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**Kinematic Orbits and the Structure of the Internal Space for
Systems of Five or More Bodies**

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Abstract

The internal space for a molecule, atom, or other n -body system can be conveniently parameterised by $3n - 9$ kinematic angles and three kinematic invariants. For a fixed set of kinematic invariants, the kinematic angles parameterise a subspace, called a kinematic orbit, of the n -body internal space. Building on an earlier analysis of the three- and four-body problems, we derive the form of these kinematic orbits (that is, their topology) for the general n -body problem. The case $n = 5$ is studied in detail, along with the previously studied cases $n = 3, 4$.

I. INTRODUCTION

The group of kinematic rotations, called here the kinematic group, is an important set of symmetries for the n -body kinetic energy. In fact, the kinematic group, to be defined precisely below, is the largest (compact, connected) group of such symmetries acting on the n -body internal space. Not surprisingly then, the orbits (see Appendix A, Ref. [1]) of the kinematic group provide a useful decomposition of the internal space. It is the purpose of this paper to analyse these orbits and to determine their topology. We have been motivated by molecular applications, but the results are quite general and could be applied to any n -body system with rotational invariance, such as atoms or nuclei.

Although many reasons exist to study kinematic rotations and their orbits, our current motivation derives from an interest in body frame singularities and their implications for the quantum dynamics of n -body systems. In two previous papers [1,2], body frame singularities in the three- and four-body problems were studied explicitly. The definition of body frame singularities, their inevitability, the flexibility one has in moving them, and their importance for quantum dynamics are all discussed in Refs. [1,2]. A detailed study of frame singularities has also been made by Pack [3]. Our earlier analysis of body frame singularities (especially the singularities of the principal axis and related frames) involved extensive use of kinematic

rotations. The present paper extends the analysis of kinematic rotations to arbitrary n and provides the basis for a future discussion of frame singularities for the general n -body problem. Although the present paper concentrates on kinematic orbits in their own right, for motivational reasons, we provide a brief two paragraph account of frame singularities, referring to Refs. [1–3] for greater detail.

An early and necessary step in many quantum n -body computations is choosing a set of body-fixed axes, that is, a body frame. The principal axis frame, in which the body-fixed axes are aligned with the principal axes, is one common choice. The body frame is a function of the shape of the system, by which we mean the positions of the bodies relative to each other; the shape may be parameterised by $3n - 6$ internal coordinates. As has been previously noted [1–3], a body frame may fail to be a smooth function of shape, and thus there may be points in the internal, or shape, space at which it is singular. (In this paper, the internal space and shape space are synonymous.) For example, in the three-body problem, the principal axis frame is singular at all oblate symmetric tops (among other shapes), and in the four-body problem, the principal axis frame is singular at all symmetric tops (among other shapes). Body frame singularities have important consequences for the form of the quantum wave function: roughly speaking, the wave function has singularities matching those of the body frame. An understanding of body frame singularities is therefore critical for understanding the singularities of the n -body wave function.

The location of the body frame singularities in shape space depends on the choice of body frame; by choosing different frames one can move these singularities about or possibly remove them altogether (as is essentially the case for the three-body problem [2,3]). Thus, for many problems one can choose a frame whose singularities are outside the physically relevant region of shape space. This is true of small vibration problems (about a noncollinear equilibrium) in which the wave function is localised around an equilibrium shape. However, for scattering states and delocalised bound states, it becomes harder to eliminate the singularities from the region of interest. For certain regions, it becomes topologically impossible to remove them completely and one must then understand their effects.

Though the study of kinematic orbits is developed here with the ultimate intent of developing a deeper understanding of frame singularities, several other reasons motivate our work. First, since the kinematic group is the largest (compact, connected) group of symmetries (of the kinetic energy) acting on shape space, the kinematic orbits provide an important foliation of shape space with which to study the kinetic energy operator. Furthermore, this foliation suggests a convenient method of defining internal, or shape, coordinates [4–11]: three internal coordinates are chosen to be kinematic invariants (for example, the three principal moments of inertia), which label a particular kinematic orbit, and the remaining $3n - 9$ internal coordinates are chosen to be kinematic angles, which parameterise the position along the kinematic orbit. Defining these angles and properly specifying their ranges requires a clear understanding of the topology of the orbits. Finally, certain large amplitude internal motions, such as pseudorotations, can be approximated by kinematic rotations. For such systems, it may be convenient to restrict the region of physical interest to a single kinematic orbit.

The kinematic group is commonly viewed as the set of discrete transformations between different conventions for Jacobi vectors. Here, however, we define the kinematic group to be a continuous symmetry group, namely $SO(n-1)$, which contains these transformations. The elements of the kinematic group $SO(n-1)$ are called kinematic rotations to distinguish them from the ordinary external $SO(3)$ rotations. (Sometimes the terminology “democracy transformations” and “democracy group” is used.) Kinematic rotations act (in the active sense) on the Jacobi vectors as shown in Eq. (2.3), from which one sees that they commute with external rotations (as shown in Eq. (2.1)). Therefore, kinematic rotations do indeed have a well-defined action on the shape of an n -body system. It is the orbits of this action of the kinematic rotations, for arbitrary n , which we compute in the present paper.

As examples of our general analysis, we specialise to the three- and four-body problems, recovering the previously known results found in Refs. [1,2,12]. The kinematic orbits for the three- and four-body cases do not exhibit the full range of diversity found in the general n -body problem and are thus somewhat special. For example, in the four-body problem the

kinematic orbits can be classified by whether a shape is an asymmetric top, a symmetric top, or a spherical top, a classification which does not hold in the general n -body case. We therefore also specialise to the five-body problem, for which the results are not previously known. As with the three- and four-body problems, the kinematic orbits for the five-body problem have particularly simple forms. However, there are seven classes of kinematic orbits, which is representative of the general n -body case.

The approach and methods used in this paper are geometrical in nature. We assume familiarity with the techniques of Refs. [1,2] and some basic understanding of Lie groups, their actions on manifolds, and the quotients by such actions. Appendix A of Ref. [1] provides a useful review, as do many basic texts [13,14].

The structure of the paper is as follows. Section II contains the principal derivations, in which we determine the isotropy subgroup of the kinematic action on shape space. This subgroup is related to the kinematic orbit via Eq. (2.5). The results of Sect. II are summarised in Table I. The results for arbitrary n are discussed briefly in Sect. III where we focus primarily on the collinear shapes. In Sect. IV we specialise the results of Sect. II to the three- and four-body problems, and these results are summarised in Tables II and III. Similarly, in Sect. V, we specialise to the five-body problem. This requires substantially more work than the three- and four-body cases which causes Sect. V to constitute almost half of the paper. The five-body results are summarised in Table IV. Our conclusions are in Sect. VI. We also include an Appendix containing three important theorems on the actions of Lie groups.

II. THE TOPOLOGY OF KINEMATIC ORBITS FOR ARBITRARY n

In the centre of mass frame, the configuration of an n -body system is parameterised by $n - 1$ (mass-weighted) Jacobi vectors $\mathbf{r}_{s\alpha}$, $\alpha = 1, \dots, n - 1$. Here, the s subscript indicates that the components of $\mathbf{r}_{s\alpha}$ are referred to a space-fixed frame. Jacobi vectors are a standard topic and we refer to the literature for more details on their definition and analysis [15,16].

For notational convenience we also introduce the $3 \times (n - 1)$ matrix F_s whose columns are the Jacobi vectors. Explicitly, $F_{si\alpha} = r_{s\alpha i}$, $i = 1, 2, 3$, $\alpha = 1, \dots, n - 1$, where $F_{si\alpha}$ and $r_{s\alpha i}$ are the components of F_s and $\mathbf{r}_{s\alpha}$ respectively.

An ordinary rotation $Q \in SO(3)$ acts on the Jacobi vectors by standard multiplication on the left

$$\mathbf{r}_{s\alpha} \mapsto Q\mathbf{r}_{s\alpha}, \quad (2.1)$$

$$F_s \mapsto QF_s. \quad (2.2)$$

We call such a rotation an external rotation to distinguish it from a kinematic rotation. A kinematic rotation $K \in SO(n - 1)$ acts by mixing up the α indices of the Jacobi vectors $\mathbf{r}_{s\alpha}$,

$$\mathbf{r}_{s\alpha} \mapsto \sum_{\beta} K_{\alpha\beta} \mathbf{r}_{s\beta}, \quad (2.3)$$

$$F_s \mapsto F_s K^T, \quad (2.4)$$

where $K_{\alpha\beta}$ denotes the components of K and T denotes the matrix transpose. Notice that kinematic rotations commute with all external rotations. Thus, the kinematic group has a well-defined action on the quotient of configuration space \mathbb{R}^{3n-3} by the group $SO(3)$ of external rotations. This quotient is called shape space, or the internal space, and its elements are called shapes. A shape thus determines the relative positions of the bodies with respect to each other. The purpose of this section is to find the topology of the orbits of the kinematic group acting on shape space.

Considering a specific configuration F_s with shape q , the kinematic orbit Γ through q is given by (that is, diffeomorphic to)

$$\Gamma = \frac{SO(n - 1)}{S}, \quad (2.5)$$

where $S \subset SO(n - 1)$ is the isotropy subgroup of the kinematic action at q . See Theorem 1 in the Appendix. The isotropy subgroup S consists of all $K \in SO(n - 1)$ which leave the shape q invariant. Our objective therefore is to determine S for each shape q . Now, $F_s K^T$

and F_s have the same shape if and only if they are related by a rotation $Q \in SO(3)$. Thus, our objective is to find all $K \in SO(n-1)$ such that there exists a $Q \in SO(3)$ satisfying

$$F_s K^T = Q F_s. \quad (2.6)$$

We use the principal value decomposition to factor F_s into

$$F_s = R \Lambda H^T, \quad (2.7)$$

where $R \in SO(3)$ and $H \in SO(n-1)$, and Λ is a $3 \times (n-1)$ matrix of the form

$$\Lambda = \begin{bmatrix} \lambda_1 & 0 & 0 & \overbrace{0 & 0 & 0 & \dots}^{n-4} \\ 0 & \lambda_2 & 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & \lambda_3 & 0 & 0 & 0 & \dots \end{bmatrix}. \quad (2.8)$$

Due to the nonuniqueness of the principal value decomposition, there is no loss of generality in assuming that $\lambda_1, \lambda_2 \geq 0$ and that the λ_i 's are ordered as

$$\lambda_1 \geq \lambda_2 \geq |\lambda_3|. \quad (2.9)$$

Using Eq. (2.7), we recast the problem of satisfying Eq. (2.6) into the following problem: for which $K \in SO(n-1)$ does there exist a $Q \in SO(3)$ such that

$$Q \Lambda (H^T K H)^T = \Lambda. \quad (2.10)$$

The above equation shows that the isotropy subgroup S of the action of the kinematic group on the shape q is conjugate to the isotropy subgroup of the action of the kinematic group on the shape of the configuration Λ . Replacing S by a conjugate subgroup in Eq. (2.5) does not effect the resulting manifold Γ (up to diffeomorphism). Thus, we assume without loss of generality that $F_s = \Lambda$, and hence we look to find all $K \in SO(n-1)$ such that there exists a $Q \in SO(3)$ satisfying

$$Q \Lambda K^T = \Lambda. \quad (2.11)$$

The answer depends on the rank of Λ , which we denote by d . The quantity d physically represents the dimensionality of the shape q . Thus, the n -body collision has $d = 0$, linear shapes have $d = 1$, planar shapes have $d = 2$, and full three-dimensional shapes have $d = 3$.

For all values of d , Λ may be “block diagonalised” in the following manner

$$\Lambda = \left[\begin{array}{c|c} \Sigma & 0 \\ \hline 0 & 0 \end{array} \right], \quad (2.12)$$

where Σ is a $d \times d$ diagonal matrix and 0 represents the zero matrices of the appropriate dimensions. Equation (2.11) can only be satisfied if Q and K are also block-diagonal, having the forms

$$K = \left[\begin{array}{c|c} A & 0 \\ \hline 0 & B \end{array} \right], \quad (2.13)$$

$$Q = \left[\begin{array}{c|c} C & 0 \\ \hline 0 & D \end{array} \right], \quad (2.14)$$

where C and A are $d \times d$ matrices, D is a $(3-d) \times (3-d)$ matrix, and B is an $(n-1-d) \times (n-1-d)$ matrix. Finding (special) orthogonal matrices K and Q satisfying Eq. (2.11) is then equivalent to finding orthogonal matrices A, B, C, D satisfying

$$C\Sigma A^T = \Sigma, \quad (2.15)$$

$$\det A \det B = 1, \quad (2.16)$$

$$\det C \det D = 1. \quad (2.17)$$

The first equation follows from Eq. (2.11). The last two equations ensure that K and Q have positive determinant.

It can be shown, due to the fact that Σ is invertible and $A, C \in O(d)$, that Eq. (2.15) can only be solved if $C = A$. This in turn allows Eq. (2.17) to be rewritten as

$$\det A \det D = 1. \quad (2.18)$$

Recall that D is of dimension $3-d$. Therefore, if $d = 3$, the matrix D is completely eliminated from consideration, and Eq. (2.18) becomes simply

$$\det A = 1. \tag{2.19}$$

However, if $d < 3$, then there always exists an orthogonal matrix D such that $\det D = \det A$. Thus, Eq. (2.18) imposes no constraint whatsoever on A .

For the sake of clarity, we now summarise the problem at hand. For an arbitrary diagonal $d \times d$ matrix Σ , with nonzero eigenvalues λ_i , $i = 1, \dots, d$ satisfying Eq. (2.9), we seek all matrices $K \in SO(n-1)$ given by Eq. (2.13), where the orthogonal $d \times d$ matrix A and orthogonal $(n-1-d) \times (n-1-d)$ matrix B satisfy

$$A\Sigma A^T = \Sigma, \tag{2.20}$$

$$\det A \det B = 1, \tag{2.21}$$

$$\det A = 1. \quad (\text{required for } d = 3 \text{ only}) \tag{2.22}$$

Notice that we have eliminated all reference to the matrix Q .

To proceed we consider each of the values of $d = 0, 1, 2, 3$ separately.

Case $d = 3$

From Eqs. (2.21) and (2.22), we see that $\det A = \det B = 1$. Thus, B is an element of $SO(n-4)$ and is independent of A . To find the allowed values of A , we consider three subcases: (i) all of the λ_i 's are distinct, (ii) two of the λ_i 's are equal, the third is distinct, (iii) all of the λ_i 's are equal. Physically, these subcases correspond to shapes which are asymmetric tops, symmetric tops, and spherical tops respectively.

Assume subcase (i). This is perhaps the most important class of shapes since three-dimensional asymmetric tops are generic in shape space. From Eq. (2.20) and the fact that Σ is diagonal, A must be one of the four matrices in the group V_4 , where

$$V_4 = \left\{ \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \right\}. \quad (2.23)$$

The group V_4 is called the viergruppe. It played a critical roll in earlier analysis of the four-body problem [1,12]; we will reproduce part of this earlier analysis in Sect. IV. Thus, K lives in a subgroup of $SO(n-1)$ isomorphic to $V_4 \times SO(n-4)$. The group $V_4 \times SO(n-4)$ is therefore the isotropy subgroup S for three-dimensional asymmetric tops.

Assume subcase (ii). Since Σ is diagonal with two equal eigenvalues, A must be block-diagonal, with a 2×2 block which can be any element $S \in O(2)$ and a 1×1 block which must be $\det S$ to ensure the condition $\det A = 1$. Thus, A lives in a subset of $SO(3)$ isomorphic to $O(2)$ and hence $O(2) \times SO(n-4)$ is the isotropy subgroup S for three-dimensional symmetric tops.

Assume subcase (iii). Since all eigenvalues of Σ are equal, Σ is proportional to the identity. Hence, A can be any element of $SO(3)$, and hence $SO(3) \times SO(n-4)$ is the isotropy subgroup S for three-dimensional spherical tops.

Case $d = 2$

We consider two subcases: (i) $\lambda_1 \neq \lambda_2$ (ii) $\lambda_1 = \lambda_2$. Physically, these correspond to asymmetric and symmetric tops respectively.

Assume subcase (i). Since Σ is diagonal with two different eigenvalues, A must be one of the four matrices in the group V_4 , where

$$V_4 = \left\{ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \right\}. \quad (2.24)$$

This is another representation of the viergruppe in Eq. (2.23). For notational simplicity, we use the same symbol for both groups; it will be clear from context which group is intended. Since $B \in O(n-3)$, the matrix K is in $V_4 \times O(n-3)$. We still must apply the one remaining

constraint given by Eq. (2.21). For this reason, we introduce the notation $V_4 \times_{\det +1} O(n-3)$ for all elements in $V_4 \times O(n-3)$ with unit determinant. Thus, $V_4 \times_{\det +1} O(n-3)$ is the isotropy subgroup S for two-dimensional asymmetric tops.

Assume subcase (ii). Since Σ is diagonal with two equal eigenvalues, Σ is proportional to the identity. Thus the matrix A can be any element of $O(2)$, and hence $O(2) \times_{\det +1} O(n-3)$ is the isotropy subgroup S for planar symmetric tops.

Case $d = 1$

Since A is in $O(1)$, A is either 1 or -1 . From Eq. (2.21), $A = \det B$. Therefore, $B \in O(n-2)$ completely determines K . Thus, $O(n-2)$ is the isotropy subgroup S for linear shapes.

Case $d = 0$

Since the dimension of A is 0 here, there is really no matrix A to worry about. That is, $K = B$. Thus, $SO(n-1)$ is the isotropy subgroup S for the n -body collision.

III. COMMENTS ON THE GENERAL RESULTS

We summarise the results from the preceding section in Table I and comment on a few special cases. First, as was to be expected the kinematic orbit passing through the n -body collision is a single point $\Gamma = SO(n-1)/SO(n-1) = \{0\}$.

A more interesting case is that of the collinear shapes. It is a well-known fact that

$$\frac{SO(k+1)}{O(k)} = \mathbb{R}P^k, \quad (3.1)$$

where $\mathbb{R}P^k$ is the k -dimensional real projective space ($k \geq 1$). The k -dimensional real projective space is the space of lines in \mathbb{R}^{k+1} . It may also be viewed as the k -dimensional

sphere S^k with antipodal points identified. A quick proof of Eq. (3.1) can be given with the aid of Theorem 1, taking

$$M = \mathbb{R}P^k = \{ \{ \hat{e}, -\hat{e} \} | \hat{e} = (\hat{e}_1, \dots, \hat{e}_{k+1}) \in S^k \subset \mathbb{R}^{k+1} \} \quad (3.2)$$

and $G = SO(k+1)$. A matrix $K \in SO(k+1)$ maps $\{ \hat{e}, -\hat{e} \}$ into $\{ K\hat{e}, -K\hat{e} \}$. If $\hat{e} = (1, 0, \dots, 0)$, then one can see that the isotropy subgroup of $\{ \hat{e}, -\hat{e} \}$ is $H = O(k)$. (In fact, H is exactly the same representation of $O(k)$, $k = n - 2$, discussed above for the case $d = 1$.) Since the orbit of the action of $SO(k+1)$ on $\mathbb{R}P^k$ is the entire space $\mathbb{R}P^k$, Eq. (3.1) follows from Theorem 2.

Applying Eq. (3.1), we see that the kinematic orbit of a collinear shape is

$$\Gamma = \frac{SO(n-1)}{O(n-2)} = \mathbb{R}P^{n-2}. \quad (3.3)$$

For the four-body problem (in three-dimensions) the two-fragment exit channels can be visualised as seven pairs of antipodal points on S^2 or, equivalently, seven points on $\mathbb{R}P^2$ [1,17]. Kinematic angles between these points were explicitly computed in Ref. [17]. These results were based on the understanding that $\mathbb{R}P^2$ is the kinematic orbit for collinear shapes in the four-body problem.¹ (The interest in collinear shapes stems from the fact that a two-fragment state becomes more and more collinear as the separation between the fragments increases.) The four-body work was an extension of well-known results for the three-body problem (in three-dimensions) in which the two-fragment exit channels can be visualised as three points on a circle $S^1 = \mathbb{R}P^1$ with certain kinematic angles between them. The result presented in Eq. (3.3) shows that in general the two-fragment exit channels can be viewed as points on $\mathbb{R}P^{n-2}$, or equivalently, pairs of antipodal points on S^{n-2} . (Some quick combinatorics gives the number of points on $\mathbb{R}P^{n-2}$ to be $2^{n-1} - 1$.) Of course, this is only

¹More precisely, the analysis of Ref. [17] is based on the fact that S^2 is the kinematic orbit for shapes in the one-dimensional four-body problem. We ignore the one-dimensional n -body problem in this paper.

a topological result, and we say nothing about the values of the kinematic angles between such points.

TABLE I. Isotropy subgroups of the kinematic action on shape space

Class	Physical Description of Class	Isotropy Subgroup S	$\dim(\Gamma)^a$
3(i)	3D asymmetric top	$V_4 \times SO(n-4)$	$3n-9$
3(ii)	3D symmetric top	$O(2) \times SO(n-4)$	$3n-10$
3(iii)	3D spherical top	$SO(3) \times SO(n-4)$	$3n-12$
2(i)	Planar asymmetric top	$V_4 \times_{\det+1} O(n-3)$	$2n-5$
2(ii)	Planar symmetric top	$O(2) \times_{\det+1} O(n-3)$	$2n-6$
1	Linear shape	$O(n-2)$	$n-2$
0	n -body collision	$SO(n-1)$	0

^a $\Gamma = \text{kinematic orbit} = SO(n-1)/S$

IV. THE THREE- AND FOUR-BODY PROBLEMS

We specialise the preceding analysis to the three- and four-body problems. These cases have been studied earlier [1,2,12]. The present analysis serves both as a check on the general results in Sect. II and as practice for the five-body problem.

We begin with the three-body problem $n = 3$. In the analysis of Sect. II we assumed for convenience that $n \geq 4$. However, by closely examining this analysis, one sees that the results presented in Table I are also valid for $n = 3$, so long as one ignores the nonsensical results for the three-dimensional classes 3(i), 3(ii), and 3(iii). For the classes 2(i) and 2(ii), the factor $O(n-3) = O(0)$ of S is to be ignored. Thus, the isotropy subgroup of the class 2(i) is the two-element group $S = \mathbb{Z}_2$ consisting of those elements of V_4 in Eq. (2.24) with unit determinant. Similarly, the isotropy subgroup of the class 2(ii) is $SO(2)$. For the class 1, the isotropy subgroup is $S = O(1) = \{+1, -1\} = \mathbb{Z}_2$. These results are summarised in Table II.

TABLE II. Isotropy subgroups and kinematic orbits for the three-body problem

	Class	Physical Description of Class	S	$\dim(\Gamma)$	Γ^a
	2(i)	Planar asymmetric top	\mathbb{Z}_2	1	S^1
	2(ii)	Planar symmetric top	$SO(2)$	0	$\{0\}$
	1	Linear shape	\mathbb{Z}_2	1	S^1
	0	3-body collision	$SO(2)$	0	$\{0\}$

^a $\Gamma = \text{kinematic orbit} = SO(2)/S$

Since the kinematic group $SO(2)$ is particularly simple, the topology of the kinematic orbits may be presented in a more direct and illuminating form than the quotient $SO(2)/S$. These forms are recorded in the rightmost column of Table II. For the three-body problem, we can provide a convenient picture of the kinematic rotations which explains why the kinematic orbits have the topologies that they do. The three-body shape space is conveniently parameterised by three internal coordinates (w_1, w_2, w_3) with ranges $-\infty < w_1, w_2 < \infty$, $0 \leq w_3 < \infty$. The kinematic rotations act on shape space via standard $SO(3)$ matrices rotating about the w_3 -axis. It so happens that the w_3 -axis consists of the planar (noncollinear) symmetric tops as well as the 3-body collision. Thus, the kinematic orbits of these shapes contain a single point, whereas the kinematic orbits of all other shapes are circles about the w_3 -axis.

Turning to the four-body problem, we specialise the entries of Table I for $n = 4$ and display the results in Table III. For the classes 3(i), 3(ii), and 3(iii) we ignore the factor $SO(n-4) = SO(0)$. For the classes 2(i) and 2(ii), the factor $O(n-3)$ reduces to $O(1) = \{+1, -1\}$. Since the choice of $+1$ or -1 in $O(1)$ is fixed by the $\det = +1$ constraint, the isotropy subgroup for classes 2(i) and 2(ii) are V_4 and $O(2)$ respectively. An interesting observation is that the results for the four-body problem are classified solely on the basis of the symmetries of the moment of inertia tensor. That is, the topology of the kinematic orbit depends only on whether a shape is a spherical top, symmetric top, or asymmetric top. (This fact is not true for $n = 3$ or $n \geq 5$.)

TABLE III. Isotropy subgroups and kinematic orbits for the four-body problem

Class	Physical Description of Class	S	$\dim(\Gamma)$	Γ^a
3(i)	3D asymmetric top	V_4	3	S^3/V_8
3(ii)	3D symmetric top	$O(2)$	2	$\mathbb{R}P^2$
3(iii)	3D spherical top	$SO(3)$	0	$\{0\}$
2(i)	Planar asymmetric top	V_4	3	S^3/V_8
2(ii)	Planar symmetric top	$O(2)$	2	$\mathbb{R}P^2$
1	Linear shape	$O(2)$	2	$\mathbb{R}P^2$
0	4-body collision	$SO(3)$	0	$\{0\}$

^a $\Gamma = \text{kinematic orbit} = SO(3)/S$

In the final column of Table III, we have again represented the topologies of the kinematic orbits in a more direct and illuminating form than simply the quotient $SO(3)/S$. We already explained in Sect. III, how the equality $SO(3)/SO(2) = \mathbb{R}P^2$ comes about. Thus, the only orbit which requires special attention here is

$$\Gamma = \frac{SO(3)}{V_4} = \frac{SU(2)}{V_8} = \frac{S^3}{V_8}. \quad (4.1)$$

Here V_8 is an eight element subgroup of $SU(2)$

$$V_8 = \{\pm 1, \pm\omega_1, \pm\omega_2, \pm\omega_3\}, \quad (4.2)$$

where $\omega_i = -i\sigma_i$, $i = 1, 2, 3$, and the σ_i 's are the usual Pauli matrices. Explicitly,

$$\omega_1 = -i\sigma_1 = \begin{bmatrix} 0 & -i \\ -i & 0 \end{bmatrix}, \quad (4.3)$$

$$\omega_2 = -i\sigma_2 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad (4.4)$$

$$\omega_3 = -i\sigma_3 = \begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix}. \quad (4.5)$$

The matrices ω_i satisfy

$$\omega_1\omega_2 = -\omega_2\omega_1 = \omega_3, \quad (4.6)$$

$$\omega_2\omega_3 = -\omega_3\omega_2 = \omega_1, \quad (4.7)$$

$$\omega_3\omega_1 = -\omega_1\omega_3 = \omega_2, \quad (4.8)$$

$$\omega_i^\dagger = \omega_i^{-1} = -\omega_i. \quad (4.9)$$

These product rules show that V_8 is the quaternion group. To prove Eq. (4.1) we recall some basic facts about $SO(3)$. First, $SU(2)$ is the double cover of $SO(3)$, and we denote the projection by $\pi : SU(2) \rightarrow SO(3)$. The kernel of π is $\mathbb{Z}_2 = \{1, -1\}$ and hence $SO(3) = SU(2)/\mathbb{Z}_2$. If $R = \pi(U)$ for some $U \in SU(2)$, then R can be given explicitly by

$$R_{ij} = -\frac{1}{2}\text{tr}(\omega_i U \omega_j U^\dagger), \quad (4.10)$$

where R_{ij} , $i, j = 1, 2, 3$, are the components of R . Using the product rules Eqs. (4.6) – (4.9) and Eq. (4.10), one can verify that $\pi(V_8) = V_4$ given in Eq. (2.23), and hence $V_4 = V_8/\mathbb{Z}_2$. We now employ Theorem 3 from the Appendix, with $G = V_8$, $H = \mathbb{Z}_2 = \{1, -1\}$, $M = SU(2)$. (It is trivial to verify that \mathbb{Z}_2 is normal in V_8 .) Hence, Eq. (A7) yields

$$\frac{SO(3)}{V_4} = \frac{SU(2)/\mathbb{Z}_2}{V_8/\mathbb{Z}_2} = \frac{SU(2)}{V_8} = \frac{S^3}{V_8}, \quad (4.11)$$

where we recall that $SU(2)$ is diffeomorphic to the three-dimensional sphere S^3 .

V. THE FIVE-BODY PROBLEM

The entries of Table I are specialised for the five-body problem, $n = 5$, and displayed in Table IV. As with the three- and four-body cases, we also represent the topology of the kinematic orbits in a more direct and illuminating form than the original quotient $\Gamma = SO(4)/S$.

Before deriving the results in Table IV, we make a few observations. First, for all classes but 2(ii) we present the kinematic orbits as products of well-studied two- and three-dimensional manifolds. In fact, all of these simpler manifolds already appear in the four-body problem, either as kinematic orbits or as the group manifold $SO(3) = \mathbb{R}P^3$. One obvious

TABLE IV. Isotropy subgroups and kinematic orbits for the five-body problem

Class	Physical Description of Class	S	$\dim(\Gamma)$	Γ^a
3(i)	3D asymmetric top	V_4	6	$S^3 \times (S^3/V_8)$
3(ii)	3D symmetric top	$O(2)$	5	$S^3 \times \mathbb{R}P^2$
3(iii)	3D spherical top	$SO(3)$	3	S^3
2(i)	Planar asymmetric top	$V_4 \times_{\det+1} O(2)$	5	$\mathbb{R}P^3 \times \mathbb{R}P^2$
2(ii)	Planar symmetric top	$O(2) \times_{\det+1} O(2)$	4	$(S^2 \times S^2)/\mathbb{Z}_2$
1	Linear shape	$O(3)$	3	$\mathbb{R}P^3$
0	5-body collision	$SO(4)$	0	$\{0\}$

^a $\Gamma = \text{kinematic orbit} = SO(4)/S$

advantage of such a simple description of the topologies of these spaces is that it simplifies the introduction of kinematic angles or some other parameterisation of the orbits. For example, in the case of a 3D asymmetric top, we may introduce six kinematic angles by taking three to be standard Euler angles on $S^3 = SU(2)$ and three to be Euler angles on S^3/V_8 . The ranges of the latter three angles must be carefully restricted to account for the fact that S^3/V_8 is only one eighth the size of S^3 . A discussion of the ranges of such angles has already been given in the context of the four-body problem [11,12,18,19]. Of course, the space S^3/V_8 can be parameterised in various other ways, such as the convenient coordinates $\tau = (\tau_1, \tau_2, \tau_3)$ suggested by Reinsch [1,20].

It is interesting to note that the kinematic orbit of a collinear shape is $\mathbb{R}P^3 = SO(3)$. A point on such an orbit (such as one of the two-fragment exit channels discussed in Sect. III) can therefore be identified with a rotation matrix and may in turn be parameterised by one of the many standard parameterisations of $SO(3)$ (Euler angles, axis-angle variables, Cayley-Klein parameters, etc.).

We proceed now to derive the results of Table IV.

A. The Projection π from $SU(2) \times SU(2)$ to $SO(4)$

With the four-body problem, we have found it useful to work with the double cover $SU(2)$ of the kinematic group $SO(3)$. With the five-body problem, we also find it useful to work with the double cover of the kinematic group. In this case, the kinematic group is $SO(4)$ and its double cover is $SU(2) \times SU(2)$. In this section we give an explicit realization of the projection from $SU(2) \times SU(2)$ to $SO(4)$.

First, we introduce the function g which maps a complex number into a corresponding 2×2 real matrix. Explicitly,

$$g(a + ib) = \begin{bmatrix} a & -b \\ b & a \end{bmatrix}, \quad (5.1)$$

where a and b are real numbers. The function g is real linear and preserves multiplication. Specifically, it is straightforward to verify the following identities

$$g(z_1 + az_2) = g(z_1) + ag(z_2), \quad (5.2)$$

$$g(z_1 z_2) = g(z_1)g(z_2), \quad (5.3)$$

$$g(z_1^*) = g(z_1)^T, \quad (5.4)$$

$$\text{tr } g(z_1) = z_1 + z_1^* = 2\text{Re } z_1, \quad (5.5)$$

$$\det g(z_1) = |z_1|^2, \quad (5.6)$$

$$\text{if } z_1 \neq 0 \text{ then } g(z_1^{-1}) = g(z_1)^{-1}, \quad (5.7)$$

where z_1 and z_2 are complex, z_1^* is the complex conjugate of z_1 , and a is real. We define g acting on a $k \times k$ complex matrix to be the $2k \times 2k$ real matrix given by

$$g \left(\begin{bmatrix} a_{11} + ib_{11} & a_{12} + ib_{12} & \dots \\ a_{21} + ib_{21} & a_{22} + ib_{22} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix} \right) = \begin{bmatrix} a_{11} & -b_{11} & a_{12} & -b_{12} & \dots \\ b_{11} & a_{11} & b_{12} & a_{12} & \dots \\ a_{21} & -b_{21} & a_{22} & -b_{22} & \dots \\ b_{21} & a_{21} & b_{22} & a_{22} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}. \quad (5.8)$$

The following identities are analogous to Eqs. (5.2) – (5.7),

$$g(M + aN) = g(M) + ag(N), \quad (5.9)$$

$$g(MN) = g(M)g(N), \quad (5.10)$$

$$g(M^\dagger) = g(M)^T, \quad (5.11)$$

$$\text{tr } g(M) = \text{tr } M + (\text{tr } M)^* = 2\text{Re}(\text{tr } M), \quad (5.12)$$

$$\det g(M) = |\det M|^2, \quad (5.13)$$

$$\text{if } M \text{ invertible then } g(M^{-1}) = g(M)^{-1}, \quad (5.14)$$

where M and N are square complex matrices, M^\dagger is the Hermitian conjugate of M , and a is a real number. Except for Eq. (5.13), these identities are relatively straightforward to prove. To prove Eq. (5.13), we first assume that M is normal and invertible, which allows us to write $M = \exp X$ for some matrix X . Then,

$$\begin{aligned} \det g(M) &= \det[g(\exp X)] = \det[\exp g(X)] = \exp[\text{tr } g(X)] = \exp[\text{tr } X + (\text{tr } X)^*] \\ &= \det(\exp X)[\det(\exp X)]^* = |\det M|^2, \end{aligned} \quad (5.15)$$

where we have used Eq. (5.12) and Eq. (5.21) (which appears below) as well as the fact that $\det \exp = \exp \text{tr}$. We now consider an arbitrary (possibly non-normal) invertible matrix M and note that it may be written as a product of normal matrices (using, for example, polar or principal value decompositions). Using this fact and Eq. (5.10), we observe that Eq. (5.13) holds for M as well. Having shown that Eq. (5.13) is valid for all invertible matrices, analytic continuation shows that it is valid for all matrices.

We now define π from $SU(2) \times SU(2)$ to $SO(4)$ by

$$\pi(U_1, U_2) = g(U_1)Pg(U_2)P^T, \quad (5.16)$$

where

$$P = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{bmatrix} \in SO(4), \quad (5.17)$$

and where $U_1, U_2 \in SU(2)$. From Eqs. (5.11) – (5.14), we observe that $g(U_1)$ and $g(U_2)$ are in $SO(4)$. Since P is also in $SO(4)$ we verify that $\pi(U_1, U_2)$ is in $SO(4)$. To verify that π is a group homomorphism we must verify the following equation

$$\pi(U_1 V_1^{-1}, U_2 V_2^{-1}) = \pi(U_1, U_2) \pi(V_1, V_2)^{-1}, \quad (5.18)$$

where $U_1, U_2, V_1, V_2 \in SU(2)$ are arbitrary. To prove Eq. (5.18), we first hypothesise that

$$g(U) [Pg(V)P^T] = [Pg(V)P^T] g(U), \quad (5.19)$$

where $U, V \in SU(2)$ are arbitrary. We postpone the proof of Eq. (5.19) temporarily in order to show how it is used to prove Eq. (5.18). To this end, we have

$$\begin{aligned} \pi(U_1 V_1^{-1}, U_2 V_2^{-1}) &= g(U_1 V_1^{-1}) P g(U_2 V_2^{-1}) P^T = g(U_1) g(V_1)^{-1} P g(U_2) g(V_2)^{-1} P^T \\ &= g(U_1) g(V_1)^{-1} [Pg(U_2)P^T] [Pg(V_2)^{-1}P^T] \\ &= [g(U_1)Pg(U_2)P^T] [Pg(V_2)^{-1}P^T g(V_1)^{-1}] \\ &= \pi(U_1, U_2) \pi(V_1, V_2)^{-1}, \end{aligned} \quad (5.20)$$

where the first equality follows from the definition Eq. (5.16), the second from Eqs. (5.10) and (5.14), the third from inserting $P^T P = I$, the fourth from Eq. (5.19), and the final equality again from Eq. (5.16).

We return now to prove Eq. (5.19). We find it convenient to work with the Lie algebras $su(2)$ and $so(4)$ of $SU(2)$ and $SO(4)$ respectively. We see from Eq. (5.11) that if $X \in su(2)$, that is X is a 2×2 anti-Hermitian matrix, then $g(X) \in so(4)$, that is, $g(X)$ is a 4×4 antisymmetric real matrix. Furthermore,

$$g(\exp X) = \exp g(X), \quad (5.21)$$

$$P \exp(X) P^T = \exp(PXP^T), \quad (5.22)$$

where Eq. (5.21) follows from Eqs. (5.9) and (5.10). Taking $U = \exp X, V = \exp Y$, Eqs. (5.21) and (5.22) allow Eq. (5.19) to be reexpressed as

$$\exp[g(X)] \exp[Pg(Y)P^T] = \exp[Pg(Y)P^T] \exp[g(X)]. \quad (5.23)$$

The above equation is valid so long as

$$[g(X), Pg(Y)P^T] = 0 \quad (5.24)$$

for arbitrary $X, Y \in su(2)$, where $[,]$ is the matrix commutator.

We prove Eq. (5.24) by using a basis of $su(2)$, which we choose to be the matrices ω_i , $i = 1, 2, 3$, given in Eqs. (4.3) – (4.5). From the product rules Eqs. (4.6) – (4.8), this basis satisfies the Lie algebra relations

$$[\omega_i, \omega_j] = 2 \sum_k \epsilon_{ijk} \omega_k. \quad (5.25)$$

It is straightforward to compute the matrices $J_i = g(\omega_i)$ and $L_i = Pg(\omega_i)P^T$,

$$J_1 = g(\omega_1) = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}, \quad (5.26)$$

$$J_2 = g(\omega_2) = \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}, \quad (5.27)$$

$$J_3 = g(\omega_3) = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad (5.28)$$

$$L_1 = Pg(\omega_1)P^T = \begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \quad (5.29)$$

$$L_2 = Pg(\omega_2)P^T = \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}, \quad (5.30)$$

$$L_3 = Pg(\omega_3)P^T = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix}. \quad (5.31)$$

The matrices J_i , $i = 1, 2, 3$ and L_i , $i = 1, 2, 3$ are a basis of the Lie algebra $so(4)$ and it is straightforward to show that they satisfy the Lie algebra relations

$$[J_i, J_j] = 2 \sum_k \epsilon_{ijk} J_k, \quad (5.32)$$

$$[L_i, L_j] = 2 \sum_k \epsilon_{ijk} L_k, \quad (5.33)$$

$$[J_i, L_j] = 0. \quad (5.34)$$

The above equations exhibit the well-known fact that $so(4) = su(2) \oplus su(2)$. Since the matrices J_i and L_i span the space of matrices of the form $g(X)$ and $Pg(Y)P^T$ respectively ($X, Y \in su(2)$), Eq. (5.34) proves Eq. (5.24), from which follows Eqs. (5.23), (5.19), and (5.18). We have thus shown π to be a group homomorphism.

The mapping π has several important properties which we will use later. First, it follows directly from the definition Eq. (5.16) that for arbitrary group elements $(U_1, U_2) \in SU(2) \times SU(2)$

$$\pi(U_1, -U_2) = \pi(-U_1, U_2) = -\pi(U_1, U_2), \quad (5.35)$$

$$\pi(-U_1, -U_2) = \pi(U_1, U_2). \quad (5.36)$$

Second, in light of Eq. (5.34), the definition of π can be conveniently reexpressed using the Lie algebra,

$$\pi(\exp X_1, \exp X_2) = \exp[g(X_1) + Pg(X_2)P^T]. \quad (5.37)$$

Since the matrices J_i and L_i form a basis of the Lie algebra $so(4)$, the above equation shows that π is surjective. However, π is obviously not injective since $\pi(I, I) = \pi(-I, -I) = I$. In fact, (I, I) and $(-I, -I)$ are the only two elements of $SU(2) \times SU(2)$ which map to $I \in SO(4)$. To prove this we consider two arbitrary elements $U_1, U_2 \in SU(2)$, expressed in axis-angle form as

$$U_1 = \cos \theta_1 I - \sin \theta_1 \hat{n}_1 \cdot \omega, \quad (5.38)$$

$$U_2 = \cos \theta_2 I - \sin \theta_2 \hat{n}_2 \cdot \omega, \quad (5.39)$$

where θ_1, θ_2 are rotation angles, \hat{n}_1, \hat{n}_2 are rotation axes, and $\omega = (\omega_1, \omega_2, \omega_3)$. Then,

$$\begin{aligned} \pi(U_1, U_2) &= (\cos \theta_1 I - \sin \theta_1 \hat{n}_1 \cdot \mathbf{J})(\cos \theta_2 I - \sin \theta_2 \hat{n}_2 \cdot \mathbf{L}) \\ &= \cos \theta_1 \cos \theta_2 I - \sin \theta_1 \cos \theta_2 (\hat{n}_1 \cdot \mathbf{J}) \\ &\quad - \cos \theta_1 \sin \theta_2 (\hat{n}_2 \cdot \mathbf{L}) + \sin \theta_1 \sin \theta_2 (\hat{n}_1 \cdot \mathbf{J})(\hat{n}_2 \cdot \mathbf{L}), \end{aligned} \quad (5.40)$$

where $\mathbf{J} = (J_1, J_2, J_3)$ and $\mathbf{L} = (L_1, L_2, L_3)$. It can easily be verified that $\{I, J_i, L_i, J_i L_j\}$ forms a basis of all 4×4 real matrices. Thus, if $\pi(U_1, U_2) = I$ then

$$\cos \theta_1 \cos \theta_2 = 1, \quad (5.41)$$

$$\sin \theta_1 \cos \theta_2 = 0, \quad (5.42)$$

$$\cos \theta_1 \sin \theta_2 = 0, \quad (5.43)$$

$$\sin \theta_1 \sin \theta_2 = 0, \quad (5.44)$$

which only occurs if $\theta_1 = \theta_2 = 0$ or $\theta_1 = \theta_2 = \pi$, corresponding to $U_1 = U_2 = I$ or $U_1 = U_2 = -I$ respectively.

In summary, we have proved that π given by Eq. (5.16) is a two-to-one surjective group homomorphism from $SU(2) \times SU(2)$ to $SO(4)$.

B. The double covers of the isotropy subgroups

For each isotropy subgroup S , we determine its double cover $\hat{S} = \pi^{-1}(S)$. That is we must find the two elements of $SU(2) \times SU(2)$ which map to each element of S . In light of Eq. (5.36), these two elements are related by a minus sign, that is, $(U_1, U_2) \in \hat{S}$ and $(-U_1, -U_2) \in \hat{S}$ map to the same element in S . Thus, the problem of determining \hat{S} reduces to finding only one element in $SU(2) \times SU(2)$ which maps to each element in S .

Since $\mathbb{Z}_2 = \{(1, 1), -(1, 1)\}$ is obviously normal in \hat{S} and $(SU(2) \times SU(2))/\mathbb{Z}_2 = SO(4)$ and $\hat{S}/\mathbb{Z}_2 = S$, we apply Theorem 3 to find

$$\Gamma = \frac{SO(4)}{S} = \frac{(SU(2) \times SU(2))/\mathbb{Z}_2}{\hat{S}/\mathbb{Z}_2} = \frac{SU(2) \times SU(2)}{\hat{S}}. \quad (5.45)$$

We will use this result extensively to determine the topology of the kinematic orbits. We analyse each class in Table IV separately.

1. The class 3(i) of 3D asymmetric tops

Considering the analysis of Sect. II, an element K of S depends on the two matrices A and B as shown in Eq. (2.13). Considering the class 3(i) for $n = 5$, the matrix B is simply the 1×1 matrix $B = 1$. The matrix A must belong to the group V_4 given by Eq. (2.23). Thus, the group S contains the following matrices

$$S = \{1, E_1, E_2, E_3\}, \quad (5.46)$$

$$E_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad (5.47)$$

$$E_2 = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad (5.48)$$

$$E_3 = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \quad (5.49)$$

From Eq. (5.16) we see that $\pi(\omega_i, \omega_i) = J_i L_i$, where J_i and L_i are given by Eqs. (5.26) – (5.31). By direct matrix multiplication, we find

$$\pi(\omega_i, \omega_i) = J_i L_i = E_i. \quad (5.50)$$

Thus, having found one element in $SU(2) \times SU(2)$ which maps to each element of S , the double cover \hat{S} is the eight element group

$$\hat{S} = \{\pm(1, 1), \pm(\omega_1, \omega_1), \pm(\omega_2, \omega_2), \pm(\omega_3, \omega_3)\} = \tilde{V}_8. \quad (5.51)$$

In the above, the tilde over V_8 has a technical meaning which we now define. If H is an arbitrary subgroup of $SU(2)$, then \tilde{H} is an isomorphic subgroup of $SU(2) \times SU(2)$ as shown in Eq. (A1). Thus, \hat{S} is isomorphic to the quaternion group in Eq. (4.2). Since \hat{S} has the form of \tilde{H} in Eq. (A1), we apply Theorem 2 from the Appendix to find

$$\Gamma = \frac{SU(2) \times SU(2)}{\hat{S}} = SU(2) \times \frac{SU(2)}{V_8} = S^3 \times \frac{S^3}{V_8}. \quad (5.52)$$

2. The class 3(ii) of 3D symmetric tops

For the class 3(ii), B is again the 1×1 matrix $B = 1$. The matrix A consists of a 2×2 block $S \in O(2)$ and a 1×1 block $\det S$. Combining these results into the single matrix K , we see that S consists of

$$S = \left\{ \left[\left[\begin{array}{c|c} S & 0 \\ \hline 0 & \det S \end{array} \right] \middle| S \in O(2) \right\} = \{1, E_1\} \left\{ \left[\begin{array}{c|c} S & 0 \\ \hline 0 & 1 \end{array} \right] \middle| S \in SO(2) \right\}, \quad (5.53)$$

where in the second equality we have factored S into the product of two groups. Having encountered the elements of the first factor earlier, we recall that $\pi(1, 1) = 1$ and (from Eq. (5.50)) that $\pi(\omega_1, \omega_1) = E_1$. Considering the second factor, we note

$$\begin{aligned} \pi(\exp(\theta\omega_3), \exp(\theta\omega_3)) &= \exp(\theta(J_3 + L_3)) = \exp\left(2\theta \left[\begin{array}{cc|c} 0 & 1 & 0 \\ -1 & 0 & 0 \\ \hline 0 & & 0 \end{array} \right]\right) \\ &= \left[\begin{array}{cc|c} \cos 2\theta & \sin 2\theta & 0 \\ -\sin 2\theta & \cos 2\theta & 0 \\ \hline 0 & & 1 \end{array} \right], \end{aligned} \quad (5.54)$$

where we used Eqs. (5.37), (5.28), and (5.31). Equation (5.54) shows that the double cover of the second factor in Eq. (5.53) is the group

$$\tilde{A} = \{(U, U) | U \in A\}, \quad (5.55)$$

where A is the group

$$A = \{\exp(\theta\omega_3) | 0 \leq \theta < 2\pi\}. \quad (5.56)$$

Note that $A = U(1) \subset SU(2)$. The double cover of S is therefore

$$\hat{S} = \{(1, 1), (\omega_1, \omega_1)\} \tilde{A} = \{(U, U) | U \in B\} = \tilde{B}, \quad (5.57)$$

where B is the group

$$B = \{1, \omega_1\}A. \quad (5.58)$$

A priori, it is perhaps not obvious that B is actually a group. To verify that B is indeed closed under multiplication and inverses, the following identity is useful

$$\omega_1 \exp(\theta\omega_3) \omega_1^\dagger = \exp(\theta\omega_1\omega_3\omega_1^\dagger) = \exp(-\theta\omega_3), \quad (5.59)$$

which derives from Eqs. (4.6) – (4.9). When forming products and inverses of the elements of B , Eq. (5.59) allows any ω_1 factors to be shifted to the left so that the final result again has the form displayed in Eq. (5.58).

Since \hat{S} has the form of Eq. (A1), we apply Theorem 2 to find

$$\Gamma = \frac{SU(2) \times SU(2)}{\hat{S}} = \frac{SU(2) \times SU(2)}{\bar{B}} = SU(2) \times \frac{SU(2)}{B}. \quad (5.60)$$

The quotient $SU(2)/B$ is diffeomorphic to $\mathbb{R}P^2$. To prove this, we first consider the quotient $SU(2)/A = SU(2)/U(1)$. It is well known that $SU(2)/U(1) = S^2$. One way of seeing this fact is to consider the action of $SU(2)$ on \mathbb{R}^3 via the 3×3 orthogonal matrices given in Eq. (4.10). The orbit of $SU(2)$ acting on $\hat{z} \in \mathbb{R}^3$ is clearly the sphere S^2 . The isotropy subgroup of the vector \hat{z} is the group A of $U(1)$ rotations about the \hat{z} -axis. Theorem 1 thus gives the desired result

$$\frac{SU(2)}{A} = S^2. \quad (5.61)$$

Furthermore, we note the following explicit identification between a right coset $[U] = AU \in SU(2)/A$ and a unit vector $\hat{n} \in S^2$ (denoting a coset with bold square brackets),

$$[U] \leftrightarrow \hat{n} = R^T \hat{z} = -\frac{1}{2} \text{tr} (\omega U^\dagger \omega_3 U), \quad (5.62)$$

where R is given by Eq. (4.10) and $\omega = (\omega_1, \omega_2, \omega_3)$. We have placed the transpose on R in order that \hat{n} be well-defined for right cosets; observe that the right hand side of Eq. (5.62) is invariant under $U \mapsto \exp(\theta \omega_3)U$.

Having computed $SU(2)/A$, we apply Theorem 3 to compute $SU(2)/B$. With regards to the notation of the theorem, we take $G = B$, $H = A$ and $M = SU(2)$. We first must verify that A is normal in B . Proving this fact reduces to showing that $\omega_1 \exp(\theta \omega_3) \omega_1^\dagger$ is in A for an arbitrary $\exp(\theta \omega_3) \in A$. This fact, in turn, follows immediately from Eq. (5.59). Thus, A is normal in B and B/A is a well-defined group isomorphic to \mathbb{Z}_2 . According to Theorem 3, the non-identity element $[\omega_1] \in B/A$ acts on $[U] \in SU(2)/A$ by $[\omega_1][U] = [\omega_1 U]$. Identifying $[U]$ with \hat{n} , the action of $[\omega_1]$ on \hat{n} is

$$[\omega_1]\hat{\mathbf{n}} = -\frac{1}{2}\text{tr} [\omega(\omega_1 U)^\dagger \omega_3(\omega_1 U)] = \frac{1}{2}\text{tr} (\omega U^\dagger \omega_3 U) = -\hat{\mathbf{n}}, \quad (5.63)$$

which follows from Eqs. (4.6) – (4.9). Thus, the quotient S^2/\mathbb{Z}_2 is $\mathbb{R}P^2$, and by Theorem 3 we have the following identifications

$$\frac{SU(2)}{B} = \frac{SU(2)/A}{B/A} = \frac{S^2}{\mathbb{Z}_2} = \mathbb{R}P^2. \quad (5.64)$$

Recalling Eq. (5.60), we find that

$$\Gamma = S^3 \times \mathbb{R}P^2. \quad (5.65)$$

3. The class 3(iii) of 3D spherical tops

For the class 3(iii), B is again the 1×1 matrix $B = 1$. The matrix A can be any matrix in $SO(3)$. Thus, the group S is

$$S = \left\{ \left[\begin{array}{c|c} A & 0 \\ \hline 0 & 1 \end{array} \right] \middle| A \in SO(3) \right\}. \quad (5.66)$$

To find the double cover of S , we consider an arbitrary matrix $U \in SU(2)$ expressed as $U = \exp(\mathbf{n} \cdot \boldsymbol{\omega})$ for some vector $\mathbf{n} = (n_1, n_2, n_3)$. Then we find from Eq. (5.37) and Eqs. (5.26) – (5.31) that

$$\pi(U, U) = \pi(\exp(\mathbf{n} \cdot \boldsymbol{\omega}), \exp(\mathbf{n} \cdot \boldsymbol{\omega})) = \exp[\mathbf{n} \cdot (\mathbf{J} + \mathbf{L})]. \quad (5.67)$$

Furthermore, from Eqs. (5.26) – (5.31), we see that

$$\mathbf{J}_1 + \mathbf{L}_1 = 2 \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad (5.68)$$

$$J_2 + L_2 = 2 \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad (5.69)$$

$$J_3 + L_3 = 2 \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \quad (5.70)$$

Thus, the matrices $J_i + L_i$ generate S , and from Eq. (5.67) the double cover of S is

$$\hat{S} = \{(U, U) | U \in SU(2)\} = \tilde{E}. \quad (5.71)$$

Applying Theorem 2, we have

$$\Gamma = \frac{SU(2) \times SU(2)}{\hat{S}} = \frac{SU(2) \times SU(2)}{\tilde{E}} = SU(2) \times \frac{SU(2)}{SU(2)} = S^3. \quad (5.72)$$

4. The class 2(i) of planar asymmetric tops

For the class 2(i), the matrices A and B are respectively in V_4 (as shown in Eq. (2.24)) and $O(2)$. These matrices must further satisfy $\det AB = 1$. For convenience, we switch the positions of A and B in Eq. (2.13). That is, we place A in the lower right block and B in the upper left block. This switch is equivalent to conjugating by a permutation and hence does not effect the topology of the quotient $SO(4)/S$. With this modification, the isotropy subgroup is

$$\begin{aligned} S &= \left\{ \left[\begin{array}{c|c} B & 0 \\ \hline 0 & A \end{array} \right] \middle| B \in O(2), A \in V_4, \det AB = 1 \right\} \\ &= \{1, E_1, -E_2, -E_3\} \left\{ \left[\begin{array}{c|c} B & 0 \\ \hline 0 & I \end{array} \right] \middle| B \in SO(2) \right\}, \end{aligned} \quad (5.73)$$

where we have again factored S into the product of two groups. Considering the elements in the first factor, we may combine Eqs. (5.35) and (5.50) to produce

$$\pi(\omega_1, \omega_1) = E_1, \quad (5.74)$$

$$\pi(\omega_2, -\omega_2) = -E_2, \quad (5.75)$$

$$\pi(-\omega_3, \omega_3) = -E_3. \quad (5.76)$$

The second factor of Eq. (5.73) is identical to the second factor of Eq. (5.53), and hence the double cover of the second factor is \tilde{A} given by Eq. (5.55). Thus, the double cover of S is

$$\begin{aligned} \hat{S} &= \{(1, 1), (\omega_1, \omega_1), (\omega_2, -\omega_2), (-\omega_3, \omega_3)\} \tilde{A} \\ &= \{(1, 1), (\omega_2, -\omega_2)\} \{(1, 1), (\omega_1, \omega_1)\} \tilde{A} = \{(1, 1), (\omega_2, -\omega_2)\} \tilde{B}, \end{aligned} \quad (5.77)$$

where \tilde{B} is given in Eq. (5.57).

We apply Theorem 3 to determine the topology of the kinematic orbit, taking $G = \hat{S}$, $H = \tilde{B}$, and $M = SU(2) \times SU(2)$. Using Eqs. (4.6) – (4.9), it is straightforward to verify that \tilde{B} is normal in \hat{S} , and hence \hat{S}/\tilde{B} is a well-defined group isomorphic to \mathbb{Z}_2 . The action of the nonidentity element $[\omega_2, -\omega_2] \in \hat{S}/\tilde{B}$ on $[U_1, U_2] \in (SU(2) \times SU(2))/\tilde{B}$ is

$$[\omega_2, -\omega_2][U_1, U_2] = [\omega_2 U_1, -\omega_2 U_2]. \quad (5.78)$$

Using Theorem 2, we previously showed that $(SU(2) \times SU(2))/\tilde{B}$ is diffeomorphic to $SU(2) \times (SU(2)/B)$. The diffeomorphism is given by Eq. (A4). Using this diffeomorphism we find that the action of $[\omega_2, -\omega_2] \in \hat{S}/\tilde{B}$ on $(U_1, [U_2]) \in SU(2) \times (SU(2)/B)$ is

$$[\omega_2, -\omega_2](U_1, [U_2]) = (-U_1, [-\omega_2 U_2]) = (-U_1, [U_2]), \quad (5.79)$$

where the last equality follows from the fact that $-\omega_2 = \omega_1 \omega_3 \in B$. (Be careful not to confuse the bold square bracket notation $[\ , \]$ used for cosets of $SU(2) \times SU(2)$ with the (nonbold) square bracket notation used for the matrix commutator.) From Eq. (5.79) we see that the quotient of $SU(2) \times (SU(2)/B)$ by \hat{S}/\tilde{B} is $\mathbb{R}P^3 \times (SU(2)/B)$. Applying Theorem 3 and recalling Eq. (5.64), we find

$$\Gamma = \frac{SU(2) \times SU(2)}{\hat{S}} = \frac{(SU(2) \times SU(2))/\tilde{B}}{\hat{S}/\tilde{B}} = \frac{SU(2) \times (SU(2)/B)}{\hat{S}/\tilde{B}} = \mathbb{R}P^3 \times \mathbb{R}P^2. \quad (5.80)$$

5. The class 2(ii) of planar symmetric tops

For the class 2(ii), the matrices A and B are both in $O(2)$ and satisfy $\det AB = 1$. Thus, the isotropy subgroup is

$$\begin{aligned} S &= \left\{ \left[\begin{array}{c|c} A & 0 \\ \hline 0 & B \end{array} \right] \middle| A, B \in O(2), \det AB = 1 \right\} \\ &= \{1, E_1\} \left\{ \left[\begin{array}{c|c} A & 0 \\ \hline 0 & I \end{array} \right] \middle| A \in SO(2) \right\} \left\{ \left[\begin{array}{c|c} I & 0 \\ \hline 0 & B \end{array} \right] \middle| B \in SO(2) \right\}, \end{aligned} \quad (5.81)$$

where we have factored S into three factors. The first two factors multiply to give the group S in Eq. (5.53). Thus, the double cover of the first two factors is the group \tilde{B} in Eq. (5.57).

Considering the last factor of Eq. (5.81), we note

$$\begin{aligned} \pi(\exp(\theta\omega_3), \exp(-\theta\omega_3)) &= \exp(\theta(J_3 - L_3)) = \exp \left(2\theta \left[\begin{array}{c|c} 0 & 0 \\ \hline 0 & \begin{array}{cc} 0 & -1 \\ 1 & 0 \end{array} \end{array} \right] \right) \\ &= \left[\begin{array}{c|c} I & 0 \\ \hline 0 & \begin{array}{cc} \cos 2\theta & -\sin 2\theta \\ \sin 2\theta & \cos 2\theta \end{array} \end{array} \right], \end{aligned} \quad (5.82)$$

where we used Eqs. (5.37), (5.28), and (5.31). Thus, the double cover of the third factor in Eq. (5.81) is the group

$$C = \{(U, U^\dagger) | U \in A\}, \quad (5.83)$$

where A is the group defined in Eq. (5.56). Therefore, the double cover of S is given by the product of \tilde{B} and C ,

$$\hat{S} = \tilde{B}C = \{(l, l), (\omega_1, \omega_1)\} \tilde{A}C = \{(l, l), (\omega_1, \omega_1)\} D, \quad (5.84)$$

where we have used Eq. (5.57) and where

$$D = \tilde{A}C = \{(U_1, U_2) | U_1, U_2 \in A\} = U(1) \times U(1). \quad (5.85)$$

We apply Theorem 3, with $G = \hat{S}$, $H = D$, and $M = SU(2) \times SU(2)$, to determine the topology of the kinematic orbit. Using Eq. (5.59), it is straightforward to verify that D is normal in \hat{S} , and hence \hat{S}/D is a well-defined group isomorphic to \mathbb{Z}_2 . Since $D = U(1) \times U(1)$, we find

$$\frac{SU(2) \times SU(2)}{D} = \frac{SU(2) \times SU(2)}{U(1) \times U(1)} = \frac{SU(2)}{A} \times \frac{SU(2)}{A} = S^2 \times S^2, \quad (5.86)$$

where we have used Eq. (5.61). From Eq. (5.63), the action of the nontrivial element $[\omega_1, \omega_1] \in \hat{S}/D$ on $(\hat{\mathbf{n}}_1, \hat{\mathbf{n}}_2) \in S^2 \times S^2$ is shown to be

$$[\omega_1, \omega_1](\hat{\mathbf{n}}_1, \hat{\mathbf{n}}_2) = (-\hat{\mathbf{n}}_1, -\hat{\mathbf{n}}_2). \quad (5.87)$$

With this understanding of the action of \mathbb{Z}_2 on $S^2 \times S^2$, we have

$$\Gamma = \frac{SU(2) \times SU(2)}{\hat{S}} = \frac{(SU(2) \times SU(2))/D}{\hat{S}/D} = \frac{S^2 \times S^2}{\mathbb{Z}_2}. \quad (5.88)$$

6. The class 1 of collinear shapes

In Sect. III we showed that for collinear shapes $\Gamma = SO(n-1)/O(n-2) = \mathbb{R}P^{n-2}$. For $n = 5$ this yields $\mathbb{R}P^3$ and no more need be said. However, for completeness and analogy with the preceding cases, we show here how this result also follows from Eq. (5.45).

The matrix B can be any matrix in $O(3)$ and the matrix A is the 1×1 matrix $A = \det B$. As in the analysis of class 2(i), we switch the positions of the blocks in K containing A and B . Specifically, the isotropy subgroup is

$$S = \left\{ \left[\begin{array}{c|c} B & 0 \\ \hline 0 & \det B \end{array} \right] \middle| B \in O(3) \right\} = \{I, -I\} \left\{ \left[\begin{array}{c|c} B & 0 \\ \hline 0 & 1 \end{array} \right] \middle| B \in SO(3) \right\}. \quad (5.89)$$

Concerning the first factor, Eq. (5.35) shows

$$\pi(-1, 1) = -1. \quad (5.90)$$

The second factor is the same as the group S given in Eq. (5.66). Thus, the double cover of the second factor is the group \tilde{E} given in Eq. (5.71) and the double cover of S is

$$\hat{S} = \{(1, 1), (-1, 1)\}\tilde{E}. \quad (5.91)$$

We apply Theorem 3 with $G = \hat{S}$, $H = \tilde{E}$, and $M = SU(2) \times SU(2)$. It is trivial to show that \tilde{E} is normal in \hat{S} and hence \hat{S}/\tilde{E} is a well-defined group isomorphic to \mathbb{Z}_2 . Recall from Eq. (5.72) that $(SU(2) \times SU(2))/\tilde{E} = SU(2)$. The nontrivial element $[-1, 1] \in \hat{S}/\tilde{E}$ maps $[U_1, U_2] \in (SU(2) \times SU(2))/\tilde{E}$ into $[-U_1, U_2]$. Using the diffeomorphism $f : (SU(2) \times SU(2))/\tilde{E} \rightarrow SU(2)$ of Eq. (A4), this results in the following action on $U \in SU(2)$,

$$[-1, 1]U = -U. \quad (5.92)$$

Thus, we find

$$\Gamma = \frac{SU(2) \times SU(2)}{\hat{S}} = \frac{(SU(2) \times SU(2))/\tilde{E}}{\hat{S}/\tilde{E}} = \frac{SU(2)}{\mathbb{Z}_2} = \mathbb{R}P^3. \quad (5.93)$$

VI. CONCLUSIONS

For the general n -body problem, we have expressed a kinematic orbit as the quotient of the kinematic group by the isotropy subgroup of the shape in question. We have computed these isotropy subgroups explicitly. For the three-, four-, and five-body cases, we have represented the kinematic orbits in terms of simple well-studied spaces of low dimension. We have also showed that the kinematic orbit of a collinear shape is $\mathbb{R}P^{n-2}$ for any n .

The natural next step for us to take is an analysis of body frame singularities for $n \geq 5$. We envision such an analysis beginning, as in the case of the three- and four-body analysis [1,2], with a detailed study of the principal axis frame and its singularities. As in the previous analysis, this would amount to finding the fundamental group of the asymmetric

top region of shape space and then relating the paths (or more precisely the equivalence classes of paths) in this group to the jumps in the principal axis frame.

In the three- and four-body problems, one can find a frame related to the principal axis frame which has a smaller set of frame singularities. In particular, the frame jumps can be completely eliminated. A natural question is whether such a frame exists for $n \geq 5$. Extending this line of inquiry, another natural question is which frames have the smallest set of singularities and what constraints are placed on one's ability to move these singularities around. We believe that the study of frames restricted to the kinematic orbits may shed some light on these issues. For example, it would be useful to know, in the language of fibre bundles, whether the $SO(3)$ bundles defined over the kinematic orbits are trivial or not.

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APPENDIX A: THEOREMS ON LIE GROUP QUOTIENTS

We present three theorems regarding the actions of Lie groups on manifolds and the corresponding quotient spaces. These results provide a rigorous mathematical foundation for many of the steps presented in the bulk of the paper. The first result is a standard theorem and is found, for example, in Bredon (Ref. [14], p. 303, Corollary 1.3).

Theorem 1 *Let G be a compact Lie group acting smoothly on a smooth manifold M . Then the orbit through a point $x \in M$ is diffeomorphic to G/H where H is the isotropy subgroup of G at x . (That is, H contains all elements of G which leave x fixed.)*

The next result is useful for simplifying the descriptions of several manifolds appearing in the five-body problem. It is similar to an exercise of Bredon (Ref. [14], p. 113, Exercise 9).

Theorem 2 *Let G be a compact Lie group and H a Lie subgroup of G . Let \tilde{H} be the following Lie subgroup of $G \times G$,*

$$\tilde{H} = \{(h, h) | h \in H\}. \quad (\text{A1})$$

Of course, \tilde{H} is trivially isomorphic to H . Then, the smooth manifolds $(G \times G)/\tilde{H}$ and $G \times (G/H)$ are diffeomorphic.

Proof

Assuming that $(G \times G)/\tilde{H}$ and G/H are the right coset spaces, we introduce the following notation for the right cosets

$$[g_1, g_2]_{\tilde{H}} = \tilde{H}(g_1, g_2) \in (G \times G)/\tilde{H} \quad g_1, g_2 \in G, \quad (\text{A2})$$

$$[g]_H = Hg \in G/H \quad g \in G. \quad (\text{A3})$$

We define a function $f : (G \times G)/\tilde{H} \rightarrow G \times (G/H)$ acting on an arbitrary $[g_1, g_2]_{\tilde{H}} \in (G \times G)/\tilde{H}$ by

$$f([g_1, g_2]_{\tilde{H}}) = (g_2^{-1}g_1, [g_2]_H). \quad (\text{A4})$$

We assert that f is a diffeomorphism. First, we verify that f is well-defined on the coset space by noting

$$f([hg_1, hg_2]_{\tilde{H}}) = ((hg_2)^{-1}(hg_1), [hg_2]_H) = (g_2^{-1}g_1, [g_2]_H) = f([g_1, g_2]_{\tilde{H}}), \quad (\text{A5})$$

where $h \in H$ is arbitrary. Next, it is straightforward to verify that the following function is well-defined and that it is the inverse of f

$$f^{-1}(g_1, [g_2]_H) = [g_2g_1, g_2]_{\tilde{H}}, \quad (\text{A6})$$

where $g_1, g_2 \in G$ are arbitrary. Since both f and f^{-1} are smooth, they are both diffeomorphisms. \mathcal{QED} .

The following theorem is a refinement of an exercise in Bredon (Ref. [14], p. 67, Exercise 1) to the case of smooth actions. We omit the straightforward proof.

Theorem 3 *Let G be a compact Lie group and H a normal Lie subgroup of G so that G/H is itself a Lie group. Let G act smoothly upon a smooth manifold M . Assume that the isotropy subgroups of this action are all conjugate to one another so that M/G and M/H are themselves smooth manifolds. Then, G/H has a well-defined action on M/H given by $[g]_H[x]_H = [gx]_H$, where $[g]_H \in G/H$ and $[x]_H \in M/H$. Furthermore, the following diffeomorphism holds*

$$\frac{M}{G} = \frac{M/H}{G/H}. \quad (\text{A7})$$

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