroup and its topology is examined carefully. Section V is devoted to the principal axis frame and its properties: its multiple branches and their connectivity under continuous deformations of shape, the restriction to a single branch by means of branch cuts, and the discontinuities across the branch cuts. We find that the jumps in the principal axis frame on going around closed loops in the internal space are directly related to the topological properties of the kinetic cube. In Sec. VI we examine the singularities of the principal axis frame, which occur at all symmetric top shapes, both oblate and prolate. We also introduce a version of the Eckart frame that has singularities on a smaller subset of the internal space than the principal axis frame, namely, on the prolate symmetric tops of one chirality only. We discuss the relation of these singular sets to the phenomenon of string singularities in the field of magnetic monopoles and indicate why no frame has singularities on a smaller subset of the internal space than the Eckart frame. Finally, in Sec. VII we present some conclusions and thoughts about future work. Three appendixes are also supplied. Appendix A explains the concept of group actions, which is central to the development of the present paper, and Appendix B concerns the various spaces that occur in the main body of the paper and the standard mathematical notation for them. Finally, Appendix C contains some material moved from the main body of the paper for purposes of continuity of flow.

## II. CONFIGURATION SPACE AND GROUP ACTIONS

The configuration space in the four-body problem, after the elimination of the center-of-mass degrees of freedom, is

TABLE I. Orbits and their isotropy subgroups for the action of external rotations on the configuration space of the four-body problem.

| Case | Orbit | Orbit dimension | Isotropy subgroup |
|---|---|---|---|
| noncollinear | SO(3) | 3 | $\{\mathsf{I}\}$ |
| collinear | $S^2$ | 2 | SO(2) |
| four-body collision | one point | 0 | SO(3) |

the space $\mathbb{R}^9$, on which the nine components of the three mass-weighted Jacobi vectors $\mathbf{r}_{s\alpha}$, $\alpha=1,2,3$, are coordinates. As in Ref. [1], we use an $s$ subscript to indicate the space or inertial frame components of a vector or tensor and use greek indices $\alpha$, $\beta$, etc., to label Jacobi vectors. We define the Jacobi vectors in the usual way by linking particle 1 to 2, then these to 3, and then linking the first three to particle 4. All other choices of Jacobi vectors are related to this choice by constant kinematic rotations (defined momentarily). As in Ref. [1], we represent a point of configuration space by $Q=\{\mathbf{r}_{s\alpha}\}$.

We introduce the $3\times3$ matrices $\mathsf{F}_s$, $\mathsf{T}_s$, and $\mathsf{J}$, defined by $F_{si\alpha}=r_{s\alpha i}$, $\mathsf{T}_s=\mathsf{F}_s\mathsf{F}_s^t$, and $\mathsf{J}=\mathsf{F}_s^t\mathsf{F}_s$, respectively, where the $t$ superscript is the matrix transpose and $i=1,2,3$ stands for $x,y,z$. These are the obvious generalizations of Eqs. (2.7), (2.8), and (2.11) of Ref. [1] to the case of four particles. The matrix $\mathsf{F}_s$ simply contains the three Jacobi vectors in its three columns and therefore it labels a point of configuration space equally as well as the symbol $Q$. We call $\mathsf{T}_s$ the moment tensor and $\mathsf{J}$ the Jacobi dot product tensor, the latter because $J_{\alpha\beta}=\mathbf{r}_{s\alpha}\cdot\mathbf{r}_{s\beta}$. As in Eq. (2.9) of Ref. [1], the moment of inertia tensor (with respect to the space frame) $\mathsf{M}_s$ is related to the moment tensor by $\mathsf{M}_s=(\mathrm{tr}\,\mathsf{T}_s)\mathsf{I}-\mathsf{T}_s$. As proved in Ref. [13], the three (necessarily non-negative) eigenvalues of $\mathsf{T}_s$ and those of $\mathsf{J}$ are identical. We call these three eigenvalues $\lambda_1$, $\lambda_2$, and $\lambda_3$; they are related to the eigenvalues of the moment of inertia tensor $\mu_1,\mu_2,\mu_3$ by Eq. (2.10) of Ref. [1].

A point $Q=\{\mathbf{r}_{s\alpha}\}$ of configuration space is acted upon by external rotations according to $\mathbf{r}'_{s\alpha}=\mathsf{R}\mathbf{r}_{s\alpha}$, where $\mathsf{R}\in\mathrm{SO}(3)$, which physically represents a rigid rotation of the four-particle system. We will write this as $Q'=RQ$ for short; see Eq. (2.1) of Ref. [1]. As in that paper, $R$ (in italics) stands for an element of SO(3) as an abstract group and $\mathsf{R}$ (in sans serif) stands for the corresponding $3\times3$ matrix. In terms of the matrix $\mathsf{F}_s$, the action of external rotations can also be written $\mathsf{F}'_s=\mathsf{R}\mathsf{F}_s$. Two configurations are considered to have the same shape if and only if they are related by some proper external rotation. The description of rotation orbits, fibers, and the fiber bundle can be taken over from the three-body case [1] almost word for word, but here we will take the opportunity to introduce and exemplify the language of group actions, orbits, and isotropy subgroups, which is so important for understanding the four-body problem. This language is explained in Appendix A.

The different cases are summarized in Table I. If the configuration $Q$ is noncollinear, then the only rotation that leaves $Q$ invariant is the identity, so the isotropy subgroup at $Q$ is just the trivial subgroup $\{\mathsf{I}\}$ containing the identity $\mathsf{I}\in\mathrm{SO}(3)$. In this case, the points of the orbit can be placed in one-to-one correspondence with rotations $\mathsf{R}\in\mathrm{SO}(3)$; equivalently, the Euler angles of those rotations can be used as coordinates along the orbit. This is what is always done in practice in defining the external Euler angles. In this case, the orbit is a three-dimensional surface that is a copy of SO(3). That is, the orbit is diffeomorphic (see Appendix B) to SO(3).

If $Q$ is a collinear configuration (all three Jacobi vectors are parallel, but at least one is nonvanishing), then rotations about the axis of collinearity do nothing to the configuration. In this case, the isotropy subgroup of $Q$ is SO(2), the subgroup of rotations about a fixed axis, which are proper orthogonal transformations in the plane perpendicular to the axis. It is obvious geometrically that the orbit of a collinear configuration under the external rotation group SO(3) is the two-sphere $S^2$ (this notation is explained in Appendix B), because a rotation can only change the direction of collinearity, and the final configuration is uniquely specified by a unit vector indicating that direction. The same fact can be expressed in the language of quotient spaces, explained in Appendix A; the points of the orbit can be placed in one-to-one correspondence with the left cosets of SO(2) within SO(3) and, as proved in Appendix B, the space of these cosets is $S^2$,

$$S^2=\frac{\mathrm{SO}(3)}{\mathrm{SO}(2)}. \tag{2.1}$$

Finally, if $Q$ is the four-body collision (all three Jacobi vectors vanish), then the isotropy subgroup is all of SO(3) and the orbit is just a point (the four-body collision itself).

Next we introduce kinematic rotations and their action on configuration space. The kinematic group, which was SO(2) in the three-body problem, is SO(3) in the four-body problem. As an abstract group, the kinematic group is the same as the external rotation group, but the action is different; if $K\in\mathrm{SO}(3)$, then the action of $K$ on $Q=\{\mathbf{r}_{s\alpha}\}$ is given by

$$\mathbf{r}'_{s\alpha}=\sum_{\beta=1}^{3}K_{\alpha\beta}\mathbf{r}_{s\beta}, \tag{2.2}$$

which is the obvious generalization of Eq. (2.2) of Ref. [1]. We will also write this as $Q'=KQ$; in terms of the $\mathsf{F}_s$ matrix, the action (2.2) is $\mathsf{F}'_s=\mathsf{F}_s\mathsf{K}^t$. In these equations, $K$ stands for an element of SO(3) as an abstract group, $\mathsf{K}$ for the corresponding $3\times3$ matrix, $K_{\alpha\beta}$ for the components of this matrix, and $\mathsf{K}^t$ for the transpose of this matrix.

The orbits of the kinematic action on configuration space are discussed in Appendix C in order not to interrupt the flow of the presentation. However, the reader may wish to return to Appendix C after reading Sec. IV below, on the kinematic orbits in shape space.

## III. SHAPE SPACE IN THE FOUR-BODY PROBLEM

Shape space is the space in which a single point represents an entire external rotation orbit in configuration space. In the three-body problem, shape space is the quotient space $\mathbb{R}^6/\mathrm{SO}(3)$, which is one-half of $\mathbb{R}^3$; this fact was not proved in Ref. [1] because it was assumed to be familiar to most readers who have worked with three-body problems. In the four-body problem, shape space is the quotient space $\mathbb{R}^9/\mathrm{SO}(3)$, which turns out to be $\mathbb{R}^6$. It is not entirely trivial to prove this, but a complete and careful proof is given in Ref. [13]; see also the work of Kuppermann [2,3], who has considered many of the same issues treated in Ref. [13].

To say that shape space is $\mathbb{R}^6$ means that there exists a set of six shape coordinates, each of which ranges from $-\infty$ to $+\infty$, such that there is a one-to-one correspondence between shapes (that is, external rotation orbits in configuration space) and coordinate sixtuplets. In the literature it is popular to use other coordinate systems, usually containing some kind of hyperspherical angles, which of course have finite ranges. Such coordinates are potentially useful for numerical integration schemes, but usually are not so convenient for understanding the global topology and structure of shape space. This is mainly because when the angular coordinates are at the ends of their ranges, they are not usually in one-to-one correspondence with shapes and the boundaries of these ranges correspond to surfaces in shape space where different regions of that space join continuously to one another. Thus it takes some extra effort to understand topological questions in such a coordinate system. For this reason, we will begin our discussion of shape space with coordinates that make it evident that shape space is $\mathbb{R}^6$.

The theory of these coordinates is given in full detail in Ref. [13]. This theory relies on two theorems, proved in Ref. [13]. The first states that if two configurations $Q$ and $Q'$ have the same $\mathsf{J}$ tensor, then they are related by either a proper or an improper rotation. As we will say, $Q$ and $Q'$ have the same shape modulo chirality. The $\mathsf{J}$ tensor is a $3\times 3$, symmetric non-negative definite matrix. The second theorem states that every $3\times 3$, symmetric non-negative definite matrix is the $\mathsf{J}$ tensor for some shape. More precisely, the second theorem states that if such a matrix has nonzero determinant, then it corresponds to precisely two shapes of nonzero volume and opposite chirality, whereas if its determinant is zero, then it corresponds to precisely one shape of zero volume, that is, a planar shape.

We will not prove these theorems here, but simply note that they are believable on several grounds. First, from the definition of $\mathsf{J}$, it follows that

$$\det \mathsf{J} = V^2, \tag{3.1}$$

where $V$ is the signed volume contained in the parallelepiped spanned by the Jacobi vectors,

$$V = \det \mathsf{F}_s = \mathbf{r}_{s1}\cdot(\mathbf{r}_{s2}\times\mathbf{r}_{s3}). \tag{3.2}$$

We will refer to shapes of positive or negative volume as shapes of positive or negative chirality, respectively, because the spatial inversion operation, which takes $\{\mathbf{r}_{s\alpha}\}$ into $\{-\mathbf{r}_{s\alpha}\}$ or $\mathsf{F}_s$ into $-\mathsf{F}_s$, also takes $V$ into $-V$.

Next, it is not hard to see for the four-body problem that knowledge of the $\mathsf{J}$ tensor implies knowledge of the shape, modulo chirality, because from the Jacobi dot products one can find the dot products of the vectors connecting the particles and from these the interparticle distances. However, the interparticle distances determine the shape of a tetrahedron modulo chirality.

These theorems suggest that we seek a parametrization of the $\mathsf{J}$ matrices. Since such matrices are symmetric, they have six independent components; the following linear combinations of these components are convenient parameters:

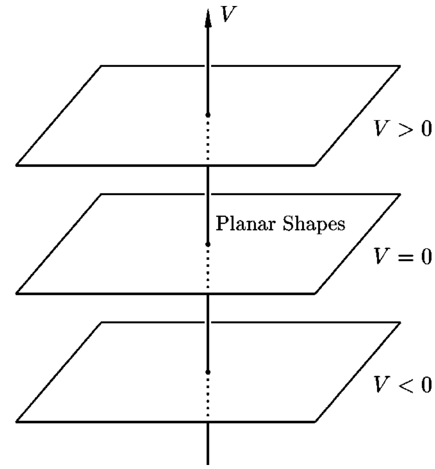


FIG. 1. The six-dimensional shape space for the four-body problem may be visualized by taking slices at constant $V$, giving a series of five-dimensional hyperplanes. The hyperplane $V=0$ contains the planar shapes.

$$\begin{aligned} w &= r_{s1}^2 + r_{s2}^2 + r_{s3}^2, \quad w_3 = \sqrt{3}\,\mathbf{r}_{s2}\cdot\mathbf{r}_{s3}, \\ w_1 &= (\sqrt{3}/2)(r_{s1}^2 - r_{s2}^2), \quad w_4 = \sqrt{3}\,\mathbf{r}_{s3}\cdot\mathbf{r}_{s1}, \\ w_2 &= \sqrt{3}\,\mathbf{r}_{s1}\cdot\mathbf{r}_{s2}, \quad w_5 = (1/2)(-r_{s1}^2 - r_{s2}^2 + 2r_{s3}^2). \end{aligned} \tag{3.3}$$

Note that $w = \operatorname{tr}\mathsf{J} = \rho^2$, where $\rho$ is the hyperradius, and that $(w_1,\dots,w_5)$ specify the symmetric, traceless part of $\mathsf{J}$. In these equations, $r_{s\alpha} = |\mathbf{r}_{s\alpha}|$.

The six quantities $(w;w_1,\dots,w_5)$ can be used locally as coordinates on shape space for the four-body problem, but are not suitable globally, for three reasons. First, they do not distinguish shapes related by chirality; second, there are values of these coordinates that are not physically meaningful because they correspond to $\mathsf{J}$ matrices that have negative eigenvalues; and third, the ranges of the coordinates that specify the boundaries of the physically meaningful region are not independent of one another.

These difficulties are analyzed in detail in Ref. [13], where it is shown that an alternative coordinate set $(V;w_1,\dots,w_5)$ solves all the problems listed. In the coordinate system $(V;w_1,\dots,w_5)$, all six coordinates range from $-\infty$ to $+\infty$ and coordinate sixtuplets stand in precisely one-to-one correspondence with shapes. These coordinates are probably the best for understanding global topological questions in the four-body shape space, although for other purposes other coordinate systems are needed (and will be introduced below).

For example, we can visualize four-body shape space as illustrated in Fig. 1, in which $\mathbb{R}^6$ is decomposed into slices of constant $V$, each of which is $\mathbb{R}^5$, a five-dimensional hyperplane. The $V=0$ slice is the hyperplane containing the planar shapes of zero volume, which separates the region $V>0$ of shapes of positive chirality from the region $V<0$ of shapes of negative chirality. Incidentally, this shows immediately that in the four-body problem, one cannot pass continuously from a shape of positive chirality to one of negative chirality without passing through a planar shape (a fact that can be seen in other ways). (This statement does not hold for $n>4$.) The volume $V$ corresponds most closely to the area coordinate $w_3$ in the three-body problem (here the analogy is stronger for the planar three-body problem, in which $w_3$ can take on negative values) and the coordinates $(w_1,\ldots,w_5)$ in the four-body problem are analogous to the coordinates $(w_1,w_2)$ in the three-body problem.

## IV. KINEMATIC ORBITS IN SHAPE SPACE

An idea developed by Zickendraht [5] and apparently rediscovered several times since is to use the Euler angles of the kinematic rotations and some set of kinematic invariants as coordinates on the shape space for the four-body problem. In light of the discussion of Appendix A, this idea obviously involves the decomposition of shape space into the orbits of the kinematic group. In this section we will examine the action of the kinematic group on shape space in detail. We first set up a suitable section of the kinematic fiber bundle (this concept is explained in Ref. [1]), consisting (within an $\mathbb{R}^5$ hyperplane at constant $V$) of a 60° sector in the $w_1$-$w_5$ plane, what we will call the principal sector. Next we classify the kinematic orbits themselves and show that they depend on whether the shape is an asymmetric top, a symmetric top, or a spherical top. Finally, we examine the kinematic orbit for the asymmetric top in some detail because it is a space that is more difficult to visualize than the others. We call this space the kinetic cube because it can be represented by a cube in certain coordinate systems, with certain ''gluing rules,'' that is, identification of points on opposite faces.

### A. A section of the kinematic fiber bundle

We begin by constructing a suitable section of the kinematic fiber bundle, that is, a surface in shape space that intersects each kinematic orbit at one point. The kinematic action on configuration space $\mathsf{F}_s'=\mathsf{F}_s\mathsf{K}^t$ for $\mathsf{K}\in \mathrm{SO}(3)$ implies a certain kinematic action on shape space. This action is captured by the transformation law for the $\mathsf{J}$ tensor under kinematic rotations,

$$\mathsf{J}'=\mathsf{K}\mathsf{J}\mathsf{K}^t, \tag{4.1}$$

which follows from the definition of $\mathsf{J}$ and implies that the old and new coordinates $(w;w_1,\ldots,w_5)$ under a kinematic rotation are related by a linear transformation. In fact, $w=\rho^2=\mathrm{tr}\,\mathsf{J}$ is invariant under kinematic rotations and $(w_1,\ldots,w_5)$ transform according to the $\ell=2$ irreducible representation of SO(3), precisely as quadrupole moment tensors transform under ordinary rotations. The $\ell=2$ irreducible representation is five dimensional and the matrix representing the transformation of the coordinates $(w_1,\ldots,w_5)$ is just the usual $D^2_{mm'}$ matrix or rather this matrix reexpressed in a nonstandard basis. The nonstandard basis is convenient for present purposes because the usual (spherical) basis is complex. The particular linear combinations shown in the definitions of $(w_1,\ldots,w_5)$ in Eq. (3.3) were chosen to be real and so that the transformation matrix [the five-dimensional irreducible representative of SO(3)] would be orthogonal. Apart from that, the choice was essentially arbitrary. Our paper [13] explains the group theory of the transformation (4.1) (why it contains the $\ell=2$ irreducible representation, etc). A different approach that reaches similar conclusions has been given by Kuppermann [2,3].

To visualize the action of the kinematic group on shape space, we first note that the volume $V$ is a kinematic invariant, $V'=\det(\mathsf{F}_s')=\det(\mathsf{F}_s\mathsf{K}^t)=\det \mathsf{F}_s=V$, since $\det \mathsf{K}=1$. Therefore, the kinematic orbits are confined to the five-dimensional hyperplanes $V=\mathrm{const}$ illustrated in Fig. 1. Within one of these hyperplanes, the five coordinates $(w_1,\ldots,w_5)$ transform linearly under kinematic rotations, as was just mentioned; these coordinates by themselves indicate the shapes through which the kinematic orbit passes since $V$ is given. Equivalently, the $\mathsf{J}$ tensor by itself identifies a shape on a constant $V$ slice since $V$ determines the chirality.

Now let $q$ be a point in one of these hyperplanes, corresponding to some $\mathsf{J}$ matrix, and consider the kinematic orbit passing through $q$. Since every symmetric matrix can be diagonalized by some orthogonal transformation, there certainly exists a point on the kinematic orbit with a diagonal $\mathsf{J}$ matrix. However, it follows from Eq. (3.3) that the diagonal $\mathsf{J}$ matrices lie on the two-dimensional subspace of the five-dimensional hyperplane given by $w_2=w_3=w_4=0$, that is, on the $w_1$-$w_5$ plane. Therefore, every kinematic orbit passes through the $w_1$-$w_5$ plane. On this plane, the $\mathsf{J}$ matrix is diagonal,

$$\mathsf{J}=\mathrm{diag}(\lambda_1,\lambda_2,\lambda_3), \tag{4.2}$$

so the three Jacobi vectors $\mathbf{r}_{s\alpha}$ are orthogonal there and $\lambda_\alpha=r^2_{s\alpha}$. Also, according to Eq. (3.3), the eigenvalues are related to the the $w$ coordinates by

$$w_1=(\sqrt{3}/2)(\lambda_1-\lambda_2),$$
$$w_5=(1/2)(-\lambda_1-\lambda_2+2\lambda_3). \tag{4.3}$$

The analog of the $w_1$-$w_5$ plane (at fixed $V$) in the four-body problem is the $w_1$ axis (at fixed $w_3$) for the three-body problem; equivalently, the analog of the three-dimensional $w_1$-$w_5$-$V$ hyperplane in the four-body problem is the $w_1$-$w_3$ plane in the three-body problem. We recall that the latter plane in the three-body problem is the one upon which the $2\times 2$ $\mathsf{J}$ tensor is diagonal and that each asymmetric top kinematic orbit intersects that plane at two points; for this reason, we had to take a subset of that plane ($w_1>0$ for the planar three-body problem) in order to obtain a section of the kinematic fiber bundle, that is, a surface that is intersected only once by each kinematic orbit. We will now see the analogs of these facts for the four-body problem.

We return to the four-body problem. All kinematic orbits intersect the $w_1$-$w_5$ plane at least once, but in fact most of them pass through this plane more than once because different diagonal matrices can be achieved by permuting the eigenvalues. As a first case, suppose all three eigenvalues $\lambda_\alpha$ are distinct (an asymmetric top). Then there are $3!=6$ distinct diagonal matrices that can be obtained by applying kinematic rotations to a given $\mathsf{J}$ matrix, according to Eq. (4.1). Therefore, the kinematic orbit passing through any asymmetric top shape intersects the $w_1$-$w_5$ plane in six points. Next, if two of the eigenvalues are equal and the third distinct (a symmetric top, either oblate or prolate), then there are three distinct permutations of the eigenvalues and each kinematic orbit passes through the $w_1$-$w_5$ plane at three points. Finally, if all three eigenvalues are equal (a spherical top), the kinematic orbit intersects the $w_1$-$w_5$ plane at just one point (the orbit is that one point).

To obtain a useful section of the kinematic fiber bundle, we require a surface that intersects each kinematic orbit only once. Taking first the case of asymmetric tops (all three eigenvalues unequal), we can achieve a unique diagonal $\mathsf{J}$ matrix by requiring that the eigenvalues be in a descending order $\lambda_1>\lambda_2>\lambda_3\geqslant 0$. However, by Eq. (4.3), we see that $\lambda_1>\lambda_2$ when $w_1>0$ and $\lambda_2>\lambda_3$ when $w_5<-w_1/\sqrt{3}$. These conditions restrict us to the region labeled I in Fig. 2, a 60° sector lying between polar angles $\theta=-90°$ and $\theta=-30°$. We will call this region the *fundamental sector* and take it to be the section of the kinematic fiber bundle in the four-body problem. Also illustrated are five other sectors, labeled II–VI, in which the ordering of the eigenvalues is permuted. The point marked by a cross in the fundamental sector represents an initial point on an asymmetric top kinematic orbit and the other points labeled by a cross, one in each sector, represent the other intersections of that kinematic orbit with the $w_1$-$w_5$ plane. One can show that such points are related to one another by reflections in the $w_5$ axis and in the two lines $w_5=\pm w_1/\sqrt{3}$.

Next we note that as we approach the $w_5$ axis (the line $w_1=0$) from within the fundamental sector, we achieve a shape for which $\lambda_1=\lambda_2>\lambda_3$, which is an oblate symmetric top (because these conditions imply $\mu_3>\mu_1=\mu_2$). Thus the negative $w_5$ axis is a half line of oblate symmetric tops, as are the other two half lines in the figure labeled $O$, rotated by $\pm 120°$ from this one. An oblate symmetric top shape is indicated by a closed circle, as are the other two intersections with the $w_1$-$w_5$ plane of the kinematic orbit passing through this shape. Similarly, as we approach the line $w_5=-w_1/\sqrt{3}$ from within the fundamental sector, we achieve the condition $\lambda_1>\lambda_2=\lambda_3$, which defines a prolate symmetric top (because these conditions imply $\mu_1<\mu_2=\mu_3$). The three half lines labeled $P$ in the figure, related to one another by 120° rotations, are the half lines of prolate top shapes. The asterisk in the figure represents a prolate symmetric top shape and the kinematic orbit passing through this shape intersects the $w_1$-$w_5$ plane in two other points, also labeled by an asterisk. Finally, the origin of the $w_1$-$w_5$ plane is a spherical top (all three eigenvalues equal); the orbit of this point intersects the $w_1$-$w_5$ plane in a single point (the origin itself).

The general picture of the kinematic section presented by Fig. 2 is independent of the value of $V$, but if $V=0$ there is one further comment. In this case, since $V^2=\lambda_1\lambda_2\lambda_3$ and the (necessarily non-negative) eigenvalues are in descending order in the fundamental sector, it follows that $\lambda_3=0$ in this sector. This means that on the half line of prolate shapes at polar angle of $\theta=-30°$, we have $\lambda_1>\lambda_2=\lambda_3=0$, which is the condition for a collinear configuration. Likewise, the other two half lines labeled $P$ are collinear configurations within the hyperplane $V=0$.

For the three-body problem in space, a section of the kinematic fiber bundle is the region $w_1,w_3>0$ of the $w_1$-$w_3$ plane (or the region $w_1>0$ in the case of the planar three-body problem, see the end of Sec. II of Ref. [1]). The analog of this region for the four-body problem is the three-dimensional wedge $S\times\mathbb{R}$, the Cartesian product of the fundamental sector $S$ in Fig. 2 with $\mathbb{R}$, the latter representing the volume $(-\infty<V<\infty)$. The wedge $S\times\mathbb{R}$ is otherwise the space of kinematic invariants; we will say more about it below.

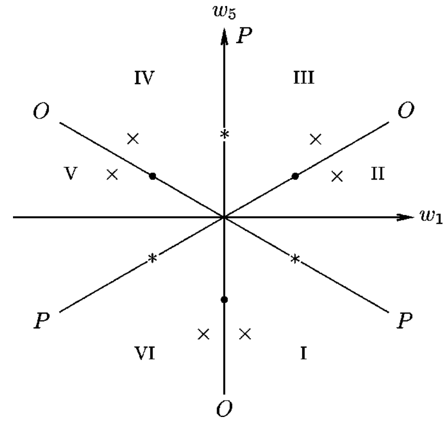


FIG. 2. The section of the kinematic fiber bundle is sector $I$ (the fundamental sector) in the $w_1$-$w_5$ plane. The interior of this sector contains asymmetric tops; the six intersections of an asymmetric top kinematic orbit with the $w_1$-$w_5$ plane are labeled $\times$. The radial half lines labeled $P$ or $O$ contain, respectively, the prolate and oblate symmetric tops. The three intersections of an oblate symmetric top kinematic orbit with the $w_1$-$w_5$ plane are labeled $\bullet$; similarly $*$ labels the prolate symmetric tops. The spherical top is at the origin.

### B. Kinematic orbits in shape space

Next we examine the nature of the kinematic orbits, which are generated by allowing all kinematic rotations to act on points of the fundamental sector (including its edges, if we want the symmetric and spherical tops). We do this by first finding the isotropy subgroups for the various cases. Since $V$ is fixed, a shape is uniquely identified by the $\mathsf{J}$ tensor, which transforms according to Eq. (4.1). It suffices to find the isotropy subgroups for points on the section since the isotropy subgroups at different points on an orbit are just conjugate subgroups and are identical as abstract groups (see Appendix A). Therefore, we choose a point on the section, where $\mathsf{J}$ is diagonal and the eigenvalues are in descending order. The different cases are summarized in Table II; we now discuss the cases in detail.

We begin with the asymmetric tops. Since all eigenvalues are unequal, there are only four kinematic rotations that leave $\mathsf{J}$ invariant under the transformation (4.1), namely, the proper orthogonal matrices that are diagonal. These matrices form a group that we denote by $V_4$,

TABLE II. Orbits and their isotropy subgroups for the kinematic action on shape space in the four-body problem.

| Case | Orbit | Orbit dimension | Isotropy subgroup |
|---|---|---|---|
| asymmetric top | $SO(3)/V_4$ | 3 | $V_4$ |
| symmetric top | $\mathbb{R}P^2$ | 2 | O(2) |
| spherical top | one point | 0 | SO(3) |

$$V_4=\left\{\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix},\begin{pmatrix}1&0&0\\0&-1&0\\0&0&-1\end{pmatrix},\begin{pmatrix}-1&0&0\\0&1&0\\0&0&-1\end{pmatrix},\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}\right\}, \tag{4.4}$$

which as an abstract group is the viergruppe $\{e,a,b,c\}$, with the multiplication law $a^2=b^2=c^2=e$, $ab=ba=c$, etc. We will also write this group as

$$V_4=\{\mathsf{I},\mathsf{K}_1(\pi),\mathsf{K}_2(\pi),\mathsf{K}_3(\pi)\}, \tag{4.5}$$

where the notation indicates rotations about the $\alpha=1,2,3$ ''axes'' by an angle of $\pi$ [as matrices, these are the same as $\mathsf{R}_x(\pi)$, etc., but the notation is changed to indicated that they are used as kinematic rotations]. The viergruppe is the isotropy subgroup of the kinematic action on an asymmetric top and therefore the kinematic orbits for asymmetric top shapes are copies of (diffeomorphic to) the quotient space $\mathrm{SO}(3)/V_4$. This quotient space is a three-dimensional space with a nontrivial topology, which is analyzed in more detail below.

For now, however, we simply comment on the analog of the space $\mathrm{SO}(3)/V_4$ for the three-body problem. In the three-body problem, action of the kinematic group [see Eq. (2.6) of Ref. [1]] on an asymmetric top has a two-element isotropy subgroup $\{\mathsf{I},-\mathsf{I}\}$, a subgroup of SO(2). As an abstract group, this is $\mathbb{Z}_2$, the two-element group $\{e,a\}$ with multiplication law $a^2=e$. The kinematic rotation $-\mathsf{I}\in\mathrm{SO}(2)$ corresponds to a kinematic angle of $\phi=\pi$ in the language of Ref. [1] and, as indicated in Fig. 3 of that reference, the period of the kinematic orbits in shape space is $\phi=\pi$. The orbits themselves are circles, that is, copies of $S^1$. From another point of view, these orbits should be copies of the quotient space $\mathrm{SO}(2)/\mathbb{Z}_2$, as indeed they are, since SO(2) itself is the circle $S^1$, and the quotient operation in question is equivalent to identifying antipodal points on the circle (points with coordinates $\phi$ and $\phi+\pi$). That is, the quotient space is the real projective space $\mathbb{R}P^1$, which otherwise is a circle again, since it is the same as a half circle with end points identified. Altogether, we have

$$\frac{\mathrm{SO}(2)}{\mathbb{Z}_2}=\frac{S^1}{\mathbb{Z}_2}=\mathbb{R}P^1=S^1 \tag{4.6}$$

for the kinematic orbits of asymmetric tops in the three-body problem. However, in a sense the final circle $S^1$ is only half as big as the first circle SO(2), which is a way of saying that the period of the kinematic orbits in shape space is $\pi$ instead of $2\pi$. In a similar manner, we will see below that the space $\mathrm{SO}(3)/V_4$ can be identified with a region of SO(3) that is 1/4

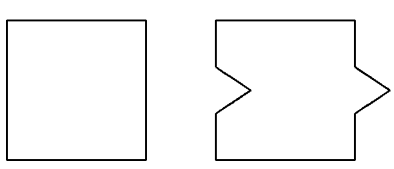

FIG. 3. The fundamental region for tessellating the plane is not unique. Similarly, the fundamental region within SO(3) representing the quotient space $\mathrm{SO}(3)/V_4$ is not unique.

the size of the whole group manifold, with certain rules for identifying points on the boundaries of the region.

We turn now to the symmetric tops. To be specific let us take a prolate symmetric top, whose $\mathsf{J}$ tensor on the section has the form

$$\mathsf{J}=\mathrm{diag}(\lambda_1,\lambda_2,\lambda_2), \tag{4.7}$$

that is, with $\lambda_2=\lambda_3$. When this $\mathsf{J}$ is acted upon by kinematic rotations according to Eq. (4.1), the proper orthogonal matrices $\mathsf{K}$ that leave it invariant have the form

$$\mathsf{K}=\begin{pmatrix}\sigma&0&0\\0&S_{11}&S_{12}\\0&S_{21}&S_{22}\end{pmatrix}, \tag{4.8}$$

where $\mathsf{S}$ (the $2\times2$ matrix on the lower diagonal) belongs to O(2) and $\sigma=\det\mathsf{S}=\pm1$. Such matrices $\mathsf{K}$ form a faithful representation of O(2), so the isotropy subgroup is O(2) as an abstract group. A similar argument applies to oblate symmetric tops; the isotropy subgroup is again O(2) as an abstract group. Therefore, the kinematic orbits of symmetric top configurations are copies of the quotient space

$$\frac{\mathrm{SO}(3)}{\mathrm{O}(2)}=\mathbb{R}P^2, \tag{4.9}$$

where the identification with $\mathbb{R}P^2$ (and the notation for the real projective space $\mathbb{R}P^2$) is explained in Appendix B.

In three-body scattering problems, it is well known that there are three exit channels that can be associated with three points on a circle. This circle can be identified as a kinematic orbit in the three-body shape space of an asymptotic (large hyperradius) collinear state, that is, a large circle centered on the origin in the $w_1$-$w_2$ plane. The kinematic rotations that connect the points on this circle are the same ones that connect the three usual choices of Jacobi coordinates in the three-body problem, each of which is particularly convenient for describing asymptotic states in one exit channel.

In a previous publication [10] we have studied the two-fragment exit channels and the kinematic rotations connecting them in collinear four-body scattering problems. In that work it was found that there are 14 two-fragment exit channels, which can be arranged as points on a certain sphere ($S^2$) and connected by kinematic rotations. The arrangement of points is particularly symmetric in the case of equal masses. Reference [10] generalized the well known facts just mentioned regarding three-body exit channels, although it was still restricted to collinear problems. It turns out that when we extend the work of Ref. [10] to four-body scattering in three spatial dimensions, the 14 exit channels become seven pairs of antipodal points on the same two-sphere as in the collinear case. Equivalently, these seven pairs of antipodal points can be seen as seven points in the space $\mathbb{R}P^2$,

TABLE III. Spaces of different kinds of tops in the four-body problem. The first $\mathbb{R}$ in each entry in column 2 stands for the volume $V$, which ranges from $-\infty$ to $+\infty$. For the asymmetric top, the space $S$ is the 60° principal sector in the $w_1$-$w_5$ plane (interior only). There are two symmetric top regions (oblate and prolate), both described by the second line; the space $\mathbb{R}^+$ is the set of positive numbers, standing for the radial lines at the edges of the principal sector (omitting the origin). For the spherical tops, the notation $\mathbb{R}^0$ stands for a single point (the first indicating the vertex of the principal sector and the second indicating that the kinetic orbit is just a single point).

| Top | Space | Dimension |
|---|---|---|
| asymmetric | $\mathbb{R}\times S\times \mathrm{SO}(3)/V_4$ | 6 |
| symmetric | $\mathbb{R}\times\mathbb{R}^+\times\mathbb{R}P^2$ | 4 |
| spherical | $\mathbb{R}\times\mathbb{R}^0\times\mathbb{R}^0$ | 1 |

which because of Eq. (4.9) is now recognized as the kinematic orbit of a symmetric top. Symmetric top orbits appear here because two-fragment asymptotic states are collinear and therefore prolate symmetric tops.

Finally, in the case of a spherical top, the $\mathsf{J}$ tensor is a multiple of the identity matrix, so all kinematic rotations leave $\mathsf{J}$ invariant according to Eq. (4.1). In this case, the isotropy subgroup is all of SO(3) and the kinematic orbit is just a point.

Altogether, we find that a five-dimensional $\mathbb{R}^5$ slice of the four-body shape space at constant $V$ can be decomposed into the product of the interior of the fundamental sector (a 60° sector) times the space $\mathrm{SO}(3)/V_4$, plus two copies (oblate and prolate) of a radial half line (the two sides of the fundamental sector) times the space $\mathbb{R}P^2$, plus a single point (the spherical top). All these are glued smoothly together to form $\mathbb{R}^5$. This decomposition applies in particular to the $\mathbb{R}^5$ hyperplane of planar shapes ($V=0$), so the collinear configurations, which lie in this hyperplane, can be represented as a single radial half line times the space $\mathbb{R}P^2$. Counting the dimension contained in the volume $V$, we see that the space of asymmetric tops is six dimensional, that of symmetric tops is four dimensional, and that of spherical tops is one dimensional. These spaces are summarized in Table III. Finally, the space of collinear shapes is three dimensional.

### C. Space $\mathrm{SO}(3)/V_4$, the kinetic cube

We now analyze more closely the kinematic orbits of asymmetric tops, which are diffeomorphic to $\mathrm{SO}(3)/V_4$. This is otherwise the space of left cosets of $V_4$ [in the $3\times3$ representation (4.4)] within SO(3), that is, the space of sets of proper orthogonal matrices of the form $(\mathsf{K}_1,\mathsf{K}_2,\mathsf{K}_3,\mathsf{K}_4)$, where the $\mathsf{K}$'s are related by $\mathsf{K}_i=\mathsf{K}_j\mathsf{V}$ for some $\mathsf{V}\in V_4$. To repeat the logic that leads to these cosets, all four of these kinematic rotations have the same effect on a diagonal asymmetric top $\mathsf{J}$ matrix according to Eq. (4.1), so any one of the four serves to label points on the asymmetric top kinematic orbit. To reduce this to a description involving only a single matrix, we proceed as follows. We start with one value of $\mathsf{K}_1$, from which the three other $\mathsf{K}$'s can be determined, producing altogether four points inside SO(3). If we allow $\mathsf{K}_1$ to range over a small region surrounding the initial point, the other three $\mathsf{K}$'s will also sweep out small regions about their initial points. As we increase the size of region swept out by $\mathsf{K}_1$, it will eventually bump into the regions being swept out by the other $\mathsf{K}$'s. When this happens, we stop moving in that direction, but continue to expand the initial region in directions that are not yet covered by the other $\mathsf{K}$'s. We keep this up until the entire group manifold SO(3) is covered by one (and only one) of the four $\mathsf{K}$'s. The region covered by $\mathsf{K}_1$ will then be 1/4 of the entire group manifold and can be taken as a "fundamental region" for representing the space of cosets. Then points in the fundamental region stand in one-to-one correspondence with points of $\mathrm{SO}(3)/V_4$. One must be careful with boundary points, however, because there will be gluing rules indicating how boundary points are to be identified in order to represent a unique point of the quotient space $\mathrm{SO}(3)/V_4$.

The construction just given can be described by saying that we have tessellated SO(3) into four identical pieces that fill up the whole group manifold with no overlap. For comparison, we note that the ordinary tessellation of the plane by unit squares can be regarded as the process of replicating the fundamental region (a given unit square) by the group of integer displacements in the $x$ and $y$ directions and that the fundamental region itself can be regarded as the quotient space resulting from dividing the plane by this group. This example also makes it clear that the fundamental region is not unique; two possible fundamental regions are illustrated in Fig. 3, which differ from one another in that some territory has been borrowed by the fundamental region from its neighbor on one side and symmetrically (under a group operation) abandoned on the other side. The situation is similar with $\mathrm{SO}(3)/V_4$; the fundamental region is not unique, but can be defined in many ways. The tessellation of the plane illustrates another point, which is that while the fundamental region (say, a unit square in the plane) represents the quotient space point for point, it does not accurately represent the topology of the quotient space, unless some gluing rules are adopted. For example, points on opposite sides of the fundamental square represent only one point in the quotient space and points near points on opposite sides, while not close to one another in the plane, actually are close to one another in the quotient space. Therefore, we must glue opposite sides of the fundamental region together to represent the topology of the quotient space accurately. In this way, we see that the quotient space is actually a two-torus, a compact manifold with no boundary. Similarly, $\mathrm{SO}(3)/V_4$ is a compact, three-dimensional manifold with no boundary.

In earlier work [11], one of us (M.R.) has shown that in coordinates we call $\boldsymbol{\tau}=(\tau_1,\tau_2,\tau_3)$, the fundamental region of SO(3) is a cube. We will call this space the kinetic cube. Recently Kuppermann [3] has also identified the fundamental region as a cube in Euler angle coordinates. These two cubes in the respective coordinate spaces do not represent the same region on SO(3) because the mapping between the two sets of coordinates is nonlinear and a cube in one coordinate space does not map onto a cube in the other. It must be that the two corresponding regions on the group manifold are related to one another as are the fundamental regions in Fig. 3, but we have not attempted to prove this in detail. Kuppermann's fundamental region is given by $0\leqslant\alpha,\beta,\gamma\leqslant\pi$ in the usual $(\alpha,\beta,\gamma)$ Euler angle coordinates; actually, the corresponding region on SO(3) is not a smooth distortion of a cube because the angles $\alpha$ and $\gamma$ are not unique when $\beta = 0,\pi$ (only $\alpha+\gamma$ has meaning when $\beta=0$ and only $\alpha-\gamma$ when $\beta=\pi$). In effect, two faces of Kuppermann's cube are pinched into a line.

Kuppermann's cube construction makes it easy to see that the fundamental region is in fact 1/4 of SO(3), but makes it hard to determine the gluing rules at the boundaries of the region and hence the topology. Another difficulty is that Kuppermann's cube positions the identity rotation at a corner of the fundamental region, instead of in the center; this in particular makes it hard to study the SO(2) subgroup of rotations about the $x$ axis, which is important for the connectivity of the principal axis frame. These difficulties are related to the usual drawbacks of the Euler angles as a coordinate system on SO(3) [the three angles are unsymmetrical among themselves, some angles are undefined at the end points of the ranges, the coordinate system is singular at the identity element, and SO(2) subgroups do not have a simple representation].

The $\boldsymbol{\tau}$ coordinates are better for these purposes. These coordinates are defined as follows. We parametrize a proper rotation by its axis $\hat{\mathbf{n}}$ and angle $\theta$, denoting the corresponding matrix by $\mathsf{R}(\hat{\mathbf{n}},\theta)$. The axis $\hat{\mathbf{n}}$ ranges over the unit sphere $S^2$ and the angle range is $0\leqslant\theta\leqslant\pi$. Points $(\hat{\mathbf{n}},\theta)$ stand in one-to-one correspondence with $\mathsf{R}\in \mathrm{SO}(3)$, except when $\theta=0$, where $\mathsf{R}(\hat{\mathbf{n}},0)$ is independent of $\hat{\mathbf{n}}$, and except for $\theta=\pi$, where $\mathsf{R}(\hat{\mathbf{n}},\pi)=\mathsf{R}(-\hat{\mathbf{n}},\pi)$. Thus, if we write $\theta\hat{\mathbf{n}}$ as a vector in $\mathbb{R}^3$, we see that SO(3) can be identified with a region that is the solid interior of a sphere in $\mathbb{R}^3$ with radius of $\pi$, with antipodal points on the surface of the sphere identified. This is the standard construction that makes it clear that SO(3) is diffeomorphic to $\mathbb{R}P^3$ (the "northern hemisphere" of $S^3$ with gluing rules at the "equator"; see Appendix B). The identity matrix is at the origin and the SO(2) subgroups representing rotations about an axis $\hat{\mathbf{n}}$ are represented by straight lines passing through the origin and connecting antipodal points on the surface. In particular, the SO(2) subgroups of rotations about the $x$, $y$, and $z$ axes are just the three coordinate axes in $\theta\hat{\mathbf{n}}$ space.

In terms of this construction, the $\boldsymbol{\tau}$ coordinates are defined by

$$\boldsymbol{\tau}=\hat{\mathbf{n}}\tan\frac{\theta}{2}. \tag{4.10}$$

The mapping from $\theta\hat{\mathbf{n}}$ space to $\boldsymbol{\tau}$ space pushes the surface of the sphere to infinity; thus points of $\boldsymbol{\tau}$ space stand in one-to-one correspondence with rotations, except when $\theta=\pi$; such rotations are not represented in $\boldsymbol{\tau}$ space. The main advantage of the $\boldsymbol{\tau}$ coordinates is that is it relatively easy to find the coordinates of the product of two rotations, given the coordinates of the two rotations themselves. Explicitly, if $\mathsf{R}(\boldsymbol{\tau}) = \mathsf{R}(\boldsymbol{\tau}_1)\mathsf{R}(\boldsymbol{\tau}_2)$, then

$$\boldsymbol{\tau}=\frac{\boldsymbol{\tau}_1+\boldsymbol{\tau}_2+\boldsymbol{\tau}_1\times\boldsymbol{\tau}_2}{1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2}. \tag{4.11}$$

The analogous formula in Euler angle coordinates is quite unpleasant.

Equation (4.11) is most easily proved in terms of spinor rotations, that is, elements of SU(2). We call on the following basic facts connecting SO(3) and SU(2). Corresponding to every $\mathsf{R}(\hat{\mathbf{n}},\theta)\in \mathrm{SO}(3)$ there are two spinor rotations in SU(2), $U(\hat{\mathbf{n}},\theta)$ and $U(\hat{\mathbf{n}},\theta+2\pi)$, which differ only by a sign. These are defined by

$$U(\hat{\mathbf{n}},\theta)=\exp\left(-\frac{i\theta\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}}{2}\right)=\cos\frac{\theta}{2}-i(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})\sin\frac{\theta}{2} \tag{4.12}$$

$$=\cos\frac{\theta}{2}(1-i\boldsymbol{\tau}\cdot\boldsymbol{\sigma}), \tag{4.13}$$

where $\boldsymbol{\sigma}$ are the Pauli matrices. To find the $R\in \mathrm{SO}(3)$ associated with a given $U\in \mathrm{SU}(2)$, we may use the formula

$$R_{ij}=\frac{1}{2}\,\mathrm{tr}(U^\dagger\sigma_i U\sigma_j). \tag{4.14}$$

In the expression $U(\hat{\mathbf{n}},\theta)$, $\hat{\mathbf{n}}$ ranges over the unit sphere $S^2$ and $0\leqslant\theta\leqslant 2\pi$. The correspondence between SU(2) and SO(3) given by Eq. (4.14) is a group representation, that is, if $U_1$ and $U_2$ correspond to $\mathsf{R}_1$ and $\mathsf{R}_2$ by Eq. (4.14), then $U_1U_2$ corresponds to $\mathsf{R}_1\mathsf{R}_2$. Finally, Eq. (4.11) follows easily by multiplying $U(\hat{\mathbf{n}}_1,\theta_1)$ and $U(\hat{\mathbf{n}}_2,\theta_2)$ and using Eqs. (4.10) and (4.13).

We return to Eq. (4.11) and allow the second angle $\theta_2$ to approach $\pi$, writing $\hat{\mathbf{n}}_2=\hat{\mathbf{e}}$ and making the notational changes $\boldsymbol{\tau}_1\to\boldsymbol{\tau}$ and $\boldsymbol{\tau}\to\boldsymbol{\tau}'$. Then we have

$$\boldsymbol{\tau}'=-\frac{\hat{\mathbf{e}}+\boldsymbol{\tau}\times\hat{\mathbf{e}}}{\boldsymbol{\tau}\cdot\hat{\mathbf{e}}}. \tag{4.15}$$

This is the equation we must use when right multiplying by elements of $V_4$ [see Eq. (4.4)] since these contain rotations by an angle of $\pi$.

It is now straightforward to show that the cube $-1 \leqslant\tau_1,\tau_2,\tau_3\leqslant+1$ in $\boldsymbol{\tau}$ space is the fundamental region for the quotient operation $\mathrm{SO}(3)/V_4$. In detail, this involves showing that if $\mathsf{K}(\boldsymbol{\tau})$ lies in the interior of the cube, then the other three rotations of the form $\mathsf{KV}$ for $\mathsf{V}\in V_4$ lie outside the cube and if $(\mathsf{K}_1,\mathsf{K}_2,\mathsf{K}_3,\mathsf{K}_4)$ are any four rotations related by right multiplication by elements of $V_4$, that is, $\mathsf{K}_i=\mathsf{K}_j\mathsf{V}$ for some $\mathsf{V}\in V_4$, then at least one of them lies either in the interior or on the surface of the cube. The proof of these facts using Eq. (4.15) is straightforward and will not be given here, partly because a more compelling (geometrical) argument will be given momentarily. In any case, the region $|\tau_i|\leqslant 1$, $i=1,2,3$, is the kinetic cube in the $\boldsymbol{\tau}$ coordinates (see Fig. 4). The identity $\mathsf{I}\in \mathrm{SO}(3)$ is at the origin $\boldsymbol{\tau}=0$ and rotations about the $x$, $y$, and $z$ axes run along the $\tau_1$, $\tau_2$, and $\tau_3$ coordinate axes. These rotations hit the walls of the cube at angles $\theta=\pm\pi/2$ and puncture its six faces in their centers.

On the boundaries of the cube, there is more than one point corresponding to a given coset, which is to say that there are gluing rules (identifications of points on the boundary) that are needed to make the correspondence one to one. Consider first the face at $\tau_3=-1$. When a point $\boldsymbol{\tau} =(\tau_1,\tau_2,-1)$ on this face is right multiplied by $\mathsf{K}_3(\pi)$,

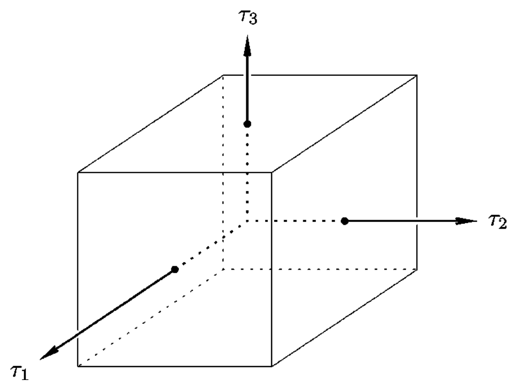


FIG. 4. The fundamental region of $SO(3)/V_4$ is the cube $|\tau_i| \leqslant 1$ in the $\boldsymbol{\tau}$ coordinates.

corresponding to $\hat{\mathbf{e}}=(0,0,1)$, then according to Eq. (4.15) it is mapped onto $(\tau_2,-\tau_1,1)$. That is, the face at $\tau_3=-1$ is mapped onto the face at $\tau_3=+1$ with a rotation by angle $-\pi/2$ about the $\tau_3$ axis. In reference to Fig. 5, we see that the face $ABCD$ is identified with the face $FGHE$. Precisely analogous statements apply to the other axes and produce the identifications $AEFB=HGCD$ and $BFGC=EHDA$. These rules in turn imply an identification of the edges, which are identical in triplets; these are $AB=FG=HD$, $BC=GH=EA$, $CD=HE=FB$, and $DA=EF=GC$. The edge identifications are indicated in Fig. 5 by the numbers 1,2,3,4, with arrows indicating the directions. Finally, the vertices are identified four at a time, with $A=F=H=C$ and $B=G=D=E$.

The kinetic cube acquires an interesting and highly symmetrical representation when expressed in terms of spinor rotations [that is, when ''lifted'' into SU(2)]. For this purpose it is best to use the Cayley-Klein parameters for SU(2), which we define by writing

$$U=x_0-i\mathbf{x}\cdot\boldsymbol{\sigma}, \tag{4.16}$$

where $\mathbf{x}=(x_1,x_2,x_3)$. Then the conditions $U^\dagger U=1$ and $\det U=1$ are equivalent to $x_0^2+x_1^2+x_2^2+x_3^2=1$. This shows that SU(2) is diffeomorphic to $S^3$, the unit sphere in the

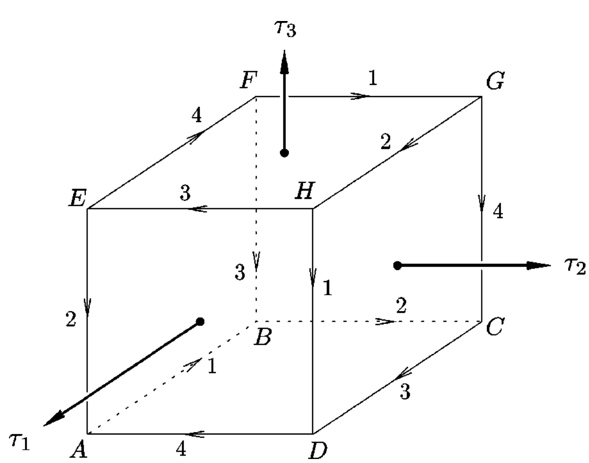


FIG. 5. Opposite faces of the kinetic cube are identified with a $\pi/2$ rotation. Similarly, edges are identified in triplets and vertices four at a time. The arrows indicate the direction of identification of the edges.

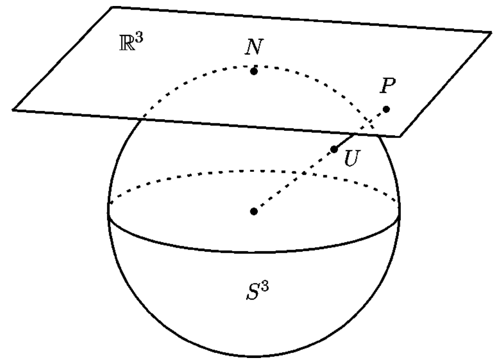


FIG. 6. The three-sphere $S^3$ is the group manifold SU(2), to which the hyperplane $\mathbb{R}^3$ is tangent at the ''north pole'' $N$. The element $U\in SU(2)$ is projected from the origin onto the tangent plane at $P$. The $\boldsymbol{\tau}$ coordinates of $U$ are the coordinates of $P$ in the tangent hyperplane.

four-dimensional space $\mathbb{R}^4$ in which $(x_0,x_1,x_2,x_3)$ are coordinates. The identity matrix $1\in SU(2)$ is at the ''north pole'' with coordinates (1,0,0,0), the ''equator'' with coordinates $(0,x_1,x_2,x_3)$ contains all rotations by an angle of $\pi$, and the ''south pole'' with coordinates $(-1,0,0,0)$ is the matrix $-1\in SU(2)$. If $\mathsf{R}\in SO(3)$ then the two $U$ matrices corresponding to $\mathsf{R}$ according to Eqs. (4.13) and (4.14) have coordinates $\{x_i\}$ and $\{-x_i\}$, that is, they lie on antipodal points of $S^3$.

Now consider the construction illustrated in Fig. 6, in which a point $U\in SU(2)$ (a point on $S^3$) is projected (as seen from the origin) onto the three-dimensional hyperplane $\mathbb{R}^3$, which is tangential to the ''north pole.'' By comparing Eqs. (4.13) and (4.16), we have $x_0=\cos(\theta/2)$ and $\mathbf{x}=\hat{\mathbf{n}}\sin(\theta/2)$ for the coordinates of $U$, in terms of the axis and angle. By scaling the four-vector $(x_0,\mathbf{x})$ by $1/\cos(\theta/2)$, we obtain a point on the tangent plane with coordinates $(1,\boldsymbol{\tau})$, where $\boldsymbol{\tau}$ is given by Eq. (4.10). Thus we see that the $(\tau_1,\tau_2,\tau_3)$ coordinates of a rotation are the same as the Cayley-Klein coordinates $(x_1,x_2,x_3)$ in the $\mathbb{R}^3$ hyperplane tangent to the north pole. This makes it obvious why the $\boldsymbol{\tau}$ coordinates diverge for rotations by an angle of $\pi$, because the corresponding $U$ matrices are on the ''equator.''

Now it is easy to see what spinor rotations correspond to the kinetic cube. We simply construct the cube $|x_i|\leqslant 1$, $i=1,2,3$, in the hyperplane tangent to the north pole and then let a point such as $P$ in Fig. 6 run over the interior (or faces) of this cube. As it does, the point $U$ in the figure fills in the region (or its boundary) in SU(2) in which the $\boldsymbol{\tau}$ coordinates have the specified ranges. This region is centered on the north pole. There is an antipodal but otherwise identical region centered on the south pole; taken together, these two regions constitute the lift into SU(2) of the kinetic cube in SO(3), that is, the set of spinor rotations that project onto the kinetic cube according to Eq. (4.14).

The meaning of these regions in $S^3$ is made more clear by Fig. 7, which is a sphere inscribed in a cube and is supposed to suggest the three-sphere $S^3$ inscribed in the four-cube (the latter being the unit cube in four dimensions). The four-cube is described by $|x_i|\leqslant 1$, $i=0,1,2,3$, and the inscribed three-sphere $S^3$ is tangential to the faces of this four-cube at eight points, where the four coordinates take on the values $\pm 1$ on

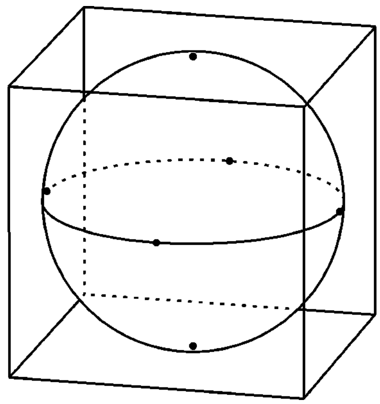

FIG. 7. A two-sphere inscribed in a three-cube suggests a three-sphere $S^3$ inscribed in a four-cube. The four-cube has eight faces, each of which is an ordinary three-cube, which project onto eight identical regions of $S^3$. These regions can be identified with the coset space $\mathrm{SU}(2)/V_8$, which is the same as the coset space $\mathrm{SO}(3)/V_4$, the kinetic cube.

the four coordinate axes. The eight faces of this four-cube are ordinary three-cubes, of which the kinetic cube in the tangential hyperplane illustrated in Fig. 6 is one. All eight three-cubes are identical and share all of their faces (ordinary squares or two-cubes) with one another. When these eight three-cubes are projected onto $S^3$ as illustrated in Fig. 6, they produce eight identical, three-dimensional regions in $S^3$ that tessellate $S^3$.

Furthermore, these eight regions are mapped into one another by the eight element subgroup of SU(2), which is the lift of $V_4$, regarded as a subgroup of SO(3), that is, those spinor rotations that correspond to the ordinary rotations in $V_4$ according to Eqs. (4.13) and (4.14). This eight element group is the set of spinor rotations $\{\pm 1, \pm U_x(\pi), \pm U_y(\pi), \pm U_z(\pi)\}$, which we will denote by $V_8$. It is otherwise the quaternion group, the eight-element group $\{\pm 1, \pm i, \pm j, \pm k\}$ with multiplication law $i^2 = j^2 = k^2 = -1$, $ij = -ji = k$, etc. It is easy to show that any one of the eight spinor rotations in $V_8$ (on right multiplication) simply permutes the eight regions among themselves. Thus any one of these regions can be taken as the fundamental region for $\mathrm{SU}(2)/V_8$. When these regions are projected onto SO(3) according to Eq. (4.14), they project in antipodal pairs onto the four regions in the tessellation of SO(3). In particular, the pair centered on the north and south poles (on the $\pm x_0$ axis) project onto the kinetic cube, the fundamental region of $\mathrm{SO}(3)/V_4$. In summary, we have found another representation of the kinetic cube as a space of cosets, this time the cosets of the quaternion group within SU(2). This is indicated by the equation

$$\frac{\mathrm{SO}(3)}{V_4} = \frac{\mathrm{SU}(2)}{V_8}. \tag{4.17}$$

This finishes our discussion of the kinematic orbits in shape space. At this point the reader may wish to examine Appendix C on the kinematic orbits in configuration space, which of course project onto the kinematic orbits in shape space when the external orientation (the position along the rotation fibers) is thrown away. The interplay between the kinematic orbits in these two spaces is important in understanding the connectivity of the principal axis frame, which is our next subject.

## V. PRINCIPAL AXIS FRAME

In this section we study the principal axis frame and its multiple branches in the four-body problem. In a sense, the analysis is a straightforward generalization of the work presented in Ref. [1] on the three-body problem, but it is necessary to invoke a more formal language because of the more exotic spaces that are involved. We begin by examining the 24 branches of the principal axis frame and the ''frame group'' of rotations that connects them. Next we study how one branch, continuously tracked around a closed loop in shape space, may end on another branch when the shape returns to its initial value. We show that the ''frame jump'' must be an element of the viergruppe $V_4$ and that it has a simple dependence on the initial branch. Next we study the dependence of the frame jump on the loop itself. As in the three-body problem, we show that the connectivity of the principal axis frame can be determined by loops generated from kinematic rotations alone. This leads us into the homotopy group of the kinetic cube, that is, the classes of topologically equivalent curves, which we are able to translate into principal axis frame jumps. Finally, we show how branch cuts may be introduced into the kinetic cube to define a single-valued principal axis frame and we show how the discontinuities across the branch cuts may be computed.

### A. Multiple branches of the principal axis frame

As in Ref. [1], we consider the principal axis frame to be defined only over the asymmetric top region of shape space, where the principal axes of the body are unique apart from a sign (their directions) and their labelings ($x$, $y$, or $z$). These ambiguities give rise to 24 principal axis frames, which is the number of ways of orienting a right-handed frame along three orthogonal lines. See Fig. 4 of Ref. [1]. These 24 frames are related by a 24-element group of rotations, generated by products and powers of $\mathsf{R}_x(\pi/2)$, $\mathsf{R}_y(\pi/2)$, and $\mathsf{R}_z(\pi/2)$. We will call this the *frame group* and denote it by $F_{24}$; it is a subgroup of SO(3). If we pick any one principal axis frame and apply the 24 rotations of the frame group to it, all 24 principal axis frames are generated. It is easy to see why there are 24 frames; since the eigenvalues of the moment tensor are distinct, there are $3! = 6$ ways of permuting them and once a permutation of eigenvalues has been selected, there remain four rotations belonging to the viergruppe $V_4$, defined in Eq. (4.4), which leave the ordering of the eigenvalues invariant but flip the directions of some of the principal axes. The viergruppe we are referring to here is composed of external rotations, whereas earlier it was composed of kinematic rotations; as a subgroup of matrices in SO(3), it is the same group.

Geometrically, the 24 branches of the principal axis frame can be seen as 24 sections of the rotation fiber bundle, that is, 24 six-dimensional surfaces in configuration space $\mathbb{R}^9$, each of which cuts the rotation fiber in one point. See Fig. 5 of Ref. [1], which illustrates two of these sections. If we denote the points of a fiber where these sections intersect it by

$Q_1,\ldots,Q_{24}$, then these points are related by elements of the frame group, that is, $Q_i = \mathsf{F}Q_j$ for some $\mathsf{F}\in F_{24}$.

Now we ask what happens as we continuously track one of the branches of the principal axis frame around a closed loop in the asymmetric region of shape space. When we return to our original shape, will we return on the same branch of the principal axis frame or will there be a ''jump'' to another branch? More generally, which branches are accessible by continuous tracking from a given initial branch? Are all 24 branches connected together or only some of them? (Actually, the word ''jump'' is misleading because the entire process is one of continuous tracking; if we were to reverse the process, we would return to the original branch.)

In fact, it is not hard to see that the branches are connected together in sets of at most four. This is because the moment of inertia tensor is diagonal at all points along the path of continuous tracking and its eigenvalues, which are distinct initially and can never cross one another during the tracking process (because that would take us outside the asymmetric top region), must necessarily return to their original values and original sequence when we return to the original shape. Therefore, the frame itself must preserve the sequencing of the eigenvalues, so the frame jump must belong to the viergruppe $V_4$ of matrices shown in Eq. (4.4). These matrices change only the signs of the eigenvectors of the moment of inertia tensor, not the eigenvalues. The viergruppe (4.4) is a subgroup of the frame group $F_{24}$. Thus the only nontrivial frame jumps that can occur on continuous tracking are rotations by $\pi$ about one of the three principal axes. This is a believable conclusion, based on experience with the three-body problem, where the only nontrivial frame jump is a rotation by $\pi$ about the $z$ axis. The question remains, however, which closed curves in shape space give rise to which jumps.

Let us precisely define the frame jump on continuously tracking the principal axis frame around a closed loop in the asymmetric top region of shape space as the rotation that maps the initial frame into the final frame or, equivalently, the initial configuration $Q_i$ (a branch of the principal axis frame) to the final one $Q_f$, both on the same rotation fiber. The frame jump must be an element of $V_4$, in the representation given by Eq. (4.4) and it is a function of both the loop and the initial branch.

However, the dependence on the initial branch is easy to determine. Suppose we choose two initial branches of the principal axis frame $Q_{i1}$ and $Q_{i2}$, which are necessarily related by some member of the frame group, say, $Q_{i2} = \mathsf{F}Q_{i1}$ where $\mathsf{F}\in F_{24}$, and suppose that on tracking these around a closed loop we reach the final branches $Q_{f1}$ and $Q_{f2}$. Then the frame jump of the first frame is the rotation $\mathsf{V}\in V_4$ such that $Q_{f1} = \mathsf{V}Q_{i1}$. Now the two branches, which are related by $\mathsf{F}$ at the initial point, must be related by some member of the frame group at all points along the continuous tracking. However, since the tracking is continuous and the elements of the frame group are discrete, in fact the two branches must be related by the same $\mathsf{F}$ at all points along the continuous tracking. In particular, we must have $Q_{f2} = \mathsf{F}Q_{f1}$ (at the final point). However, this implies $Q_{f2} = (\mathsf{F}\mathsf{V}\mathsf{F}^{-1})Q_{i2}$. Here we note that $V_4$ is a normal subgroup of $F_{24}$, which means that $\mathsf{F}\mathsf{V}\mathsf{F}^{-1}$ is a member of $V_4$ for all $\mathsf{F}\in F_{24}$.

In summary, if we pick one branch of the principal axis frame as a reference and label the other branches by the elements of $F_{24}$ that map the reference into them and if we determine the frame jump $\mathsf{V}\in V_4$ of the reference branch on going around a loop in the asymmetric top region, then the frame jump on the branch labeled by $\mathsf{F}$ is $\mathsf{F}\mathsf{V}\mathsf{F}^{-1}\in V_4$.

### B. Frame jump and homotopy classes of the kinetic cube

Next we determine how the frame jump depends on the closed loop in the asymmetric top region. We begin with the basic topological fact (discussed in Ref. [1]) that the frame jump must be the same for any two closed loops that can be continuously deformed into one another. In algebraic topology [12], two closed loops in some space (starting at a given point) are said to be *homotopic* or to lie in the same *homotopy class* if they can be continuously deformed into one another. Thus we see that the frame jump is a function of the homotopy class that the loop in the asymmetric region of shape space belongs to. For comparison, we note that in the three-body problem, the homotopy classes of the asymmetric top region of shape space are specified by the number of times the closed loop goes around the $w_3$ axis; thus the homotopy classes are labeled by a winding number $\nu$, an integer that ranges from $-\infty$ to $+\infty$. Also, we recall that in the three-body problem, all closed loops in the asymmetric top region could be continuously deformed into kinematic orbits, so it sufficed to use only kinematic orbits to determine frame jumps. In fact, the frame jump in the three-body problem turned out to be $\mathsf{R}_z(\pi)^\nu = \mathsf{R}_z(\nu\pi)$.

Returning now to the four-body problem, suppose we start at some initial point $q_0$ in the asymmetric top region of shape space and go around some closed loop and suppose the frame jump is $\mathsf{V}_1\in V_4$. Then suppose we go around another closed loop, again starting from $q_0$, and suppose we find the frame jump $\mathsf{V}_2$. Then according to the discussion in Sec. V A, the frame jump on going around both loops in tandem is $(\mathsf{V}_1\mathsf{V}_2\mathsf{V}_1^{-1})\mathsf{V}_1 = \mathsf{V}_1\mathsf{V}_2$. However, in algebraic topology [12], the catenation of two loops is regarded as the product of the loops and it is shown that this product respects homotopy classes. (The product $ab$ of loop $a$ times loop $b$, both assumed to begin at the same point, is the loop obtained by going around $a$ first and then $b$.) In other words, the homotopy class of the product of loops is defined to be the product of the classes. Also, the inverse of a loop (going around in the reverse direction) defines the inverse class. With these definitions, one can show that the homotopy classes form a group, the *fundamental group* of the manifold $M$ upon which the loops are defined, denoted $\pi_1(M)$ in standard notation. For example, the fundamental group of the asymmetric top region in the three-body problem is $\mathbb{Z}$, the group of integers (winding numbers) under addition, and the fundamental group of any simply connected space (such as $\mathbb{R}^3$ or $S^2$) is the trivial group $\{e\}$ since all loops can be contracted to a point. Thus, in the language of algebraic topology, we see that the frame jump corresponding to the product of two homotopy classes is the product of the frame jumps. In other words, we have established a group homomorphism between the fundamental group of the asymmetric top region and the group $V_4$ of frame jumps.

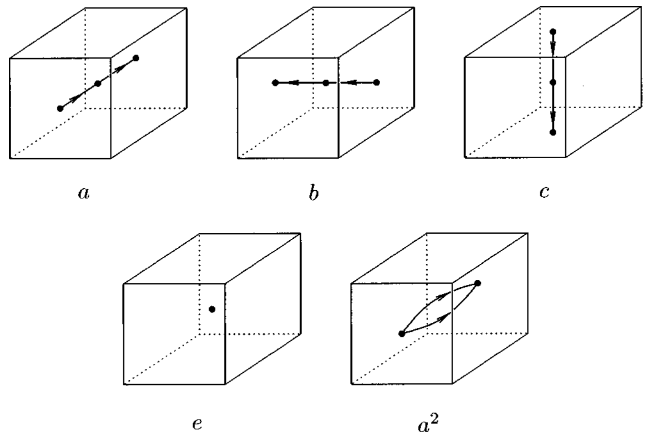


FIG. 8. By experimenting with closed curves in the kinetic cube, we can find the homotopy classes. The axes are assumed to be aligned with the cube as in Fig. 5. The identity element $e$ contains any curve that can be contracted to a point. Elements $a$, $b$, and $c$ run along the subgroups of rotations along the 1, 2, and 3 axes, respectively, starting at angle 0, going to angle $-\pi/2$, and then passing from angle $+\pi/2$ back to angle 0. Curves $a^2$, $b^2$, and $c^2$ are homotopically equivalent. The homotopy classes turn out to form the quaternion group $V_8$.

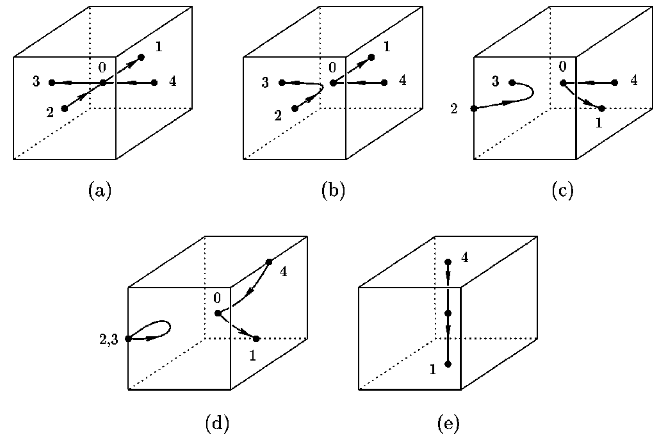


FIG. 9. Illustration of the class multiplication law $ab=c$.

It turns out in the four-body problem that every closed loop in the asymmetric top region of shape space can be continuously deformed into a closed loop composed entirely of kinematic rotations. This is the obvious generalization of an analogous fact shown in Ref. [1] for the three-body problem and it shows that kinematic rotations alone suffice to determine the connectivity of the principal axis frame. In other words, one can ignore any variation in the kinematic invariants (the volume $V$ and the labels $w_1,w_5$ of the kinematic orbit or any equivalent set of kinematic invariants such as the eigenvalues $\lambda_i$ of the $\mathsf{J}$ tensor) when considering the frame change around a closed loop. Only the variation in the kinematic Euler angles need be considered. Thus the fundamental group of the asymmetric top region is the same as the fundamental group of the kinetic cube $\pi_1[\mathrm{SO}(3)/V_4]$.

This property can be understood with reference to the first row of Table III, where $S$ is the interior of the 60° principal sector of the kinematic section. A closed loop in the asymmetric top region of shape space can be thought of as a combination of a closed loop in the space of kinematic invariants (the wedge $\mathbb{R}\times S$), with a closed loop in the kinetic cube $\mathrm{SO}(3)/V_4$. However, the wedge is simply connected, so the part of the loop in this space (the variation in the kinematic invariants) can be continuously deformed into a point, leaving only the variation in the kinetic cube.

Therefore, we need the homotopy classes and the class multiplication law for the kinetic cube $\mathrm{SO}(3)/V_4$. There are two approaches to finding these. In one approach, we start drawing closed curves in the kinetic cube, paying attention to the gluing rules at the boundaries and simply experiment to find the homotopy classes and their multiplication law. The process, illustrated in Fig. 8, is not rigorous, but in this case it is effective. The identity class consists of any curve that can be contracted to a point, such as the curve that starts at the identity element $\mathsf{K}=\mathsf{I}$ inside the cube and goes nowhere. This is the class $e$ in the second row of the figure. Another closed curve, labeled $a$ in the figure (first row), starts at the identity element $\mathsf{K}=\mathsf{I}$, goes to the center of the face $\tau_1=-1$, which, according to the gluing rules, is the same point as the center of the face $\tau_1=+1$ and then returns to the identity element. Because of the gluing rules, this curve $a$ is a closed curve in the kinetic cube. It cannot, however, be contracted to a point because if we move the point on one face, the point on the other face must move in such a way as to satisfy the gluing rules. Thus there is no way to bring the two end points together and the class $a$ is distinct from the class $e$. The curve $a$ consists of kinematic rotations along the ''$x$ axis'' (that is, the 1 axis), with angles decreasing from 0 to $-\pi/2$ and then from $+\pi/2$ back to 0. In a similar way we construct curves or homotopy classes $b$ and $c$, illustrated in the figure, which run along the $y$ and $z$ axes, respectively, with decreasing angles.

Further classes can be obtained by taking inverses, products, and powers of the ones found so far. For example, the inverse of curve $a$, call it $-a$ (not shown in the figure), is a curve that goes in the opposite direction from $a$, that is, with increasing angles; one can show that it is not homotopically equivalent to $a$. Similarly, we obtain homotopy classes $-b$ and $-c$. The curve $a^2$, obtained by following $a$ twice (second row of figure), belongs to yet a new homotopy class, which is distinct from $a$ and the others mentioned so far; but it turns out to be identical to $b^2$ and $c^2$ (not illustrated in the figure). We will call this class $-e=a^2=b^2=c^2$. With this we have found all the homotopy classes (there are eight).

The multiplication law is obtained by catenating curves and continuously deforming the result. For example, we can show that $ab=c$, as illustrated in Fig. 9. In Fig. 9(a) we first start at 0 (the identity element $\mathsf{K}=\mathsf{I}$ in the kinetic cube), go to 1 on the $\tau_1=-1$ face, which is the same as 2, and then return to 0. This is curve $a$. Next we go from 0 to 3, which is the same as 4, and then return to 0. This is curve $b$ and the whole journey is the product $ab$. In Fig. 9(b) we continuously deform the product curve, retracting from 2 and 3 to pull the middle away from 0. In Fig. 9(c) we have moved 1 down to the middle of the edge $\tau_1=\tau_3=-1$, which, according to the gluing rules, forces 2 (which is the same as 1) to move horizontally to the middle of the edge $\tau_1=+1$, $\tau_2=-1$. The curve is still traversed in the order $0\rightarrow 1=2\rightarrow 3=4\rightarrow 0$. In Fig. 9(d) we move 3 over to coincide with 2, which by the gluing rules forces 4 upward to the midpoint of the edge $\tau_2=\tau_3=+1$. Now all four points 1,2,3,4 are identical. Next we contract the small loop $2\rightarrow3=2$ to a point, so the history of the product loop is $0\rightarrow1=4\rightarrow0$. Finally, we move 1 to the center of the bottom face, which forces 4 to move to the center of the top face. The result (see Fig. 8) is loop $c$. This proves that $ab=c$. We defined the loops $a$, $b$, and $c$ to go in the direction of decreasing angles so that this result would come out. In this manner we can fill out the multiplication table for the homotopy classes of the kinetic cube and we recognize it as the same as the quaterion group $V_8$, with $\{\pm e,\pm a,\pm b,\pm c\}$ identified with $\{\pm 1,\pm i,\pm j,\pm k\}$ for quaterions or $\{\pm 1,\pm U_x(\pi),\pm U_y(\pi),\pm U_z(\pi)\}$ for SU(2) matrices.

A more efficient route to the same answer is to recognize that any closed curve in $\mathrm{SO}(3)/V_4$ starting and ending at the identity is the projection of a curve on $\mathrm{SU}(2)=S^3$ that starts at the identity 1 and ends at some point on SU(2) that is symmetrically related to the identity by some member of $V_8$. That is, the curve must end on a member of $V_8$, regarded as a subgroup of SU(2). Furthermore, any continuous deformation of the closed curve in $\mathrm{SO}(3)/V_4$, holding the starting point fixed, must correspond to a continuous deformation of the curve in SU(2) that does not change the starting or ending points (because that would create a curve that was not closed upon projection). Furthermore, since $\mathrm{SU}(2)=S^3$ is simply connected, any two curves that start and end at given points can be continuously deformed into one another. Therefore, the homotopy classes of the kinetic cube can be placed in one-to-one correspondence with the elements of $V_8$ and elements of $V_8$ can be used to label the homotopy classes. In fact, if we label the homotopy classes by the inverse of the element of $V_8$ upon which the curve in SU(2) terminates, then it can be shown that class multiplication is equivalent to group multiplication within $V_8$. We omit the proof of this fact, which is straightforward. For example, the curve $a$, which is closed in the kinetic cube, lifts into a curve that starts at 1 and ends at $U_x(-\pi)$ in SU(2). Therefore, we would label curve $a$ by the SU(2) matrix $U_x(\pi)$ (an element of $V_8$). Thus the fundamental group of the kinetic cube is the quaternion group $V_8$,

$$\pi_1[\mathrm{SO}(3)/V_4]=\pi_1[\mathrm{SU}(2)/V_8]=V_8. \tag{5.1}$$

One might say this equation is obvious: Since SU(2) is simply connected, any nontrivial topology comes from the quotient operation.

### C. Frame jump as a function of the homotopy class

To return to the principal axis frame, we have now established that the frame jump (an external rotation in $V_4$) must be a function of the homotopy class in the kinetic cube, which is labeled by a member of $V_8$. Moreover, this function must be a group homomorphism. Regarding $V_8=\{\pm 1,\pm U_x(\pi),\pm U_y(\pi),U_z(\pi)\}$ as a subgroup of SU(2) and $V_4$ as a subgroup of SO(3) as in Eq. (4.4), an obvious guess is that the homomorphism is given simply by throwing away the $\pm$ sign in the SU(2) matrices and keeping the axis and the angle constant, to produce $V_4=\{\mathsf{I},\mathsf{R}_x(\pi),\mathsf{R}_y(\pi),\mathsf{R}_z(\pi)\}$. We write $\mathsf{R}$ for these matrices instead of $\mathsf{K}$ because the frame jump is an external rotation. This mapping from $V_8$ to $V_4$ is just the usual homomorphism between SU(2) and SO(3), as expressed by Eq. (4.14), restricted to the subgroup $V_8$ of SU(2).

To prove this systematically, we proceed as follows. Let us choose a shape $q_0$ in the asymmetric top region of the principal sector of the kinematic section (such as the point marked by a cross in sector I in Fig. 2), which will serve as an initial condition for a kinematic orbit. We wish to choose a principal axis frame on the external rotation fiber labeled by $q_0$ and then to track this frame as we follow some closed curve in the kinetic cube, representing a sequence of shapes that start and end at $q_0$. We must then find the jump in the frame when the curve returns to $q_0$.

To choose a principal axis frame at $q_0$, we note first that the $\mathsf{J}$ tensor is diagonal on the kinematic section [see Eq. (4.2)], so all three Jacobi vectors are orthogonal there and the squares of the Jacobi vectors are equal to the eigenvalues $\lambda_1,\lambda_2,\lambda_3$. Therefore, we choose a frame specified by the configuration $Q_0=\{\mathbf{r}_{s0\alpha}\}$,

$$\mathbf{r}_{s01}=a_1\hat{\mathbf{x}},\quad \mathbf{r}_{s02}=a_2\hat{\mathbf{y}},\quad \mathbf{r}_{s03}=a_3\hat{\mathbf{z}}, \tag{5.2}$$

where $a_i^2=\lambda_i$ and $a_1>a_2>|a_3|\geqslant 0$. This is the analog of Eq. (2.23) of Ref. [1]. We let $a_3$ carry the sign of $V=a_1a_2a_3$ (the chirality), much as we did with $a_2$ in Eq. (2.36) of Ref. [1]. The set $(a_1,a_2,a_3)$ forms a convenient choice for the kinematic invariants; we note that $a_3$ is smooth as $V$ crosses from positive to negative values. The frame given by Eq. (5.2) is a principal axis frame.

One must not think that Eq. (5.2) defines a left-handed frame when $a_3<0$. It does not. In fact, it is impossible to define a left-handed frame in the formalism of this paper since a body frame is equivalent to a choice of a reference point on an external rotation fiber and all such points are related by proper rotations. When $a_3$ is negative, the vector $\mathbf{r}_{s30}$ simply points in the $-z$ direction; the frame itself is always right handed.

To track the principal axis frame continuously as we change the shape we call on the fact discussed in Ref. [1], namely, that the kinematic orbits in configuration space automatically follow the principal axis frame. Suppose, for example, that we wish to start at a shape $q_0$ in the kinematic section and to go around the closed loop specified by $-a$, which is labeled by the SU(2) matrix $-U_x(\pi)=U_x(-\pi)\in V_8$. This loop runs in the opposite direction to the loop $a$ illustrated in Fig. 8. We obtain loop $-a$ by letting the family of kinematic rotations $K_x(\phi)$ act on $q_0$, where $-\pi/2\leqslant\phi<\pi/2$. The alternative range $0\leqslant\phi<\pi$ works just as well since any two kinematic rotations related by an element of $V_4$ [in this case we are thinking of $K_x(\pi)$] have the same effect on a shape. As $\phi$ ranges from 0 to $\pi$, we let $K_x(\phi)$ act on the principal axis body frame (5.2) according to Eq. (2.2), which generates a continuous sequence of principal axis frames. When $\phi=\pi$, we find $Q_1=\{\mathbf{r}_{s1\alpha}\}=K_x(\pi)Q_0$, where

$$\mathbf{r}_{s11}=a_1\hat{\mathbf{x}},\quad \mathbf{r}_{s12}=-a_2\hat{\mathbf{y}},\quad \mathbf{r}_{s13}=-a_3\hat{\mathbf{z}}. \tag{5.3}$$

However, this is related to the original frame by the external rotation $R_x(\pi)$. In other words, we have

$$K_x(\pi)Q_0=R_x(\pi)Q_0, \tag{5.4}$$

which should be compared with Eq. (2.12) of Ref. [1].

Thus we have established that the homotopy class labeled by $U_x(-\pi)$ corresponds to the external rotation $R_x(\pi)$. Similarly, we find that $U_x(\pi)$ corresponds to (the same) $R_x(\pi)$, $\pm U_y(\pi)=U_y(\pm\pi)$ corresponds to $R_y(\pi)$, etc. This is precisely the homomorphism between $V_8$ and $V_4$ that we guessed above.

In summary, homotopy classes $\pm e$, $\pm a$, $\pm b$, and $\pm c$ in Fig. 8 correspond respectively to frame jumps $\mathsf{I}$, $\mathsf{R}_x(\pi)$, $\mathsf{R}_y(\pi)$, and $\mathsf{R}_z(\pi)$. This concludes our discussion of how the frame jump depends on the closed loop in the asymmetric top region of shape space.

### D. Branch cuts and a single-valued principal axis frame

The principal axis frame can be made single valued at the expense of introducing branch cuts in shape space. The effect of the branch cuts is to make the asymmetric top region simply connected, so a single-valued principal axis frame can be defined. The frame is continuous as we move around in shape space, as long as we do not cross the branch cuts. However, the frame (and any wave function with $J\neq 0$ that is referred to the frame) is discontinuous across the branch cuts, so to use this construction it is important to know what the discontinuities are.

In the three-body problem [1], a convenient branch cut in shape space is the region $w_1<0$ of the $w_1$-$w_3$ plane, which is otherwise the surface $\phi=\pm\pi/2$. Here $\phi$ is the kinematic angle and the kinematic section (the surface $\phi=0$) is the region $w_1>0$ of the $w_1$-$w_3$ plane, as discussed in Ref. [1]. The discontinuity in the frame as we cross the branch cut may be defined as the external rotation that maps the old frame to the new one. In the three-body problem, this rotation is $R_z(\pi)$ and is independent of the direction in which we cross the branch cut [because $R_z(\pi)^{-1}=R_z(\pi)$]. We note that in the three-body problem, the branch cut is a two-dimensional surface in shape space that emanates from the one-dimensional line of singularities of the principal axis frame, namely, the $w_3$ axis.

In the four-body problem, we can make the asymmetric top region simply connected by declaring that the surface of the kinetic cube is a branch cut. As noted previously, the space of kinematic invariants (the wedge $\mathbb{R}\times S$; see Table III) is already simply connected, so to make the whole asymmetric top region simply connected we need only make the kinetic cube simply connected. Topologically speaking, the surface of the kinetic cube is really the surface of a cube when viewed as the boundary of the fundamental region in SO(3), but because of the gluing rules it has a more complicated topology when viewed as a subset of the kinematic orbit, that is, the space $SO(3)/V_4$.

The interior of the kinetic cube is a simply connected region over which we can define a single-valued principal axis frame. We do this by arbitrarily choosing one principal axis frame at the center of the kinetic cube (where $\mathsf{K}=\mathsf{I}$, representing a point on the fundamental sector of the kinematic section) and then by continuously tracking the frame along curves that emanate from the center but do not cross the branch cuts on the faces of the cube. The frame we get at the end point of such a continuous tracking depends only on the end point and not on the path because the interior of the cube is simply connected and any two paths starting at the center and ending at the same point can be continuously deformed into one another. Equation (6.1) below is an explicit expression for the principal axis frame constructed in this manner.

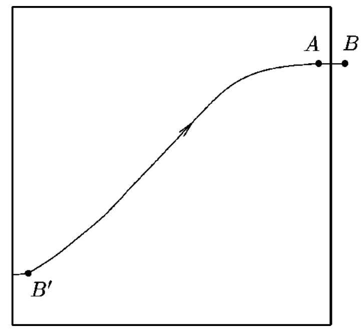


FIG. 10. The square represents a slice through the kinetic cube, interpreted either as a region of SO(3) [the fundamental region under $SO(3)/V_4$] or as the space of asymmetric tops related by kinematic rotations. In the latter interpretation, there are gluing rules at the boundaries. As a region of SO(3), $A$ and $B$ are nearby points on opposite sides of the boundary of the fundamental region; in the space of asymmetric tops, point $B'$ is the same as $B$, according to the gluing rules. The curve passing between the boundary near $B'$ to the boundary near $A$ is a closed loop in the space of asymmetric tops and the discontinuity in the principal axis frame on passing from $A$ to $B$ is the same as the frame jump on going around that closed loop.

As in the three-body problem, we may define the discontinuity as we cross the branch cut as the external rotation that maps the old frame to the new one. This discontinuity is a function of where we are on the branch cut surface, not (as above) of any loop or history that took us to where we are. However, the discontinuity at a point on the branch cut can be mapped into a frame jump associated with a closed loop. Consider Fig. 10, in which the square represents a slice through the kinetic cube and points $A$ and $B$ are just on opposite sides of the branch cut (a face of the cube). As seen in the space $SO(3)/V_4$ (or, equivalently, in shape space along a kinematic orbit of the asymmetric top region), the motion from $A$ to $B$ takes us back inside the kinetic cube to a point $B'$, whose location can be determined by the gluing rules. In shape space, the points $A$ and $B=B'$ are infinitesimally close and effectively lie on the same external rotation fiber, so it makes sense to talk about the external rotation that maps the (single-valued) principal axis frame at $A$ to the principal axis frame at $B'$. This is the discontinuity across the branch cut. However, it is also the frame jump associated with the curve that begins on one face at $B'$ and passes through the interior of the cube to the equivalent point (according to the gluing rules) $A$ on the opposite face. This curve is closed in the kinetic cube, like the curve $a$ in Fig. 8, and since the principal axis frame is continuous in the interior of the cube, the frame jump (obtained by continuous tracking) is the same as the discontinuity.

In this way we see that the frame discontinuity across the faces $\tau_1=\pm 1$ of the kinetic cube is $\mathsf{R}_x(\pi)$, the same as the frame jump for loops $\pm a$. As in the three-body problem, the frame discontinuity is independent of the direction in which we cross the branch cut. Similarly, the frame jumps across the faces $\tau_2=\pm 1$ and $\tau_3=\pm 1$ are $\mathsf{R}_y(\pi)$ and $\mathsf{R}_z(\pi)$, respectively.

This concludes our discussion of the multiple branches of the principal axis frame. In the next section we will study the singularities of the principal axis frame and compare them to those of the Eckart frame.

## VI. FRAME SINGULARITIES

The singularities of the principal axis frame in the four-body problem occur at the symmetric top configurations, both prolate and oblate, where the moment of inertia tensor is degenerate and its eigenframe is not unique (even modulo the senses of the axes). The character of the singularities is almost precisely as in the three-body problem, that is, the principal axis frame does not approach a unique value as a symmetric top configuration is approached and the derivatives of the principal axis frame with respect to shape become infinite there. (One difference is that in the three-body problem, the principal axis frame is singular only at the oblate symmetric top configurations.)

One can define a version of the Eckart frame in the four-body problem that is very similar to the Eckart frame discussed in Ref. [1] for the three-body problem. This Eckart frame is well defined, single valued, continuous, and differentiable everywhere in shape space except at prolate symmetric top configurations of one chirality only. Thus there are no issues of multiple branches, frame jumps, or frame discontinuities with the Eckart frame. The singularities of the Eckart frame are on a smaller subset of shape space than those of the principal axis frame; in fact, one can show that no other frame has singularities on a smaller subset of shape shape than the Eckart frame. In this section we elaborate on these facts.

### A. Singularities of the principal axis frame

We begin by giving an explicit, parametric representation of the principal axis frame over the asymmetric top region of shape space. We have already given an explicit expression for a principal axis frame on the kinematic section, Eq. (5.2). This frame is easily extended to the entire asymmetric top region by applying kinematic rotations. We let $q_0$ be a shape on the kinematic section (the principal sector in Fig. 2), we let $Q_0$ be the frame over this shape according to Eq. (5.2), and we write $Q^{PA}=KQ_0$, $q=Kq_0$, where $K\in \mathrm{SO}(3)$ is a kinematic rotation and where we attach a $PA$ superscript to the configuration $Q^{PA}$ to indicate that it lies on the principal axis section. If we parametrize points on the kinematic section by the kinematic invariants $(a_1,a_2,a_3)$ and if we parametrize the kinematic rotations by kinematic Euler angles $(\theta_1,\theta_2,\theta_3)$, then the Jacobi vectors of $Q^{PA}=\{\mathbf{r}^{PA}_{s\alpha}\}$ are given by

$$\mathbf{r}^{PA}_{s\alpha}(a_1,a_2,a_3;\theta_1,\theta_2,\theta_3)=\sum_\beta K_{\alpha\beta}(\theta_1,\theta_2,\theta_3)a_\beta \mathbf{e}_\beta, \tag{6.1}$$

where $\mathbf{e}_\beta$, $\beta=1,2,3$, represents the unit vectors $\hat{\mathbf{x}},\hat{\mathbf{y}},\hat{\mathbf{z}}$. The kinematic Euler angles can be replaced by other coordinates on SO(3), such as the $\boldsymbol{\tau}$ coordinates, if desired. If a single-valued principal axis frame is required, we can limit the kinematic Euler angles [or other coordinates on SO(3)] to the fundamental region of $\mathrm{SO}(3)/V_4$, the kinetic cube. In Eq. (6.1), the coordinates of $q$ (the shape coordinates) are nicely broken up into three kinematic invariants (the $a$'s) and three kinematic Euler angles (the $\theta$'s), and the equation itself is an explicit, parametric representation of the principal axis frame in these shape coordinates. It is an obvious generalization of Eq. (2.31) of Ref. [1].

The principal axis frame has singularities at all oblate symmetric top shapes. We denote one of these by $q_{ost}$, such as the point marked by a closed circle in Fig. 2. This point is on the edge of the kinematic section (the principal sector in the figure), at which the two largest eigenvalues of $\mathsf{J}$ are equal, $\lambda_1=\lambda_2$, so that $a_1=a_2$. The isotropy subgroup of this point contains the kinematic rotations $\mathsf{K}_3(\phi)$, which are rotations in the 1-2 plane. Now consider an asymmetric top shape $q_0$ in the interior of the principal sector, which we allow to approach the point $q_{ost}$. By continuity, the kinematic rotations $\mathsf{K}_3(\phi)$, which leave the point $q_{ost}$ invariant, must have only a small effect on $q_0$. In fact, as $\phi$ ranges between $\pm\pi/2$, the curve in shape space swept out by allowing $\mathsf{K}_3(\phi)$ to act on $q_0$ is a small circle that contracts onto $q_{ost}$ as $q_0\to q_{ost}$. The principal axis frame is defined over this circle according to Eq. (6.1) and is given explicitly by

$$\mathsf{K}_3(\phi)Q_0=\begin{pmatrix}\mathbf{r}^{PA}_{s1}\\ \mathbf{r}^{PA}_{s2}\\ \mathbf{r}^{PA}_{s3}\end{pmatrix}=\begin{pmatrix}\cos\phi & -\sin\phi & 0\\ \sin\phi & \cos\phi & 0\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}a_1\hat{\mathbf{x}}\\ a_2\hat{\mathbf{y}}\\ a_3\hat{\mathbf{z}}\end{pmatrix}$$
$$=\begin{pmatrix}a_1\cos\phi\hat{\mathbf{x}}-a_2\sin\phi\hat{\mathbf{y}}\\ a_1\sin\phi\hat{\mathbf{x}}+a_2\cos\phi\hat{\mathbf{y}}\\ a_3\hat{\mathbf{z}}\end{pmatrix}, \tag{6.2}$$

which may be compared to Eq. (2.31) of Ref. [1]. As $q_0\to q_{ost}$ at fixed $\phi$, $a_1\to a_2$ and the principal axis frame approaches a definite limit, but one that depends on $\phi$. Therefore, the frame is singular at $q_{ost}$. A similar argument applies to other oblate symmetric tops, obtained by applying kinematic rotations to $q_{ost}$; the only difference is that the isotropy subgroups are conjugate to the one used in Eq. (6.2), as explained in Appendix A.

The prolate symmetric tops are similar, except for the special treatment of the case $V=0$. Consider a prolate symmetric top shape $q_{pst}$, such as the point marked by an asterisk in Fig. 2, at which the two smallest eigenvalues of $\mathsf{J}$ are equal, $\lambda_2=\lambda_3$. For $V>0$ this implies $a_2=a_3>0$ and for $V<0$ it implies $a_2=-a_3=|a_3|$. We will defer the case $V=0$ for a moment. Also, let $q_0$ be an asymmetric top shape near $q_{pst}$. Now the isotropy subgroup of $q_{pst}$ contains the kinematic rotations $K_1(\phi)$, which sweep out a small circle when acting on $q_0$. The principal axis frames defined over this circle are given by

$$\mathsf{K}_1(\phi)Q_0=\begin{pmatrix}\mathbf{r}^{PA}_{s1}\\ \mathbf{r}^{PA}_{s2}\\ \mathbf{r}^{PA}_{s3}\end{pmatrix}=\begin{pmatrix}1 & 0 & 0\\ 0 & \cos\phi & -\sin\phi\\ 0 & \sin\phi & \cos\phi\end{pmatrix}\begin{pmatrix}a_1\hat{\mathbf{x}}\\ a_2\hat{\mathbf{y}}\\ a_3\hat{\mathbf{z}}\end{pmatrix}$$
$$=\begin{pmatrix}a_1\hat{\mathbf{x}}\\ a_2\cos\phi\hat{\mathbf{y}}-a_3\sin\phi\hat{\mathbf{z}}\\ a_2\sin\phi\hat{\mathbf{y}}+a_3\cos\phi\hat{\mathbf{z}}\end{pmatrix}. \tag{6.3}$$

When $q_0 \to q_{pst}$, we have $a_2 \to |a_3|$, the limit of the frame is $\phi$ dependent, and we have a frame singularity of the same character as in the oblate case.

However, $V=0$ implies $a_3=0$, so at $q_{pst}$ we have $a_2 = a_3 = 0$, which is the condition for a collinear configuration. It also means that as the limit $a_2 \to |a_3| = 0$ is taken, the configuration $Q^{PA} = \{\mathbf{r}_{s\alpha}^{PA}\}$ approaches a limit that is independent of $\phi$. However, a collinear configuration cannot define a frame, so the principal axis frame must still be considered singular at such configurations. In fact, the collinear configurations are singular in the strongest senses of any configurations in the four-body problem, as we will see momentarily.

### B. Eckart frame

We now introduce a version of the Eckart frame, closely following the steps taken in Ref. [1]. The standard definition of the Eckart frame in constraint form is given by Eq. (2.16) of Ref. [1]. The definition involves an ''equilibrium'' configuration $Q_e = \{\mathbf{r}_{se\alpha}\}$, which we define as follows. First we define an equilibrium shape $q_e$ as a spherical top with hyperradius $\rho_e > 0$, so that $V>0$ and $w_1 = \cdots = w_5 = 0$ at $q_e$. Next we define a frame $Q_e = \{\mathbf{r}_{se\alpha}\}$ over $q_e$ by $\mathbf{r}_{se1} = k\hat{\mathbf{x}}$, $\mathbf{r}_{se2} = k\hat{\mathbf{y}}$, $\mathbf{r}_{se3} = k\hat{\mathbf{z}}$, where $k = \rho_e/\sqrt{3}$. This is both an Eckart frame and a principal axis frame. Next we let $q_0$ be an arbitrary asymmetric top shape on the kinematic section and we define the frame $Q_0 = \{\mathbf{r}_{s0\alpha}\}$ over $q_0$ by Eq. (5.2). As noted above, this is a principal axis frame, but it is also an Eckart frame, as follows immediately from the definition, Eq. (2.16) of Ref. [1]. Next we define a frame over all of the asymmetric top region by setting

$$\begin{aligned} Q^E = \{\mathbf{r}_{s\alpha}^E\} &= R(\theta_1, \theta_2, \theta_3) Q^{PA} \\ &= R(\theta_1, \theta_2, \theta_3) K(\theta_1, \theta_2, \theta_3) Q_0, \end{aligned} \tag{6.4}$$

where $Q^{PA}$ is defined by Eq. (6.1) and the Euler angles $\theta_i$ are the same as in that equation (the kinematic and external Euler angles are equal). Equation (6.4) should be compared with Eq. (2.24) of Ref. [1]. Finally, we show that $Q^E$ actually is an Eckart frame relative to the equilibrium $Q_e$, following Eqs. (2.28) and (2.29) of Ref. [1].

The Eckart frame defined by Eq. (6.4) is single valued because the external rotation in Eq. (6.4) cancels out the frame jump in the principal axis frame on going around any closed loop in shape space. For example, the frame jump on going around homotopy class $a$ is $R_x(\pi)$, as noted above, but Eq. (6.4) supplies another factor of $R_x(\pi)$, which cancels the first.

The Eckart frame is also well defined and nonsingular at all oblate symmetric tops. To show this we apply Eq. (6.4) to the principal axis frame over the small circle about $q_{ost}$, shown in Eq. (6.2). This gives

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

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

$$\mathbf{r}_{s3}^E = a_3\hat{\mathbf{z}}. \tag{6.5}$$

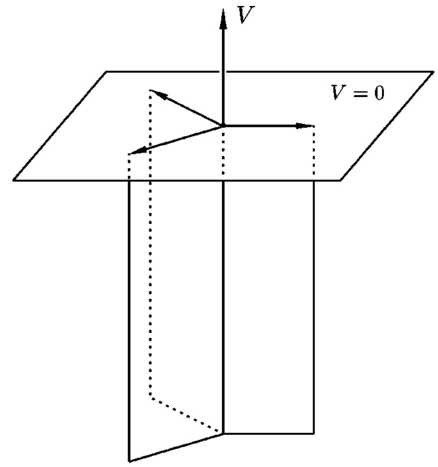


FIG. 11. The Eckart frame is singular on a four-dimensional surface that can be visualized as sheets hanging down from the collinear configurations into regions of negative $V$. These sheets (the singular set) consist of all prolate symmetric tops of one chirality only ($V \le 0$). The three radial half lines in the hyperplane $V=0$ represent the collinear shapes, which are prolate symmetric tops of zero volume, and are identified with the three half lines of Fig. 2.

Now when $a_1 \to a_2$, the frame approaches a definite value [the one given by Eq. (5.2)], independent of $\phi$, and there is no singularity.

As for the prolate symmetric tops, the Eckart frame is well defined and nonsingular there only for $V>0$. We see this by applying Eq. (6.4) to the principal axis frame over the small circle about $q_{pst}$, shown in Eq. (6.3). This gives

$$\mathbf{r}_{s1}^E = a_1\hat{\mathbf{x}},$$

$$\mathbf{r}_{s2}^E = (a_2\cos^2\phi + a_3\sin^2\phi)\hat{\mathbf{y}} + (a_2 - a_3)\sin\phi\cos\phi\hat{\mathbf{z}},$$

$$\mathbf{r}_{s3}^E = (a_2 - a_3)\sin\phi\cos\phi\hat{\mathbf{y}} + (a_2\sin^2\phi + a_3\cos^2\phi)\hat{\mathbf{z}}. \tag{6.6}$$

If $V>0$, then as $q_0 \to q_{pst}$ we have $a_2 \to a_3$ and the Eckart frame approaches a limit independent of $\phi$. In this case there is no singularity. However when $V<0$, $a_2 \to -a_3$ and the limit of the Eckart frame does depend on $\phi$, producing a singularity much like those of the principal axis frame at any symmetric top configuration.

Altogether, we see that the Eckart frame has singularities at the prolate symmetric top configurations of one chirality only ($V \le 0$). The singular set (the set of shapes upon which the frame is singular) is a four-dimensional surface in shape space that begins on the three-dimensional surface of collinear shapes and extends ''downward'' into regions of negative $V$.

One approach to visualizing this singular set is Fig. 11, in which the collinear shapes (the prolate symmetric tops of zero volume) are represented by three radial half lines inside the hyperplane $V=0$. More precisely, these three half lines are identified with the three half lines labeled $P$ in Fig. 2 in the hyperplane $V=0$, which are just the part of the space of collinear configurations that intersects the $w_1$-$w_5$ plane. (The entire space of collinear configurations is obtained by allowing the kinematic rotations to act on one of the radial half lines.)

The singular set for the Eckart frame may be said to be only 1/4 as large as the singular set for the principal axis frame because the latter frame is singular on both prolate and oblate symmetric top configurations of both chiralities. Thus there are frames for which the singular set is larger than that of the Eckart frame. However, there are no frames with a smaller singular set, as we will now argue. In particular, there are no frames that are free of singularities everywhere.

As in the three-body problem, the singular set in the four-body problem can be moved to different regions of shape space by means of gauge transformations (changes of body frame); for example, if the equilibrium point is chosen to be a spherical top of negative volume, then the singular set of the Eckart frame will lie on prolate symmetric tops of positive chirality ($V \geqslant 0$) and the sheets in Fig. 11 will extend upward. Thus there is nothing intrinsically singular about prolate tops of negative chirality; frame singularities occur there only for specific choices of frame.

On the other hand, the collinear shapes are singular for all choices of frame and the singular set of any choice of frame will be a surface that will include the collinear shapes. In effect, changes of frame can pivot the sheets in Fig. 11 about the collinear configurations or even bend them about, but never detach them from the collinear configurations. Thus we may call the collinear configurations the set of intrinsic singularities (independent of choice of body frame). This is much as in the three-body problem (the planar three-body problem forms a better analogy than the three-body problem in space), in which the singular set is a line (the string of the monopole) emanating from the three-body collision, which is the intrinsically singular set. The three-body collision in the three-body problem is analogous to the collinear configurations in the four-body problem and the string in the three-body problem is analogous to the singular set in the four-body problem. Notice that in both cases, the singular set has codimension 2, while the intrinsically singular set has codimension 3.

In the three-body problem, the singular set (the string) starts at the three-body collision and goes out to infinity. For example, one can show that the string cannot simply terminate somewhere or turn around and reattach to the three-body collision. This is done by proving that the fiber bundle is nontrivial over any sphere in shape space of constant hyperradius, no matter how large.

Similarly, in the four-body problem, the singular set is necessarily a four-dimensional surface that attaches to the three-dimensional manifold of collinear shapes and extends to infinity in shape space. In this case the proof proceeds by first constructing a certain two-sphere in shape space that lies in a three-dimensional surface transverse to the three-dimensional surface of collinear shapes. This sphere surrounds the single collinear shape that lies in the transverse surface. Then the SO(3) fiber bundle of external rotations is restricted to the lift of this sphere in shape space and this restricted bundle is proved to be nontrivial. Thus there is at least one point on the sphere where the gauge potential must be singular. By carrying out this construction for every collinear shape, a four-dimensional singular set is generated. The details of this proof involve standard techniques from the topology of fiber bundles, but they are outside the intended scope of this paper. We will provide a complete proof in future work.

## VII. CONCLUSIONS

In the future we plan to write another paper on all types of singularities in the internal space of the $n$-body problem, a paper that will call on the general theory presented in this paper but will be explicit about the various frames, coordinate systems, and basis sets that are used in current practice. This paper will deal with other types of singularities besides frame singularities. Based on conversations with researchers in the field, such a paper seems timely and desirable. This paper will present another perspective on many of the issues raised by Pack [15] and will also discuss the cases $n=4$ and $n \geqslant 5$.

Finally, we will make some comments on the practical impact of frame singularities for four-body quantum calculations. These comments cannot be comprehensive because there are so many different approaches to such calculations and, moreover, new methods may be invented in the future. However, certain things can be said.

In some circumstances it may be that frame singularities will not present serious difficulties. For example, if the exact wave function is expanded in terms of some complete set of functions, which themselves are eigenfunctions of some solvable problem, then those eigenfunctions will carry the frame singularities. (The expansion coefficients will be just numbers and will be perfectly well behaved.) For example, the basis functions might be hyperspherical harmonics or other eigenfunctions on the hypersphere. Even in this case, however, it will be important to know about the frame singularities, if only for working out the formulas for the exact eigenfunctions or for purposes of display.

On the other hand, in the case of grid or related methods (such as discrete variable representations or distributed Gaussian bases), the singularities, discontinuities, and other bad behavior of the internal wave function will have to be taken into account at the locations in the internal space where they occur. Or it may be necessary to use more than one frame in different parts of the internal space. This latter possibility seems unattractive at first sight, but it might be workable if carefully done. In this regard, we may note that the standard mathematical theory of fiber bundles requires the use of overlapping patches on the base space, in which a single gauge convention (the analog of a body frame in the present context) is used in each patch. Only in this way can singularities be systematically avoided. If this construction is used, it will be necessary to change frames in the overlap regions.

Moreover, even if a basis set expansion is used, it will still be necessary to deal with frame singularities if the basis set itself is determined by some numerical method, as is common already in three-body work. This is because the frame singularities will appear in the basis functions and will make trouble for the numerical methods used to determine them.

Of course, if the wave function is localized in the internal space, then it may be possible to choose a frame in which all singularities exist outside the region where the wave function is effectively nonzero. This commonly happens in three-body scattering calculations of sufficiently low energy, in which the singularities of the principal axis frame on the line of symmetric oblate top shapes lie deep in a classically forbidden region. It also commonly happens in bound-state problems.

In any case, there can be no question that it is important to know about the existence of frame singularities and to be careful about them. If they do make trouble, it will be important to know the extent to which the singularities can be moved about and how their impact can be minimized. This paper has provided the necessary foundation for understanding such problems.

## ACKNOWLEDGMENTS

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## APPENDIX A: GROUP ACTIONS

The concepts of group actions, orbits, isotropy subgroups, quotient spaces, etc., are very useful in understanding the spaces that occur in the $n$-body problem, especially when $n > 3$. Quite generally, these concepts arise wherever the word ''modulo'' is used, as in ''two configurations of the same shape are equal modulo a proper rotation'' or ''two configurations with the same $\mathsf{J}$ tensor have the same shape, modulo chirality.''

If $G$ is a group and $M$ is a space, then an *action* of $G$ on $M$ is a representation of $G$ by means of transformation operators or mappings that map $M$ onto itself. These mappings need not be linear (in any sense). If $g,h \in G$ are group elements and $T_g, T_h$ the corresponding mappings, then we require $T_g T_h = T_{gh}$. If $x$ is a point of $M$ and $g$ is a group element, then $T_g$ causes $x$ to get up and move to a (possibly) new point $x'$, which we denote by $x' = T_g x$. The group element $g$ is conceptually distinct from the mapping $T_g$, but we can be sloppy with notation and write simply $x' = gx$. This is what is done in the body of the paper when we write $Q' = RQ$ [confusing the transformation operator on configuration space with the rotation $R \in SO(3)$ itself] or $Q' = KQ$, $q' = Kq$, etc.

If $x$ is a point of a space $M$ upon which a group $G$ acts, then the set of points $x'$ of $M$ that can be reached from $x$ by means of the operators $T_g$ is called the *orbit* of $x$ under the action of $G$. In other words, the orbit is the set $\{T_g x | g \in G\}$, that is, the set of points swept out by letting all possible group elements act on $x$. Depending on circumstances, the orbit may be either a discrete set or a continuous one, or something more complicated.

The orbits of a group action on a space $M$ are disjoint subsets of that space. That is, if any two orbits have one point in common, then they have all points in common and are identical orbits; otherwise they are disjoint. This is important because it means that a point of $M$ can be uniquely identified by a label of the orbit in which it lies, plus a label indicating where it lies within that orbit. To prove this property, suppose $x'$ and $y'$ are on the orbits of points $x$ and $y$, that is, suppose $x' = T_g x$ and $y' = T_h y$ for some $g,h \in G$. Then suppose $x' = y'$. Then all points on the $y$ orbit belong to the $x$ orbit and, conversely, because if $y'' = T_k y$ for some $k \in G$, then $y'' = T_k T_{h^{-1}} T_g x$, etc.

The identity element (call it $e \in G$) does nothing to any point of $M$, that is, $T_e x = x$ for all $x \in M$. However, depending on the point $x$ and the nature of the group action, there may be other group elements that also leave $x$ invariant. Let $g$ and $h$ be two group elements that leave $x$ invariant, $T_g x = x$ and $T_h x = x$. Then $T_{gh} x = T_g T_h x = T_g x = x$, so the product $gh$ also leaves $x$ invariant. Thus the set of group elements that leave a given point $x$ invariant forms a group, the *isotropy subgroup* of $G$ at $x$, which we denote by $I_x$. In general the isotropy subgroup depends on $x$. The isotropy subgroup is the set $I_x = \{g \in G | T_g x = x\}$.

One extreme case is when all group elements leave a point $x$ invariant, so that the orbit of $x$ is just the point $x$ itself and $I_x = G$. Another extreme is when only the identity $e \in G$ leaves $x$ invariant, so that $I_x = \{e\}$, the trivial subgroup. In this case the orbit is effectively a copy of $G$ because it is possible to place points of the orbit in one-to-one correspondence with elements of $G$ (that is, $e \leftrightarrow x$, $g \leftrightarrow T_g x$, etc). In this case one can use group elements as labels or coordinates of points along the orbits (this is what is done with the noncollinear orbits of the external rotations acting on configuration space; the external Euler angles label the group element that identifies the orientation of the configuration). Intermediate cases are possible too, assuming $G$ has subgroups of intermediate size (that is, proper subgroups). A general rule is the larger the isotropy subgroup, the smaller the orbit, and conversely. This rule is clearly seen in Tables I and II.

When two things are said to be equivalent modulo a certain property, it does not mean that they are equal, but that they would be equal if we ignored the certain property. Often the property in question is that of being related by a group action, that is, of lying on the same orbit of a group action. For example, 3 and 18 are congruent modulo 5; this means they are related by the discrete group of displacements by integer multiples of 5 (they lie on the same orbit of this group). For another example, antipodal points of the two-sphere $S^2$ can be said to be equivalent modulo parity, that is, they lie on the same orbit of the two-element group $\{I,P\}$, where $P$ is the parity or spatial inversion operator.

If the isotropy subgroup $I_x$ of a point $x$ is the trivial subgroup $\{e\}$, then, as mentioned above, the points on the orbit can be labeled or coordinated by group elements $g$. If the isotropy subgroup $I_x$ is not trivial, then the point $x$ is labeled not only by the identity element $e$ but equally well by any member $h \in I_x$ (they all map $x$ to $x$). As for another point on the orbit, say, $x' = T_g x$ for some $g \in G$ where $x' \neq x$, it can be labeled by $g$, but equally well by $gh$ for any $h \in I_x$. For given $g \in G$, the set $\{gh | h \in I_x\}$ is a left coset of $I_x$ in $G$. Thus, in the general case of a nontrivial isotropy subgroup, the points on the orbit can be labeled by, that is, placed in one-to-one correspondence with, the left cosets of $I_x$ in $G$.

The cosets (both left and right) of a subgroup $H$ of $G$ are disjoint subsets of $G$ that are themselves orbits of group actions. This is a useful point of view because it subsumes the concept of cosets within the concept of group orbits. In the case of right cosets the action is that of $H$ on $G$ defined by $T_h g = hg$ for $h \in H$ and $g \in G$ (here $G$ has taken the role of $M$ and $H$ that of $G$). Thus the orbit of $g$ under this action is the set $\{hg | h \in H\}$, which is a right coset of $H$. The left cosets are orbits of a different action of $H$ on $G$, defined by $T_h g = gh^{-1}$. To say that two elements in $g$ belong to the same (left or right) coset of $H$ means that they are equivalent modulo (right or left) multiplication by some element of $H$.

If a space $M$ is acted upon by a group $G$, we can create a new space in which a single point represents an entire orbit in $M$, that is, a set of points in $M$ that are related by the action of the group. This new space is the *quotient space* and is denoted by $M/G$. The quotient space is only defined relative to the particular action of $G$ on $M$, which must be understood when using the notation $M/G$.

Suppose $x$ and $y$ are two points on the same orbit of a group $G$ acting on $M$ and the two isotropy subgroups are $I_x$ and $I_y$. Then $I_x$ and $I_y$ are conjugate subgroups within $G$, that is, they are identical as abstract groups, but in general are different subgroups of $G$. In fact, it is easy to show that if $y = T_a x$ for $a \in G$, then $I_y = a I_x a^{-1}$. For example, the collinear configurations in Table I have the isotropy subgroups SO(2) in SO(3); these subgroups consist physically of the rotations about the axis of collinearity. This axis is different for rotated configurations (different points on the orbit $S^2$), so the SO(2) subgroups are different, but these SO(2) subgroups are all conjugate to one another.

## APPENDIX B: SPACES OCCURRING IN THE FOUR-BODY PROBLEM

This appendix explains the standard mathematical notation for various spaces that occur in the four-body problem and fills in a few other mathematical points that were used in the paper. The following mathematical spaces are used in this paper. The notation $\mathbb{R}^n$ represents the usual space of $n$-tuples of real numbers. The $n$-sphere $S^n$ is the set of points at unit distance from the origin in $\mathbb{R}^{n+1}$. For example, $S^1$ is the circle and $S^2$ the usual two-sphere. The set of integers (positive, negative, and zero) is $\mathbb{Z}$. The set $\mathbb{Z}_2$ stands for the integers modulo 2, that is, the set {0,1}, which forms a group under addition modulo 2. As an abstract group, it is the same as the two-element group $\{e,a\}$ with multiplication law $a^2 = e$.

Two spaces are said to be diffeomorphic if there exists a smooth, invertible mapping between them, for which the inverse map is also smooth. This means the two manifolds have the same topology and also (intuitively speaking) that there are no kinks in the two manifolds or in the mappings between them. In the body of Ref. [1] and this paper, sometimes we say that the two manifolds are ''copies'' of each other when we mean that they are diffeomorphic.

The real projective space $\mathbb{R}P^n$ is the quotient space $S^n/\mathbb{Z}_2$, that is, a point of $\mathbb{R}P^n$ can be identified with a pair of antipodal points in $S^n$. The space $\mathbb{R}P^1$ is the circle with antipodal points identified, which is the same as a semicircle with end points identified, which is the same as a circle again. That is, $S^1/\mathbb{Z}_2 = S^1$. The space $\mathbb{R}P^2$ is an ordinary two-sphere $S^2$ with antipodal points identified, which is the same as a hemisphere with antipodal points on the equator identified.

The groups SO(2), SO(3), O(2), and SU(2) are standard Lie groups that can also be viewed as manifolds. The group manifold SO(2) is the circle $S^1$, SO(3) is the real projective space $\mathbb{R}P^3$, and SU(2) is the three-sphere $S^3$.

Now we will prove Eq. (2.1), which says that the space of left cosets of SO(2) in SO(3) is the two-sphere $S^2$. Here SO(2) is understood to be a subgroup of SO(3) consisting of rotations about a fixed axis; we will work with the $z$ axis. First we note that two rotations $R_1, R_2 \in \mathrm{SO}(3)$ belong to the same left coset of SO(2) if $R_1 = R_2 S$ for some $S \in \mathrm{SO}(2)$. Also, a rotation is uniquely specified by its action on an orthonormal frame, that is, a rotation maps a fixed old frame into a unique new frame, and a given new frame specifies a unique rotation. (Of course we are speaking of proper rotations and right-handed frames.) However, since $S$ leaves the $z$ axis invariant, we see that two rotations $R_1$ and $R_2$ belonging to the same left coset map the old $z$ axis into the same new $z$ axis. Conversely, if $R_1$ and $R_2$ produce the same new $z$ axis when acting on the old frame, then $R_2^{-1} R_1$ maps the old $z$ axis into itself, which means that $R_2^{-1} R_1 = S$ for some $S \in \mathrm{SO}(2)$, so that $R_1$ and $R_2$ belong to the same left coset. Therefore, the new $z$ axes stand in one-to-one correspondence with the left cosets. However, the space of new $z$ axes is the space of unit vectors in $\mathbb{R}^3$, which is $S^2$.

The proof of Eq. (4.9) is similar. Now we wish to consider the subgroup O(2) of SO(3), where the matrices belonging to the representation of O(2) have the form indicated in Eq. (4.8), that is, they are proper rotations in three dimensions that either leave the $x$ axis invariant or flip its sign. As viewed in the $y$-$z$ plane, these rotations are either proper or improper orthogonal transformations. The argument is much as in the preceding paragraph; two rotations $R_1, R_2 \in \mathrm{SO}(3)$ belong to the same left coset of O(2) if and only if they map the old $x$ axis onto the same new $x$ axis, with the possibility of a reversal of the sense of this axis. Therefore, the space of cosets is the same as the space of lines passing through the origin in $\mathbb{R}^3$, which is $\mathbb{R}P^2$.

## APPENDIX C: KINEMATIC ORBITS IN CONFIGURATION SPACE

In the three-body problem, we saw in Ref. [1] that for asymmetric tops the (one-dimensional) kinematic orbits were not tangential to the (three-dimensional) external rotation orbits; see Fig. 1 of Ref. [1]. To say this another way, if an asymmetric top configuration $Q$ is acted upon by three independent, infinitesimal external rotations, it generates three vectors in configuration space that are tangential to the rotation orbit; if it is acted upon by an infinitesimal kinematic rotation, it generates another vector that is tangent to the kinematic orbit. For asymmetric tops, these four vectors (in $\mathbb{R}^6$) are linearly independent, that is, for small kinematic angles, the kinematic orbit goes off in a direction that is independent of the rotations. However, for oblate symmetric tops, we saw that the infinitesimal kinematic rotations are tangential to the external rotation orbits. In fact, in this case, the entire kinematic orbit lies within the rotation orbit. This appendix generalizes these facts to the case of the four-body problem.

First we classify the orbits. If $Q$ is a configuration in the four-body problem, then the orbit of $Q$ under the kinematic group is either SO(3), $S^2$, or a single point, according to whether $Q$ is noncollinear, collinear, or the four-body collision, exactly as indicated by Table I for the external rotations. This follows from the fact that there is a complete mathematical symmetry between external rotations and kinematic rotations, most easily seen in terms of the $\mathsf{F}_s$ matrix, where external rotations act on the $i=1,2,3$ index and kinematic rotations act on the $\alpha=1,2,3$ index. Effectively, one group acts on rows, the other on columns. However, the three cases, noncollinear, collinear, and four-body collision, are equivalent to $r\geqslant 2$, $r=1$, and $r=0$, respectively, where $r=\operatorname{rank}\mathsf{F}_s$ and the rank is the number of linearly independent rows or columns (it does not matter which). Therefore, the isotropy subgroup and the topology of the orbits depend only on $r$ and not on whether the group acts on the rows or columns of $\mathsf{F}_s$.

This is to say that the external rotation orbit and the kinematic orbit of a given point $Q$ have the same topology and in fact are diffeomorphic as submanifolds of configuration space; they are not, however, the same submanifold in general. First consider the case of a noncollinear configuration, in which both orbits are three-dimensional copies of SO(3). If the configuration is an asymmetric top, then the three directions tangential to the external rotation orbit and the three directions tangential to the kinematic orbit are linearly independent (as vectors in $\mathbb{R}^9$). In other words, for asymmetric tops, all three independent, infinitesimal kinematic rotations change the shape of $Q$, that is, move us to a different rotation fiber. This means that Fig. 1 of Ref. [1] is schematically accurate for asymmetric top configurations in the four-body problem if the fibers $F_R$ and $F_K$ are interpreted as three-dimensional surfaces in $\mathbb{R}^9$. For symmetric tops (still noncollinear), there is one infinitesimal kinematic rotation that is tangential to the external rotation orbit, and conversely; this is equivalent to the fact that there is a one-parameter subgroup of the kinematic group [an SO(2) subgroup] consisting of kinematic rotations with the same effect on $Q$ as an external rotation [in fact, an SO(2) subgroup of the external rotations]. Kinematic rotations in this subgroup do not change the shape of the configuration (only its orientation). Finally, for the spherical top (still noncollinear), the entire external rotation orbit and kinematic rotation orbit [both copies of SO(3)] coincide, which follows from the fact that the $\mathsf{F}_s$ matrix is a multiple of the identity in this case. In this case, no kinematic rotation changes the shape.

Next, for collinear configurations, both the external rotation orbit and kinematic orbit of a given configuration $Q$ are two-spheres $S^2$, but they are not identical two-spheres. In fact, the two two-dimensional tangent spaces to these two-spheres at the point $Q$ are linearly independent (they span altogether a four-dimensional subspace of $\mathbb{R}^9$). This means that any infinitesimal kinematic rotation that moves $Q$ does so in such a way as to change the shape (the point $Q$ does not simply move down its external rotation orbit). Finally, for the four-body collision, neither external nor kinematic rotations do anything to $Q$; both orbits consist of the single point $Q$ itself.


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