QUATERNIONS AND ROTATIONS IN $\mathbb{R}^3$

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ABSTRACT. In this expository note, we show that (a) rotations in 3-dimensional space are completely described by an axis of rotation and an angle of rotation about that axis. It is then natural to enquire about the axis and angle of rotation of the composite of two rotations whose axes and angles of rotation are given. We then (b) use the algebra of quaternions to answer this question.

1. ROTATIONS

We recall that Euclidean space $\mathbb{R}^n$ comes equipped with the natural *dot product* or *inner product* defined by

$$\langle v, w\rangle = \sum_{i=1}^{n} v_i w_i$$

for two vectors $v = (v_1, .., v_n)$ and $w = (w_1, ..., w_n) \in \mathbb{R}^n$. We will denote the i-th basis vector $(0, .., 1, ..0)$ with 1 in the i-th spot and 0 elsewhere by e_i. The collection $\{e_i\}_{i=1}^n$ is called the *standard basis* of $\mathbb{R}^n$. If $v = \sum_{i=1}^n v_i e_i$ is a vector in $\mathbb{R}^n$, its *length* or *norm* is defined as $\|v\| = \langle v, v\rangle^{1/2} = \left(\sum_{i=1}^n v_i^2\right)^{1/2}$. A set of vectors $\{v_1, ..., v_r\}$ is called an *orthonormal set* if $\langle v_i, v_j\rangle = \delta_{ij}$ for all $1 \leq i, j \leq r$ (Here δ_{ij} is the *Kronecker delta* symbol defined by $\delta_{ij} = 1$ if $i = j$, and $\delta_{ij} = 0$ if $i \neq j$).

If an orthonormal set is a basis, it is called an *orthonormal basis*. For example, the standard basis $\{e_i\}_{i=1}^n$ of $\mathbb{R}^n$ is an orthonormal basis.

Definition 1.1 (Orthogonal transformations and rotations in $\mathbb{R}^n$)**.** A linear transformation $T : \mathbb{R}^n \to \mathbb{R}^n$ is called an *orthogonal transformation* if it preserves all inner products. i.e. if $\langle Tv, Tw\rangle = \langle v, w\rangle$ for all $v, w \in \mathbb{R}^n$. The set of all orthogonal transformations of $\mathbb{R}^n$ is denoted as $O(n)$. An orthogonal transformation T is called a *rotation* if its determinant $\det T > 0$. The set of all rotations of $\mathbb{R}^n$ is denoted as $SO(n)$. Thus $SO(n) \subset O(n)$.

We note that a linear transformation $T : \mathbb{R}^n \to \mathbb{R}^n$ determines an $n \times n$ matrix with respect to the standard basis as follows. We expand the the image of the j-th standard basis vector e_j under T in terms of the standard basis:

$$Te_j = \sum_{i=1}^{n} T_{ij} e_i \tag{1}$$

Thus the j-th *column* of the matrix $[T_{ij}]$ is the image Te_j of the j-th basis vector e_j. Clearly, with this same prescription we are free to define the matrix of a linear transformation with respect to *any fixed chosen basis* of $\mathbb{R}^n$, though in the present discussion we will mostly use the standard basis. If $v = \sum_{j=1}^n v_j e_j$, then for the linear transformation T we have from the relation (1) above:

$$Tv = T\left(\sum_j v_j e_j\right) = \sum_j v_j Te_j = \sum_{i=1}^{n}\left(\sum_{j=1}^{n} T_{ij} v_j\right) e_i$$

In other words, if we use the common representation of the vector v as a column vector (with column entries v_i), also denoted by v, then the column vector representing Tv is given by the matrix product $T.v$.

We next examine the condition on T_{ij} for T to be an orthogonal transformation, and for it to be a rotation.

Proposition 1.2 (Matrix characterisation of orthogonal transformations and rotations)**.** The linear transformation $T : \mathbb{R}^n \to \mathbb{R}^n$ is an orthogonal transformation if and only if $T^tT = TT^t = I$, where T^t denotes the *transpose of* T defined by $T^t_{ij} = T_{ji}$. This is summarised by saying that the column vectors (resp. row vectors) of the matrix of T form an orthonormal set. For an orthogonal transformation T, $\det T = \pm 1$. Finally, an orthogonal transformation T is a rotation if $\det T = 1$.

Proof: If T is orthogonal we have $\delta_{ij} = \langle e_i, e_j \rangle = \langle Te_i, Te_j \rangle$ for all i and j. Plugging in $Te_i = \sum_k T_{ki} e_k$ and $Te_j = \sum_m T_{mj} e_m$, we find $\delta_{ij} = \langle Te_i, Te_j \rangle = \sum_{k,m} T_{ki} T_{mj} \langle e_k, e_m \rangle = \sum_{k,m} T_{ki} T_{mj} \delta_{km} = \sum_k T^t_{ik} T_{kj} = (T^tT)_{ij}$. Thus T is orthogonal implies $T^tT = I$. This shows that $T^t = T^{-1}$, and hence also that $TT^t = I$.

Conversely, if $T^tT = I$, it follows by reversing the steps above that $\langle Te_i, Te_j \rangle = \langle e_i, e_j \rangle$ for all i and j. This implies that $\langle Tv, Tw \rangle = \sum_{i,j} v_i w_j \langle Te_i, Te_j \rangle = \sum_{i,j} v_i w_j \langle e_i, e_j \rangle = \langle v, w \rangle$ for all $v, w \in \mathbb{R}^n$. This proves the first assertion. Writing out the relation $T^tT = I$ (resp. $TT^t = I$) shows that the column (resp. row) vectors of T form an orthonormal set.

Since T orthogonal imples $T^tT = I$, we have $\det(T^tT) = \det(T^t) \det T = (\det T)^2 = \det I = 1$. Hence $\det T = \pm 1$. The second and third assertions follow. $\square$

The above matrix description of orthogonal transformations and rotations leads to the following important property of the sets $O(n)$ and $SO(n)$.

Proposition 1.3 (The group structure on $O(n)$ and $SO(n)$)**.** The sets $G = O(n)$ or $SO(n)$ are *groups.* That is, they have a *product* or *group operation* defined by composition : $T.S := T \circ S$, where $(T \circ S)v = T(Sv)$ for $v \in \mathbb{R}^n$. Furthermore, this operation satisfies the following axioms of a group:

(i): *(Associativity)* $T.(S.R) = (T.S).R$ for all $T, S, R \in G$.
(ii): *(Existence of identity)* There is an identity transformation $I \in G$ such that $T.I = I.T = T$ for all $T \in G$.
(iii): *(Existence of inverse)* For each $T \in G$, there exists an element $T^{-1} \in G$ such that $T.T^{-1} = T^{-1}.T = I$.

Indeed, since $SO(n) \subset O(n)$ inherits the group operation from $O(n)$, we call $SO(n)$ a *subgroup* of $O(n)$. The group $O(n)$ is called the *orthogonal group of* $\mathbb{R}^n$ and $SO(n)$ the *special orthogonal group* of $\mathbb{R}^n$.

Proof: We first remark that the matrix of the composite transformation $T.S$, by definition, is given by :

$$(T.S)e_j = \sum_i (T.S)_{ij} e_i$$

However the left hand side, by definition and (1), is

$$T(Se_j) = T\left(\sum_k S_{kj} e_k\right) = \sum_k S_{kj}(Te_k) = \sum_k S_{kj}\left(\sum_i T_{ik} e_i\right) = \sum_i \left(\sum_k T_{ik} S_{kj}\right) e_i$$

which implies that $(T.S)_{ij} = \sum_k T_{ik} S_{kj}$. That is, if we compose orthogonal transformations, the matrix of the composite transformation is the product of their respective matrices.

Let $T, S \in O(n)$. Since $\langle (T.S)v, (T.S)w \rangle = \langle T(Sv), T(Sw) \rangle = \langle Sv, Sw \rangle = \langle v, w \rangle$ from the fact that T and $S \in O(n)$, it follows that $T.S \in O(n)$. If further $S, T \in SO(n)$, then $\det T = \det S = 1$. But then $\det(T.S) = (\det T)(\det S) = 1$, showing that $S.T \in SO(n)$ as well. This proves the existence of a *binary operation* on $O(n)$ and $SO(n)$.

The assertion (i) follows because multiplication of matrices (or for that matter, composition of maps) is easily verified to be associative. The statement (ii) is obvious, since the identity transformation $I \in SO(n)$ and in $O(n)$ as well. The assertion (iii) follows by the previous Proposition 1.2, where we saw that $T^t = T^{-1}$, and also that $T \in O(n)$ implies $T^t \in O(n)$, because the conditions $TT^t = I$ and $T^tT = I$ are equivalent. Further $T \in SO(n)$ implies $\det T^t = \det T = 1$, so that $T^{-1} = T^t \in SO(n)$ as well. $\square$

2. Rotations in $\mathbb{R}^2$ and $\mathbb{R}^3$

The following propositions give a quantitative characterisation of all the matrices that define rotations in $\mathbb{R}^2$ and $\mathbb{R}^3$.

Proposition 2.1 (Planar Rotations)**.** If $T \in SO(2)$, then the matrix of T is given by:

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

which, geometrically, describes a counterclockwise rotation in $\mathbb{R}^2$ by the angle $\theta \in [0, 2\pi)$. If we denote this rotation by R_θ, then it is easily checked that $R_\theta.R_\phi = R_{\theta+\phi} = R_{\phi+\theta}$. (Here $\theta + \phi$ means we go modulo 2π, viz. integer multiples of 2π have to be subtracted to get the value of $\theta + \phi$ to lie in $[0, 2\pi)$). In particular, the group $SO(2)$ is *abelian*, viz $T.S = S.T$ for all $T, S \in SO(2)$. Geometrically, we can think of the group $SO(2)$ as the group S^1, defined as the circle consisting of complex numbers in $\mathbb{C}$ of modulus 1 (and group operation being multiplication of complex numbers).

Proof: We know that $T \in SO(2)$ implies firstly that $T \in O(2)$, so that by the Proposition 1.2 above, the matrix:

$$T = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

satisfies the condition $T^tT = I$, which implies that $a_{11}^2 + a_{21}^2 = 1 = a_{12}^2 + a_{22}^2$ and $a_{11}a_{12} + a_{21}a_{22} = 0$. The first relation implies, since a_{ij} are all real numbers, that $a_{11} = \cos\theta$ and $a_{21} = \sin\theta$ for some $\theta \in [0, 2\pi)$. The conditions $a_{11}a_{12} + a_{21}a_{22} = 0$ and $a_{12}^2 + a_{22}^2 = 1$ now imply that $(a_{12}, a_{22}) = \pm(-\sin\theta, \cos\theta)$. The sign $+$ is now determined by the condition that $\det T = a_{11}a_{22} - a_{12}a_{21} = 1$ since $T \in SO(2)$. This shows that T is of the form stated. The second assertion is an easy consequence of trigonometric formulas, and is left to the reader.

For the last remark, note that if we write a vector $v = xe_1 + ye_2 \in \mathbb{R}^2$ as the complex number $z = x + iy$ (where $i = \sqrt{-1}$), then $e^{i\theta}z = (\cos\theta + i\sin\theta)(x + iy) = (x\cos\theta - y\sin\theta) + i(x\sin\theta + y\cos\theta)$. Thus the components of $e^{i\theta}z$ are exactly the same as those of the rotated vector $R_\theta v$. $\square$.

Exercise 2.2. Describe the matrix of a general element $T \in O(2)$.

Now we can understand rotations in $\mathbb{R}^3$. The next proposition says that a rotation in $\mathbb{R}^3$ is only slightly more complicated than a planar rotation. Indeed, once we pin down the "axis of rotation", it is just a planar rotation in the plane perpendicular to this axis.

Proposition 2.3 (Rotations in 3-space)**.** Let $T \in SO(3)$. Then there is a vector $v \in \mathbb{R}^3$ such that the line $\mathbb{R}\,v \subset \mathbb{R}^3$ is fixed by T. This line is called the *axis of rotation of* T. If we restrict T to the plane H which is perpendicular to v (denoted by $H = (\mathbb{R}v)^\perp$), then this restriction $T_{|H}$ is just a planar rotation as described in the last proposition.

In fact, if we choose a new basis of $\mathbb{R}^3$ defined by $f_3 = \frac{v}{\|v\|}$, and f_1, f_2 an orthonormal basis of H such that the vector cross product $f_1 \times f_2 = f_3$ (viz. $\{f_1, f_2, f_3\}$ gives a *right-handed* orthonormal basis of $\mathbb{R}^3$) then the matrix of T with respect to the new basis $\{f_i\}_{i=1}^3$ is given by:

$$T = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Proof: We need to use the *characteristic polynomial* of T defined by:

$$P_T(X) := \det(XI - T)$$

It is easily seen that :

$$P_T(X) = X^3 + aX^2 + bX - 1$$

where $a, b \in \mathbb{R}$, and the constant term is $-\det T$, which is -1 because $T \in SO(3)$. A root ot this characteristic polynomial P_T is called an *eigenvalue of* T. We first make the

Claim 1: 1 is an eigenvalue of T.

If β is any real root of P_T, then $P_T(\beta) = \det(\beta I - T) = 0$. This implies that $(\beta I - T)$ is a *singular* linear transformation of $\mathbb{R}^3$, and hence must kill some non-zero vector $v \in \mathbb{R}^3$. This implies: $(\beta I - T)v = 0$, i.e. $\beta v = Tv$. That is, $v \in \mathbb{R}^3$ is an *eigenvector* of T corresponding to the real *eigenvalue* β. Furthermore $T \in O(n)$ implies $\beta^2 \langle v, v\rangle = \langle \beta v, \beta v\rangle = \langle Tv, Tv\rangle = \langle v, v\rangle$, and since $v \neq 0$, $\langle v, v\rangle > 0$, so that $\beta^2 = 1$. Hence *a real root* β *of* P_T *is forced to be* ± 1. Also, the real cubic polynomial P_T has either (i) two non-real complex conjugate roots $\alpha, \overline{\alpha}$ and a real root β, or (ii) all three real roots.

The negative of the constant term $= 1$ is the product of the roots. So in the first case (i) we get $1 = |\alpha|^2 \beta$. This implies that $\beta > 0$, and hence $\beta = 1$. In the second case (ii), all the three real roots are ± 1, and all cannot be (-1) since their product is 1. Hence in both cases $\beta = 1$ is a root of P_T (i.e. an eigenvalue). This proves Claim 1.

Thus the eigenvector v corresponding to the eigenvalue 1 satisfies $Tv = v$, i.e. it is *fixed* by T. Since T is linear, all scalar multiples of v, viz. all of the line $\mathbb{R}v$ in the direction v, is fixed by T. This is the required "axis of rotation" of T.

Now, set $H := (\mathbb{R}v)^{\perp} := \{w \in \mathbb{R}^3 : \langle w, v\rangle = 0\}$, the *orthogonal plane* to v. The relation $Tv = v$ and the fact that T is an orthogonal transformation implies $\langle Tw, v\rangle = \langle Tw, Tv\rangle = \langle v, w\rangle = 0$ for each $w \in H$. This shows that T sends vectors in H to other vectors in H. The restriction $T_{|H}$ is then an orthogonal transformation of H (it still preserves inner products). It is clear that $\det T = \det\, T_{|H}.1$, and hence $T_{|H}$ also has determinant 1. Now the matrix from of T follows from Proposition 2.1. $\square$

Main question of this note: Suppose we are given two rotations $A, B \in SO(3)$ in terms of their axes and angles of rotation in accordance with the Proposition 2.3 above. Can we figure out the axis of rotation and angle or rotation of the composite $A.B$ in terms of the given data ?

The following sections will be devoted to answering this question. First we need some preliminaries on the algebra of quaternions.

3. The Algebra of Quaternions

Definition 3.1 (Quaternion multiplication)**.** We rename the standard basis of $\mathbb{R}^4$ as 1, i, j, k. The algebra of quaternions is defined as the 4-dimensional vector space:

$$\mathbb{H} := \{x_0.1 + x_1 i + x_2 j + x_3 k : x_i \in \mathbb{R}\}$$

with multiplication defined by linearity and the relations $i.1 = 1.i = i$; $j.1 = 1.j = j$; $k.1 = 1.k = k$; $1.1 = 1$; $ij = -ji = k$; $ki = -ik = j$; $jk = -kj = i$; $i^2 = j^2 = k^2 = -1$. From this one easily deduces that :

$$(x_0.1 + x_1 i + x_2 j + x_3 k)(y_0.1 + y_1 i + y_2 j + y_3 k) = z_0.1 + z_1.i + z_2 j + z_3.k$$

where : $z_0 = x_0y_0 - x_1y_1 - x_2y_2 - x_3y_3$, $z_1 = x_0y_1 + x_1y_0 + x_2y_3 - x_3y_2$, $z_2 = x_0y_2 + x_2y_0 + x_3y_1 - x_1y_3$ and $z_3 = x_0y_3 + x_3y_0 + x_1y_2 - x_2y_1$.

For a quaternion $x = x_0.1 + x_1 i + x_2 j + x_3 k$ we define its *conjugate* as $\overline{x} = x_0 - x_1 i - x_2 j - x_3 k$.

Notation 3.2. To simplify notation, we will now write the quaternion x above as $x_0 + x_1 i + x_2 j + x_3 k$, suppressing the basis vector 1 from the first term. Because of the way multiplication is defined, this causes no confusion. Also x_0 is called the *real part of* x, denoted $\operatorname{Re} x$ and $x_1 i + x_2 j + x_3 k$ is called the *imaginary part of* x, denoted $\operatorname{Im} x$.

Proposition 3.3 (Properties of quaternion multiplication)**.** The multiplication of quaternions has the following properties :

(i): $x\overline{x} = \overline{x}x = \|x\|^2 = \sum_{i=0}^{3} x_i^2$ for all $x \in \mathbb{H}$. Furthermore, $\|xy\| = \|x\|\,\|y\|$ for all $x, y \in \mathbb{H}$.

(ii): If $x \neq 0$ is a quaternion, then $xx^{-1} = x^{-1}x = 1$ for $x^{-1} := \frac{\overline{x}}{\|x\|^2}$. In particular, if x is of unit length (i.e. a *unit quaternion*), then x^{-1} is of unit length as well.

(iii): The set $\mathbb{H}$ forms a non-commutative, associative algebra over $\mathbb{R}$. The fact that non-zero elements have inverses makes it what is called a *division algebra*. In particular, by (i) and (ii) above, the set $Spin(3) := \{v \in \mathbb{H} : \|v\| = 1\}$ forms a non-commutative group called the *group of unit quaternions*.

(iv): If $x \in \mathbb{H}$ is of unit length, then left and right multiplications by x (denote them by L_x and R_x respectively) are elements of $SO(4)$.

Proof: The statements (i), (ii) and (iii) are straighforward verifications following from the definitions in 3.1.

To see (iv), one just brutally writes down the 4×4 matrices corresponding to L_x and R_x. To write the matrix of L_x, we need to apply L_x to the basis vectors $e_1 = 1$, $e_2 = i$, $e_3 = j$, $e_4 = k$ of $\mathbb{H} = \mathbb{R}^4$ and write them down as columns as noted immediately after Definition 1.1. That is, we left multiply the basis vectors 1, i, j and k by x, and obtain the four columns of L_x. Thus the matrix representation of L_x is:

$$L_x = \begin{pmatrix} x_0 & -x_1 & -x_2 & -x_3 \\ x_1 & x_0 & -x_3 & x_2 \\ x_2 & x_3 & x_0 & -x_1 \\ x_3 & -x_2 & x_1 & x_0 \end{pmatrix}$$

Since $\|x\|^2 = \sum_{i=0}^{3} x_i^2 = 1$, we see that each column has norm 1. All the columns are mutually orthogonal by inspection. Hence by Proposition 1.2, L_x is an element of $O(4)$. Also, one can compute the determinant of this matrix brutally, and using the fact that $\|x\|^2 = 1$, check that $\det L_x = 1$. Hence $L_x \in SO(4)$. The matrix computations for R_x are similar. The details are left to the energetic reader. $\square$

4. The angle and axis of rotation of the composite of two rotations

Notation 4.1. In this section it will be useful to denote vectors in $\mathbb{R}^4$, viz. quaternions, by small letters (such as v) as we have been doing earlier, and vectors in $\mathbb{R}^3$ by boldface letters (such as $\mathbf{v}$). We also note that we are applying the "corkscrew or right-hand rule" for rotations, viz: The unit vector $\mathbf{v}$ points in the direction of a screw that is being rotated by the given angle θ. Since a counterclockwise rotation by θ is the same as a clockwise rotation by $2\pi - \theta$, we may change the vector $\mathbf{v}$ to $-\mathbf{v}$, and thus assume without loss of generality, that $\theta \in [0, \pi]$.

Definition 4.2 (Spin Representation)**.** The group of unit quaternions $G = Spin(3)$ (see (iii) of Proposition 3.3 above for the definition) acts on $\mathbb{R}^3$ as follows. Let $v = v_0.1 + v_1 i + v_2 j + v_3 k$ be a quaternion of unit length in G. Let $y = y_0.1 + y_1 i + y_2 j + y_3 k \in \mathbb{H} = \mathbb{R}^4$ be any quaternion. Consider the action of G on $\mathbb{H}$ by quaternionic conjugation or *adjoint* action:

$$\begin{aligned} G \times \mathbb{H} &\to \mathbb{H} \\ (v, y) &\mapsto (\operatorname{Ad} v)(y) := vyv^{-1} = vy\overline{v} = (L_v.R_{\overline{v}})y \end{aligned}$$

where $\overline{v} = v_0.1 - v_1 i - v_2 j - v_3 k = v^{-1}$ is the conjugate of v. Note that this action pointwise fixes the scalars $\mathbb{R}.1 \subset \mathbb{H}$. Since L_v and $R_{\overline{v}}$ are in $SO(4)$ by (iv) of Proposition 3.3, it follows that $\operatorname{Ad} v \in SO(4)$. Since it fixes $\mathbb{R}.1$, $\operatorname{Ad} v$ sends the orthogonal space consisting of imaginary quaternions $\mathbb{R}^3 := \mathbb{R}i + \mathbb{R}j + \mathbb{R}k \subset \mathbb{H}$ to imaginary quaternions. Thus G acts on $\mathbb{R}^3$ via $SO(3)$ elements, and we get the famous *spin representation of* $G = Spin(3)$ on $SO(3)$, viz.

$$\begin{aligned} \rho : G &\to SO(3) \\ v &\mapsto \rho(v) \end{aligned}$$

where $\rho(v).(\mathbf{y}) = \mathrm{Im}\,[(\mathrm{Ad}\,v)\mathbf{y}] = (\mathrm{Ad}\,v)\mathbf{y}$, where $\mathbf{y} = y_1 i + y_2 j + y_3 k \in \mathbb{R}^3$ is regarded as a pure imaginary quaternion, and "Im" denotes imaginary part. This map ρ is easily checked to be a homomorphism (viz. it satisfies $\rho(vw) = \rho(v)\rho(w)$ for all v, w) since $\mathrm{Ad}\,vw = (\mathrm{Ad}\,v)(\mathrm{Ad}\,w)$. The kernel of ρ is $\rho^{-1}(Id) = \mathbb{Z}_2 = \{+1, -1\}$.

We now come to a key lemma needed for proving the main proposition of this note.

Lemma 4.3 (Surjectivity of the homomorphism ρ)**.** The homomorphism ρ is surjective. If A is a rotation of angle θ about the axis $\mathbf{v} \in \mathbb{R}^3$ (with the right-hand corkscrew rule of Notation 4.1) then $A = \rho(v)$ where $v \in Spin(3)$ is given by:

$$v = \cos\frac{\theta}{2} + \sin\frac{\theta}{2}(v_1 i + v_2 j + v_3 k) \tag{2}$$

where $\theta \in [0, \pi]$.

Proof: If $A = \rho(v)$ for some $v = v_0.1 + v_1 i + v_2 j + v_3 k \in Spin(3)$, then let us determine the axis in $\mathbb{R}^3$ that it fixes. Clearly the unit quaternion v is fixed by conjugation $\mathrm{Ad}\,v$, since $\mathrm{Ad}\,v(v) = v.v.v^{-1} = v$. Also the real part $\mathrm{Re}(v) = v_0.1$ is fixed by this conjugation. Thus

Claim 1: The fixed axis of $\rho(v)$ in $\mathbb{R}^3$ is the $\mathbb{R}$-span of $\mathrm{Im}\,v = v_1 i + v_2 j + v_3 k$ which we identify as $\mathbf{v} = \sum_{i=1}^3 v_i e_i$. Note that if $\mathrm{Im}\,v = 0$, then $v = \pm 1$ and $\rho(v) = Id$. In this case there is nothing to be done. Thus we assume from now on (without loss of generality) that A is not the identity, and hence that $\theta \in (0, \pi]$.

What is the interpretation of v_0? Note that for a rotation $A \in SO(3)$, if we write it as a $\theta \in (0, \pi]$ rotation about the axis $\mathbf{v}$, and complete $\mathbf{v}$ into a orthonormal basis $\{\mathbf{a}, \mathbf{b}, \mathbf{v}\}$ which is right handed (viz. $\mathbf{a} \times \mathbf{b} = \mathbf{v}$), then by the last assertion of Proposition 2.3 above, with respect to this basis, A will have the matrix representation given by:

$$A = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Claim 2: The angle of rotation θ of the rotation A above is determined by the formula :

$$2\cos\theta = \mathrm{tr}A - 1$$

where $\mathrm{tr}\,A$ is the *trace* of A, the sum of its diagonal entries. We note here the fundamental fact that the trace is a property of the linear transformation, and not of the basis chosen for its matrix representation. Which is why we used the convenient basis $\{\mathbf{a}, \mathbf{b}, \mathbf{v}\}$ described above to assert this formula for θ.

We will now show that for $v = v_0 + v_1 i + v_2 j + v_3 k \in G$ a unit quaternion, the matrix representing $\mathrm{Ad}\,v = v(-)v^{-1} = v(-)\overline{v}$ in the basis $\{1, i, j, k\}$ of $\mathbb{H}$ is given by:

$$\mathrm{Ad}\,v = \begin{pmatrix} 1 & * & * & * \\ 0 & v_0^2 + v_1^2 - v_2^2 - v_3^2 & * & * \\ 0 & * & v_0^2 + v_2^2 - v_1^2 - v_3^2 & * \\ 0 & * & * & v_0^2 + v_3^2 - v_1^2 - v_3^2 \end{pmatrix}$$

where the asterisks denote some entries that we are not of interest here. Clearly $\mathrm{Ad}\,v(1) = 1$, which yields the first column above. For the second column, note that the i-component of $\mathrm{Ad}\,v(i) = v.i.v^{-1}$ is just the term containing i in

$$v.i.v^{-1} = (v_0 + v_1 i + v_3 j + v_3 k).i.(v_0 - v_1 i - v_3 j - v_3 k)$$

which is easily computed to be $v_0^2 + v_1^2 - v_2^2 - v_3^2$.

Compute likewise for the j-component and k-component of $\mathrm{Ad}\,v(k)$. It follows that the 4×4 matrix for $\mathrm{Ad}\,v$ has the diagonal entries shown above.

Clearly since $\mathbb{R}.1$ is fixed by $\mathrm{Ad}v$, and $\rho(v)$ is the restriction of $\mathrm{Ad}v$ to $(\mathbb{R}.1)^\perp$, it follows that:

$$\mathrm{tr}\,\rho(v) = \mathrm{tr}\,(\mathrm{Ad}\,v) - 1 = 3v_0^2 - v_1^2 - v_2^2 - v_3^2 = 4v_0^2 - 1$$

since $\|v\|^2 = \sum_{i=0}^3 v_i^2 = 1$. Thus, by using Claim 2 above, the angle of rotation θ of $\rho(v)$ about the axis $\mathbf{v} = v_1e_1 + v_2e_2 + v_3e_3$ is given by:

$$2\cos\theta = \mathrm{tr}\rho(v) - 1 = 4v_0^2 - 2$$

which leads to $v_0^2 = \cos^2\frac{\theta}{2}$, or

$$\cos\frac{\theta}{2} = \pm v_0 \tag{3}$$

The two signs correspond to the fact that both $\rho(v)$ and $\rho(-v)$ give exactly the same rotation of $\mathbb{R}^3 = \mathrm{Im}\,\mathbb{H}$. Note that since we are requiring that $\theta \in (0,\pi]$, $\cos\frac{\theta}{2}$ is always non-negative, and thus we may change v to $-v$ if necessary, so as to make v_0 non-negative. Hence, choosing the positive sign for v_0, it follows that

$$v = \cos\frac{\theta}{2} + \sin\frac{\theta}{2}(v_1i + v_2j + v_3k)$$

where the coefficient $\sin\frac{\theta}{2}$ in the last three terms is needed to make v a *unit* quaternion, since $\mathbf{v} = \sum_{i=1}^3 v_ie_i$ is assumed to be a unit vector in the statement. This finishes the proof of our Lemma.

□

Example 4.4. To check that our computation above is correct, let us take $\mathbf{v} = e_3$, say. As an imaginary quaternion, this $\mathbf{v}$ is k. Then take a rotation A about $\mathbf{v}$ of angle θ (in the sense of the corkscrew rule). The Lemma 2 above says that $A = \rho(v)$ where $v = \cos\frac{\theta}{2} + \sin\frac{\theta}{2}k$. Then $\rho(v)i = \mathrm{Ad}v(i) = v.i.\overline{v} = \left(\cos\frac{\theta}{2} + \sin\frac{\theta}{2}k\right) i \left(\cos\frac{\theta}{2} - \sin\frac{\theta}{2}k\right) = \left(\cos\frac{\theta}{2} + \sin\frac{\theta}{2}k\right)\left(\cos\frac{\theta}{2}i + \sin\frac{\theta}{2}j\right) = \left(\cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2}\right)i + 2\cos\frac{\theta}{2}\sin\frac{\theta}{2}j$ $= \cos\theta.i + \sin\theta.j$. Similarly compute $\rho(v)j = \left(\cos\frac{\theta}{2} + \sin\frac{\theta}{2}k\right) j \left(\cos\frac{\theta}{2} - \sin\frac{\theta}{2}k\right) = -\sin\theta.i + \cos\theta.j$.

This shows that the matrix of A is :

$$A = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

as indeed, it should be, because rotating counterclockwise by θ in the xy plane moves a corkscrew in the direction of $\mathbf{v} = e_3$ in keeping of the right hand rule of Notation 4.1.

Remark 4.5. Incidentally, the reader may well wonder whether the Lemma 2 above gives a formula for a"continuous section" for ρ (viz. a continuous map $\sigma : SO(3) \to Spin(3)$ satisfying $\rho\circ\sigma = \mathrm{Id}_{SO(3)}$). *The answer is no.* The prescription above does not give a clear way for deciding what to do when $\theta = \pi$. In this case, the π rotations about both $\mathbf{v}$ and $-\mathbf{v}$ are the same, and so we have no way of prescribing a consistent choice between v and $-v$ to define σ all over $SO(3)$ so as to make it continuous.

However, if we take the open subset U of all rotations in $SO(3)$ which rotate by an angle *strictly less than* π, the prescription given in the proof of Lemma 2 above provides a continuous map $\sigma : U \to Spin(3)$ satisfying $\rho\circ\sigma = \mathrm{Id}_U$. In fact, it is interesting to note that U can be topologically identified with a 3-dimensional open ball of radius π. This topological equivalence comes from identifying the $\theta \in [0,\pi)$ rotation about the unit vector $\mathbf{v} \in \mathbb{R}^3$ with the vector $\theta\mathbf{v} \in \mathbb{R}^3$.

Now we are ready to answer the main question of this note.

Proposition 4.6 (Angle and axis of composite rotations)**.** Let $A, B \in SO(3)$. Let $\mathbf{v}$, (resp. $\mathbf{w}$) $\in \mathbb{R}^3$ be the axis of rotation of A (resp. B), by an amount $\theta \in [0,\pi]$ (resp. $\phi \in [0,\pi]$). Assume (for computational convenience) that both these vectors $\mathbf{v}, \mathbf{w}$ are *unit vectors*. Also we avoid the trivial case of A or B being the identity transformation by stipulating that θ, ϕ are both non-zero. Finally, we also stipulate that the unit vectors $\mathbf{v}$ and $\mathbf{w}$ are not linearly dependent, because in that case $\mathbf{v} = \pm\mathbf{w}$, and both rotations are in the same plane and the answer is obvious from Proposition 2.1.

Then the axis of rotation of AB is the axis defined by the vector

$$\cos\frac{\phi}{2}\sin\frac{\theta}{2}\mathbf{v}+\sin\frac{\phi}{2}\cos\frac{\theta}{2}\mathbf{w}+\sin\frac{\theta}{2}\sin\frac{\phi}{2}(\mathbf{v}\times\mathbf{w})$$

(Note that this last defined vector may not be a unit vector). Also the angle of rotation of AB is given by ψ where

$$\cos\frac{\psi}{2}=\cos\frac{\theta}{2}\cos\frac{\phi}{2}-\sin\frac{\theta}{2}\sin\frac{\phi}{2}\langle\mathbf{v},\mathbf{w}\rangle$$

Proof: Note that, in view of our stipulation that θ,ϕ are both non-zero, we have $\theta,\phi\in(0,\pi]$. This implies that $\sin\frac{\theta}{2}\sin\frac{\phi}{2}\neq 0$. Because $\mathbf{v}$ and $\mathbf{w}$ are stipulated to be linearly independent, this means that $\sin\frac{\theta}{2}\sin\frac{\phi}{2}(\mathbf{v}\times\mathbf{w})$ is a non-zero vector. Since the vector $\mathbf{v}\times\mathbf{w}$ is perpendicular to the plane of the unit vectors $\mathbf{v}$ and $\mathbf{w}$, it follows the vector claimed to be the axis of rotation of $A.B$ in the statement is also a *non-zero* vector. If A is a rotation by $\theta\in(0,\pi]$ with direction of rotation defined by $\mathbf{v}=\sum_{i=1}^{3}v_ie_i$ with $\sum_{i=1}^{3}v_i^2=1$, then by the Lemma 2 above, $A=\rho(v)$ where the unit quaternion $v\in G=Spin(3)$ is given by:

$$v=\cos\frac{\theta}{2}+\sin\frac{\theta}{2}(v_1i+v_2j+v_3k)$$

Likewise, if the second rotation B has direction of rotation $\mathbf{w}=\sum_{i=1}^{3}w_ie_i$ by an angle $\phi\in(0,\pi]$, then $B=\rho(w)$, where $w\in G$ is the unit quaternion given by

$$w=\cos\frac{\phi}{2}+\sin\frac{\phi}{2}(w_1i+w_2j+w_3k)$$

By Claim 1 in the proof of Lemma 2 above, the fixed direction of $AB=\rho(v)\rho(w)=\rho(vw)$ is then given by computing the imaginary part of the quaternion $v.w$. Indeed,

$$\begin{aligned}
\mathrm{Im}\,(v.w) &= \left[w_1\sin\frac{\phi}{2}\cos\frac{\theta}{2}+v_1\sin\frac{\theta}{2}\cos\frac{\phi}{2}+\sin\frac{\theta}{2}\sin\frac{\phi}{2}(v_2w_3-v_3w_2)\right]i\\
&+\left[w_2\sin\frac{\phi}{2}\cos\frac{\theta}{2}+v_2\sin\frac{\theta}{2}\cos\frac{\phi}{2}+\sin\frac{\theta}{2}\sin\frac{\phi}{2}(v_3w_1-v_1w_3)\right]j\\
&+\left[w_3\sin\frac{\phi}{2}\cos\frac{\theta}{2}+v_3\sin\frac{\theta}{2}\cos\frac{\phi}{2}+\sin\frac{\theta}{2}\sin\frac{\phi}{2}(v_1w_2-v_2w_1)\right]k\\
&= \sin\frac{\theta}{2}\cos\frac{\phi}{2}\mathbf{v}+\cos\frac{\theta}{2}\sin\frac{\phi}{2}\mathbf{w}+\sin\frac{\theta}{2}\sin\frac{\phi}{2}(\mathbf{v}\times\mathbf{w})
\end{aligned}$$

which proves the first part of the proposition (where, as usual, $\mathrm{Im}\,\mathbb{H}$ is being identified with $\mathbb{R}^3$ by $i\mapsto e_1$, $j\mapsto e_2$, $k\mapsto e_3$) .

To see the angle of rotation ψ, we know that by Claim 2 in the proof of Lemma 2, $\cos\frac{\psi}{2}$ is the real part of the product quaternion vw. Thus it is

$$\begin{aligned}
\cos\frac{\psi}{2}=\mathrm{Re}(vw) &= \cos\frac{\theta}{2}\cos\frac{\phi}{2}-\sin\frac{\theta}{2}\sin\frac{\phi}{2}(v_1w_1+v_2w_2+v_3w_3)\\
&= \cos\frac{\theta}{2}\cos\frac{\phi}{2}-\sin\frac{\theta}{2}\sin\frac{\phi}{2}\langle\mathbf{v},\mathbf{w}\rangle
\end{aligned}$$

which is exactly the second part of the proposition. The proposition follows. Notice how the dot product $\langle\mathbf{v},\mathbf{w}\rangle$ enters into the formula for the angle, and the cross product $\mathbf{v}\times\mathbf{w}$ enters into the formula for the axis of rotation. □

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