Chapter 16

Unit Quaternions and Rotations in $\mathbf{SO}(3)$

This chapter is devoted to the representation of rotations in $\mathbf{SO}(3)$ in terms of unit quaternions. Since we already defined the unitary groups $\mathbf{SU}(n)$, the quickest way to introduce the *unit quaternions* is to define them as the elements of the group $\mathbf{SU}(2)$.

The skew field $\mathbb{H}$ of quaternions and the group $\mathbf{SU}(2)$ of unit quaternions are discussed in Section 16.1. In Section 16.2, we define a homomorphism $r\colon \mathbf{SU}(2) \to \mathbf{SO}(3)$ and prove that its kernel is $\{-I, I\}$. We compute the rotation matrix R_q associated with the rotation r_q induced by a unit quaternion q in Section 16.3. In Section 16.4, we prove that the homomorphism $r\colon \mathbf{SU}(2) \to \mathbf{SO}(3)$ is surjective by providing an algorithm to construct a quaternion from a rotation matrix. In Section 16.5 we define the exponential map $\exp\colon \mathfrak{su}(2) \to \mathbf{SU}(2)$ where $\mathfrak{su}(2)$ is the real vector space of skew-Hermitian 2×2 matrices with zero trace. We prove that exponential map $\exp\colon \mathfrak{su}(2) \to \mathbf{SU}(2)$ is surjective and give an algorithm for finding a logarithm. We discuss quaternion interpolation and prove the famous *slerp interpolation formula* due to Ken Shoemake in Section 16.6. This formula is used in robotics and computer graphics to deal with interpolation problems. In Section 16.7, we prove that there is no "nice" section $s\colon \mathbf{SO}(3) \to \mathbf{SU}(2)$ of the homomorphism $r\colon \mathbf{SU}(2) \to \mathbf{SO}(3)$, in the sense that any section of r is neither a homomorphism nor continuous.

16.1 The Group $\mathbf{SU}(2)$ of Unit Quaternions and the Skew Field $\mathbb{H}$ of Quaternions

Definition 16.1. The *unit quaternions* are the elements of the group $\mathbf{SU}(2)$, namely the group of 2×2 complex matrices of the form

$$\begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix} \qquad \alpha, \beta \in \mathbb{C},\ \alpha\overline{\alpha} + \beta\overline{\beta} = 1.$$

The *quaternions* are the elements of the real vector space $\mathbb{H} = \mathbb{R}\,\mathbf{SU}(2)$.

Let $\mathbf{1}, \mathbf{i}, \mathbf{j}, \mathbf{k}$ be the matrices

$$\mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \mathbf{i} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \qquad \mathbf{j} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad \mathbf{k} = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix},$$

then $\mathbb{H}$ is the set of all matrices of the form

$$X = a\mathbf{1} + b\mathbf{i} + c\mathbf{j} + d\mathbf{k}, \quad a, b, c, d \in \mathbb{R}.$$

Indeed, every matrix in $\mathbb{H}$ is of the form

$$X = \begin{pmatrix} a + ib & c + id \\ -(c - id) & a - ib \end{pmatrix}, \quad a, b, c, d \in \mathbb{R}.$$

It is easy (but a bit tedious) to verify that the quaternions $\mathbf{1}, \mathbf{i}, \mathbf{j}, \mathbf{k}$ satisfy the famous identities discovered by Hamilton:

$$\begin{aligned} \mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = \mathbf{ijk} &= -\mathbf{1}, \\ \mathbf{ij} = -\mathbf{ji} &= \mathbf{k}, \\ \mathbf{jk} = -\mathbf{kj} &= \mathbf{i}, \\ \mathbf{ki} = -\mathbf{ik} &= \mathbf{j}. \end{aligned}$$

Thus, the quaternions are a generalization of the complex numbers, but there are three square roots of $-\mathbf{1}$ and multiplication is not commutative.

Given any two quaternions $X = a\mathbf{1} + b\mathbf{i} + c\mathbf{j} + d\mathbf{k}$ and $Y = a'\mathbf{1} + b'\mathbf{i} + c'\mathbf{j} + d'\mathbf{k}$, Hamilton's famous formula

$$\begin{aligned} XY = {} & (aa' - bb' - cc' - dd')\mathbf{1} + (ab' + ba' + cd' - dc')\mathbf{i} \\ & + (ac' + ca' + db' - bd')\mathbf{j} + (ad' + da' + bc' - cb')\mathbf{k} \end{aligned}$$

looks mysterious, but it is simply the result of multiplying the two matrices

$$X = \begin{pmatrix} a + ib & c + id \\ -(c - id) & a - ib \end{pmatrix} \quad \text{and} \quad Y = \begin{pmatrix} a' + ib' & c' + id' \\ -(c' - id') & a' - ib' \end{pmatrix}.$$

It is worth noting that this formula was discovered independently by Olinde Rodrigues in 1840, a few years before Hamilton (Veblen and Young [184]). However, Rodrigues was working with a different formalism, homogeneous transformations, and he did not discover the quaternions.

If

$$X = \begin{pmatrix} a + ib & c + id \\ -(c - id) & a - ib \end{pmatrix}, \quad a, b, c, d \in \mathbb{R},$$

it is immediately verified that

$$XX^* = X^*X = (a^2 + b^2 + c^2 + d^2)\mathbf{1}.$$

Also observe that

$$X^* = \begin{pmatrix} a - ib & -(c + id) \\ c - id & a + ib \end{pmatrix} = a\mathbf{1} - b\mathbf{i} - c\mathbf{j} - d\mathbf{k}.$$

This implies that if $X \neq 0$, then X is invertible and its inverse is given by

$$X^{-1} = (a^2 + b^2 + c^2 + d^2)^{-1} X^*.$$

As a consequence, it can be verified that $\mathbb{H}$ is a skew field (a noncommutative field). It is also a real vector space of dimension 4 with basis $(\mathbf{1}, \mathbf{i}, \mathbf{j}, \mathbf{k})$; thus as a vector space, $\mathbb{H}$ is isomorphic to $\mathbb{R}^4$.

Definition 16.2. A concise notation for the quaternion X defined by $\alpha = a + ib$ and $\beta = c + id$ is

$$X = [a, (b, c, d)].$$

We call a the *scalar part* of X and (b, c, d) the *vector part* of X. With this notation, $X^* = [a, -(b, c, d)]$, which is often denoted by $\overline{X}$. The quaternion $\overline{X}$ is called the *conjugate* of X. If q is a unit quaternion, then $\overline{q}$ is the multiplicative inverse of q.

16.2 Representation of Rotations in SO(3) by Quaternions in SU(2)

The key to representation of rotations in **SO**(3) by unit quaternions is a certain group homomorphism called the *adjoint representation of* **SU**(2). To define this mapping, first we define the real vector space $\mathfrak{su}(2)$ of skew Hermitian matrices.

Definition 16.3. The (real) vector space $\mathfrak{su}(2)$ of 2×2 *skew Hermitian matrices with zero trace* is given by

$$\mathfrak{su}(2) = \left\{ \begin{pmatrix} ix & y + iz \\ -y + iz & -ix \end{pmatrix} \;\middle|\; (x, y, z) \in \mathbb{R}^3 \right\}.$$

Observe that for every matrix $A \in \mathfrak{su}(2)$, we have $A^* = -A$, that is, A is skew Hermitian, and that $\mathrm{tr}(A) = 0$.

Definition 16.4. The *adjoint representation* of the group **SU**(2) is the group homomorphism $\mathrm{Ad}\colon \mathbf{SU}(2) \to \mathbf{GL}(\mathfrak{su}(2))$ defined such that for every $q \in \mathbf{SU}(2)$, with

$$q = \begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix} \in \mathbf{SU}(2),$$

we have

$$\mathrm{Ad}_q(A) = qAq^*, \quad A \in \mathfrak{su}(2),$$

where q^* is the inverse of q (since **SU**(2) is a unitary group) and is given by

$$q^* = \begin{pmatrix} \overline{\alpha} & -\beta \\ \overline{\beta} & \alpha \end{pmatrix}.$$

One needs to verify that the map Ad_q is an invertible linear map from $\mathfrak{su}(2)$ to itself, and that Ad is a group homomorphism, which is easy to do.

In order to associate a rotation ρ_q (in $\mathbf{SO}(3)$) to q, we need to embed $\mathbb{R}^3$ into $\mathbb{H}$ as the pure quaternions, by

$$\psi(x, y, z) = \begin{pmatrix} ix & y + iz \\ -y + iz & -ix \end{pmatrix}, \quad (x, y, z) \in \mathbb{R}^3.$$

Then q defines the map ρ_q (on $\mathbb{R}^3$) given by

$$\rho_q(x, y, z) = \psi^{-1}(q\psi(x, y, z)q^*).$$

Therefore, modulo the isomorphism ψ, the linear map ρ_q is the linear isomorphism Ad_q. In fact, it turns out that ρ_q is a rotation (and so is Ad_q), which we will prove shortly. So, the representation of rotations in $\mathbf{SO}(3)$ by unit quaternions is just the adjoint representation of $\mathbf{SU}(2)$; its image is a subgroup of $\mathbf{GL}(\mathfrak{su}(2))$ isomorphic to $\mathbf{SO}(3)$.

Technically, it is a bit simpler to embed $\mathbb{R}^3$ in the (real) vector spaces of Hermitian matrices with zero trace,

$$\left\{ \begin{pmatrix} x & z - iy \\ z + iy & -x \end{pmatrix} \;\middle|\; x, y, z \in \mathbb{R} \right\}.$$

Since the matrix $\psi(x, y, z)$ is skew-Hermitian, the matrix $-i\psi(x, y, z)$ is Hermitian, and we have

$$-i\psi(x, y, z) = \begin{pmatrix} x & z - iy \\ z + iy & -x \end{pmatrix} = x\sigma_3 + y\sigma_2 + z\sigma_1,$$

where $\sigma_1, \sigma_2, \sigma_3$ are the *Pauli spin matrices*

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Matrices of the form $x\sigma_3 + y\sigma_2 + z\sigma_1$ are Hermitian matrices with zero trace.

It is easy to see that every 2×2 Hermitian matrix with zero trace must be of this form. (observe that $(i\sigma_1, i\sigma_2, i\sigma_3)$ forms a basis of $\mathfrak{su}(2)$. Also, $\mathbf{i} = i\sigma_3$, $\mathbf{j} = i\sigma_2$, $\mathbf{k} = i\sigma_1$.)

Now, if $A = x\sigma_3 + y\sigma_2 + z\sigma_1$ is a Hermitian 2×2 matrix with zero trace, we have

$$(qAq^*)^* = qA^*q^* = qAq^*,$$

so qAq^* is also Hermitian, and

$$\mathrm{tr}(qAq^*) = \mathrm{tr}(Aq^*q) = \mathrm{tr}(A),$$

and qAq^* also has zero trace. Therefore, the map $A \mapsto qAq^*$ preserves the Hermitian matrices with zero trace. We also have

$$\det(x\sigma_3 + y\sigma_2 + z\sigma_1) = \det \begin{pmatrix} x & z - iy \\ z + iy & -x \end{pmatrix} = -(x^2 + y^2 + z^2),$$

and

$$\det(qAq^*) = \det(q)\det(A)\det(q^*) = \det(A) = -(x^2 + y^2 + z^2).$$

We can embed $\mathbb{R}^3$ into the space of Hermitian matrices with zero trace by

$$\varphi(x, y, z) = x\sigma_3 + y\sigma_2 + z\sigma_1.$$

Note that

$$\varphi = -i\psi \quad \text{and} \quad \varphi^{-1} = i\psi^{-1}.$$

Definition 16.5. The unit quaternion $q \in \mathbf{SU}(2)$ induces a map r_q on $\mathbb{R}^3$ by

$$r_q(x, y, z) = \varphi^{-1}(q\varphi(x, y, z)q^*) = \varphi^{-1}(q(x\sigma_3 + y\sigma_2 + z\sigma_1)q^*).$$

The map r_q is clearly linear since φ is linear.

Proposition 16.1. *For every unit quaternion $q \in \mathbf{SU}(2)$, the linear map r_q is orthogonal, that is, $r_q \in \mathbf{O}(3)$.*

Proof. Since

$$-\|(x, y, z)\|^2 = -(x^2 + y^2 + z^2) = \det(x\sigma^3 + y\sigma^2 + z\sigma_1) = \det(\varphi(x, y, z)),$$

we have

$$\begin{aligned} -\|r_q(x, y, z)\|^2 &= \det(\varphi(r_q(x, y, z))) = \det(q(x\sigma_3 + y\sigma_2 + z\sigma_1)q^*) \\ &= \det(x\sigma_3 + y\sigma_2 + z\sigma_1) = -\left\|(x, y, z)^2\right\|, \end{aligned}$$

and we deduce that r_q is an isometry. Thus, $r_q \in \mathbf{O}(3)$. $\square$

In fact, r_q is a rotation, and we can show this by finding the fixed points of r_q. Let q be a unit quaternion of the form

$$q = \begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix}$$

with $\alpha = a + ib$, $\beta = c + id$, and $a^2 + b^2 + c^2 + d^2 = 1$ $(a, b, c, d \in \mathbb{R})$.

If $b = c = d = 0$, then $q = I$ and r_q is the identity so we may assume that $(b, c, d) \neq (0, 0, 0)$.

Proposition 16.2. *If $(b, c, d) \neq (0, 0, 0)$, then the fixed points of r_q are solutions (x, y, z) of the linear system*

$$\begin{aligned} -dy + cz &= 0 \\ cx - by &= 0 \\ dx - bz &= 0. \end{aligned}$$

This linear system has the nontrivial solution (b, c, d) and has rank 2. Therefore, r_q has the eigenvalue 1 with multiplicity 1, and r_q is a rotation whose axis is determined by (b, c, d).

Proof. We have $r_q(x, y, z) = (x, y, z)$ iff

$$\varphi^{-1}(q(x\sigma_3 + y\sigma_2 + z\sigma_1)q^*) = (x, y, z)$$

iff

$$q(x\sigma_3 + y\sigma_2 + z\sigma_1)q^* = \varphi(x, y, z),$$

and since

$$\varphi(x, y, z) = x\sigma_3 + y\sigma_2 + z\sigma_1 = A$$

with

$$A = \begin{pmatrix} x & z - iy \\ z + iy & -x \end{pmatrix},$$

we see that $r_q(x, y, z) = (x, y, z)$ iff

$$qAq^* = A \quad \text{iff} \quad qA = Aq.$$

We have

$$qA = \begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix} \begin{pmatrix} x & z - iy \\ z + iy & -x \end{pmatrix} = \begin{pmatrix} \alpha x + \beta z + i\beta y & \alpha z - i\alpha y - \beta x \\ -\overline{\beta}x + \overline{\alpha}z + i\overline{\alpha}y & -\overline{\beta}z + i\overline{\beta}y - \overline{\alpha}x \end{pmatrix}$$

and

$$Aq = \begin{pmatrix} x & z - iy \\ z + iy & -x \end{pmatrix} \begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix} = \begin{pmatrix} \alpha x - \overline{\beta}z + i\overline{\beta}y & \beta x + \overline{\alpha}z - i\overline{\alpha}y \\ \alpha z + i\alpha y + \overline{\beta}x & \beta z + i\beta y - \overline{\alpha}x \end{pmatrix}.$$

By equating qA and Aq, we get

$$\begin{aligned} i(\beta - \overline{\beta})y + (\beta + \overline{\beta})z &= 0 \\ 2\beta x + i(\alpha - \overline{\alpha})y + (\overline{\alpha} - \alpha)z &= 0 \\ 2\overline{\beta}x + i(\alpha - \overline{\alpha})y + (\alpha - \overline{\alpha})z &= 0 \\ i(\beta - \overline{\beta})y + (\beta + \overline{\beta})z &= 0. \end{aligned}$$

The first and the fourth equation are identical and the third equation is obtained by conjugating the second, so the above system reduces to

$$\begin{aligned} i(\beta - \overline{\beta})y + (\beta + \overline{\beta})z &= 0 \\ 2\beta x + i(\alpha - \overline{\alpha})y + (\overline{\alpha} - \alpha)z &= 0. \end{aligned}$$

Replacing α by $a + ib$ and β by $c + id$, we get

$$\begin{aligned} -dy + cz &= 0 \\ cx - by + i(dx - bz) &= 0, \end{aligned}$$

which yields the equations

$$
\begin{aligned}
-dy + cz &= 0 \\
cx - by &= 0 \\
dx - bz &= 0.
\end{aligned}
$$

This linear system has the nontrivial solution (b, c, d) and the matrix of this system is

$$
\begin{pmatrix} 0 & -d & c \\ c & -b & 0 \\ d & 0 & -b \end{pmatrix}.
$$

Since $(b, c, d) \neq (0, 0, 0)$, this matrix always has a 2×2 submatrix which is nonsingular, so it has rank 2, and consequently its kernel is the one-dimensional space spanned by (b, c, d). Therefore, r_q has the eigenvalue 1 with multiplicity 1. If we had $\det(r_q) = -1$, then the eigenvalues of r_q would be either $(-1, 1, 1)$ or $(-1, e^{i\theta}, e^{-i\theta})$ with $\theta \neq k2\pi$ (with $k \in \mathbb{Z}$), contradicting the fact that 1 is an eigenvalue with multiplicity 1. Therefore, r_q is a rotation; in fact, its axis is determined by (b, c, d). □

In summary, $q \mapsto r_q$ is a map r from $\mathbf{SU}(2)$ to $\mathbf{SO}(3)$.

Theorem 16.3. *The map* $r\colon \mathbf{SU}(2) \to \mathbf{SO}(3)$ *is a homomorphism whose kernel is* $\{I, -I\}$.

Proof. This map is a homomorphism, because if $q_1, q_2 \in \mathbf{SU}(2)$, then

$$
\begin{aligned}
r_{q_2}(r_{q_1}(x, y, z)) &= \varphi^{-1}(q_2 \varphi(r_{q_1}(x, y, z)) q_2^*) \\
&= \varphi^{-1}(q_2 \varphi(\varphi^{-1}(q_1 \varphi(x, y, z) q_1^*)) q_2^*) \\
&= \varphi^{-1}((q_2 q_1) \varphi(x, y, z) (q_2 q_1)^*) \\
&= r_{q_2 q_1}(x, y, z).
\end{aligned}
$$

The computation that showed that if $(b, c, d) \neq (0, 0, 0)$, then r_q has the eigenvalue 1 with multiplicity 1 implies the following: if $r_q = I_3$, namely r_q has the eigenvalue 1 with multiplicity 3, then $(b, c, d) = (0, 0, 0)$. But then $a = \pm 1$, and so $q = \pm I_2$. Therefore, the kernel of the homomorphism $r\colon \mathbf{SU}(2) \to \mathbf{SO}(3)$ is $\{I, -I\}$. □

Remark: Perhaps the quickest way to show that r maps $\mathbf{SU}(2)$ into $\mathbf{SO}(3)$ is to observe that the map r is continuous. Then, since it is known that $\mathbf{SU}(2)$ is connected, its image by r lies in the connected component of I, namely $\mathbf{SO}(3)$.

Proposition 16.2 showed that if $u = (b, c, d) \neq (0, 0, 0)$, then r_q is a rotation whose axis is determined by $u = (b, c, d)$. The angle θ of this rotation can also be determined. The following result is proven in Gallier [72] (Chapter 9).

Theorem 16.4. *Let* $r\colon \mathbf{SU}(2) \to \mathbf{SO}(3)$ *be the homomorphism of Definition 16.5. For every unit quaternion*

$$q = \begin{pmatrix} a+ib & c+id \\ -(c-id) & a-ib \end{pmatrix},$$

we have $r_q = I_3$ *iff* $u = (b,c,d) = 0$ *iff* $|a| = 1$. *If* $u \neq 0$, *then either* $a = 0$ *and* r_q *is a rotation by* π *around the axis of rotation determined by the vector* $u = (b,c,d)$, *or* $0 < |a| < 1$ *and* r_q *is the rotation around the axis of rotation determined by the vector* $u = (b,c,d)$ *and the angle of rotation* $\theta \neq \pi$ *with* $0 < \theta < 2\pi$, *is given by*

$$\tan(\theta/2) = \frac{\|u\|}{a}.$$

Here we are assuming that a basis (w_1, w_2) *has been chosen in the plane orthogonal to* $u = (b,c,d)$ *such that* (w_1, w_2, u) *is positively oriented, that is,* $\det(w_1, w_2, u) > 0$ *(where* w_1, w_2, u *are expressed over the canonical basis* (e_1, e_2, e_3), *which is chosen to define positive orientation).*

Remark: Under the orientation defined above, we have

$$\cos(\theta/2) = a, \quad 0 < \theta < 2\pi.$$

Note that the condition $0 < \theta < 2\pi$ implies that θ is uniquely determined by the above equation. This is not the case if we choose π such that $-\pi < \theta < \pi$ since both θ and $-\theta$ satisfy the equation, and this shows why the condition $0 < \theta < 2\pi$ is preferable. If $0 < a < 1$, then $0 < \theta < \pi$, and if $-1 < a < 0$, then $\pi < \theta < 2\pi$. In the second case, r_q is also the rotation of axis $-u$ and of angle $-(2\pi - \theta) = \theta - 2\pi$ with $0 < 2\pi - \theta < \pi$, but this time the orientation of the plane orthogonal to $-u = (b,c,d)$ is the opposite orientation from before. This orientation is given by (w_2, w_1), so that $(w_2, w_1, -u)$ has positive orientation. Since the quaternions q and $-q$ define the same rotation, we may assume that $a > 0$, in which case $0 < \theta < \pi$, but we have to remember that if $a < 0$ and if we pick $-q$ instead of q, the vector defining the axis of rotation becomes $-u$, which amounts to flipping the orientation of the plane orthogonal to the axis of rotation.

The map r is surjective, but this is not obvious. We will return to this point after finding the matrix representing r_q explicitly.

16.3 Matrix Representation of the Rotation r_q

Given a unit quaternion q of the form

$$q = \begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix}$$

with $\alpha = a + ib$, $\beta = c + id$, and $a^2 + b^2 + c^2 + d^2 = 1$ $(a, b, c, d \in \mathbb{R})$, to find the matrix representing the rotation r_q we need to compute

$$q(x\sigma_3 + y\sigma_2 + z\sigma_1)q^* = \begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix} \begin{pmatrix} x & z - iy \\ z + iy & -x \end{pmatrix} \begin{pmatrix} \overline{\alpha} & -\beta \\ \overline{\beta} & \alpha \end{pmatrix}.$$

First, we have

$$\begin{pmatrix} x & z - iy \\ z + iy & -x \end{pmatrix} \begin{pmatrix} \overline{\alpha} & -\beta \\ \overline{\beta} & \alpha \end{pmatrix} = \begin{pmatrix} x\overline{\alpha} + z\overline{\beta} - iy\overline{\beta} & -x\beta + z\alpha - iy\alpha \\ z\overline{\alpha} + iy\overline{\alpha} - x\overline{\beta} & -z\beta - iy\beta - x\alpha \end{pmatrix}.$$

Next, we have

$$\begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix} \begin{pmatrix} x\overline{\alpha} + z\overline{\beta} - iy\overline{\beta} & -x\beta + z\alpha - iy\alpha \\ z\overline{\alpha} + iy\overline{\alpha} - x\overline{\beta} & -z\beta - iy\beta - x\alpha \end{pmatrix} =$$

$$\begin{pmatrix} (\alpha\overline{\alpha} - \beta\overline{\beta})x + i(\overline{\alpha}\beta - \alpha\overline{\beta})y + (\alpha\overline{\beta} + \overline{\alpha}\beta)z & -2\alpha\beta x - i(\alpha^2 + \beta^2)y + (\alpha^2 - \beta^2)z \\ -2\overline{\alpha}\overline{\beta}x + i(\overline{\alpha}^2 + \overline{\beta}^2)y + (\overline{\alpha}^2 - \overline{\beta}^2)z & -(\alpha\overline{\alpha} - \beta\overline{\beta})x - i(\overline{\alpha}\beta - \alpha\overline{\beta})y - (\alpha\overline{\beta} + \overline{\alpha}\beta)z \end{pmatrix}$$

Since $\alpha = a + ib$ and $\beta = c + id$, with $a, b, c, d \in \mathbb{R}$, we have

$$\begin{aligned} \alpha\overline{\alpha} - \beta\overline{\beta} &= a^2 + b^2 - c^2 - d^2 \\ i(\overline{\alpha}\beta - \alpha\overline{\beta}) &= 2(bc - ad) \\ \alpha\overline{\beta} + \overline{\alpha}\beta &= 2(ac + bd) \\ -\alpha\beta &= -ac + bd - i(ad + bc) \\ -i(\alpha^2 + \beta^2) &= 2(ab + cd) - i(a^2 - b^2 + c^2 - d^2) \\ \alpha^2 - \beta^2 &= a^2 - b^2 - c^2 + d^2 + i2(ab - cd). \end{aligned}$$

Using the above, we get

$$(\alpha\overline{\alpha} - \beta\overline{\beta})x + i(\overline{\alpha}\beta - \alpha\overline{\beta})y + (\alpha\overline{\beta} + \overline{\alpha}\beta)z = (a^2 + b^2 - c^2 - d^2)x + 2(bc - ad)y + 2(ac + bd)z,$$

and

$$\begin{aligned} -2\alpha\beta x - i(\alpha^2 + \beta^2)y + (\alpha^2 - \beta^2)z = 2(-ac + bd)x + 2(ab + cd)y + (a^2 - b^2 - c^2 + d^2)z \\ - i[2(ad + bc)x + (a^2 - b^2 + c^2 - d^2)y + 2(-ab + cd)z]. \end{aligned}$$

If we write

$$q(x\sigma_3 + y\sigma_2 + z\sigma_1)q^* = \begin{pmatrix} x' & z' - iy' \\ z' + iy' & -x' \end{pmatrix},$$

we obtain

$$\begin{aligned} x' &= (a^2 + b^2 - c^2 - d^2)x + 2(bc - ad)y + 2(ac + bd)z \\ y' &= 2(ad + bc)x + (a^2 - b^2 + c^2 - d^2)y + 2(-ab + cd)z \\ z' &= 2(-ac + bd)x + 2(ab + cd)y + (a^2 - b^2 - c^2 + d^2)z. \end{aligned}$$

In summary, we proved the following result.

Proposition 16.5. *The matrix representing r_q is*

$$R_q = \begin{pmatrix} a^2+b^2-c^2-d^2 & 2bc-2ad & 2ac+2bd \\ 2bc+2ad & a^2-b^2+c^2-d^2 & -2ab+2cd \\ -2ac+2bd & 2ab+2cd & a^2-b^2-c^2+d^2 \end{pmatrix}.$$

Since $a^2+b^2+c^2+d^2=1$, this matrix can also be written as

$$R_q = \begin{pmatrix} 2a^2+2b^2-1 & 2bc-2ad & 2ac+2bd \\ 2bc+2ad & 2a^2+2c^2-1 & -2ab+2cd \\ -2ac+2bd & 2ab+2cd & 2a^2+2d^2-1 \end{pmatrix}.$$

The above is the rotation matrix in Euler form induced by the quaternion q, which is the matrix corresponding to ρ_q. This is because

$$\varphi = -i\psi, \quad \varphi^{-1} = i\psi^{-1},$$

so

$$r_q(x,y,z) = \varphi^{-1}(q\varphi(x,y,z)q^*) = i\psi^{-1}(q(-i\psi(x,y,z))q^*) = \psi^{-1}(q\psi(x,y,z)q^*) = \rho_q(x,y,z),$$

and so $r_q = \rho_q$.

We showed that every unit quaternion $q \in \mathbf{SU}(2)$ induces a rotation $r_q \in \mathbf{SO}(3)$, but it is not obvious that every rotation can be represented by a quaternion. This can shown in various ways.

One way to is use the fact that every rotation in $\mathbf{SO}(3)$ is the composition of two reflections, and that every reflection σ of $\mathbb{R}^3$ can be represented by a quaternion q, in the sense that

$$\sigma(x,y,z) = -\varphi^{-1}(q\varphi(x,y,z)q^*).$$

Note the presence of the negative sign. This is the method used in Gallier [72] (Chapter 9).

16.4 An Algorithm to Find a Quaternion Representing a Rotation

Theorem 16.6. *The homomorphism $r\colon \mathbf{SU}(2) \to \mathbf{SO}(3)$ is surjective.*

Here is an algorithmic method to find a unit quaternion q representing a rotation matrix R, which provides a proof of Theorem 16.6.

Let

$$q = \begin{pmatrix} a+ib & c+id \\ -(c-id) & a-ib \end{pmatrix}, \quad a^2+b^2+c^2+d^2=1,\ a,b,c,d \in \mathbb{R}.$$

First observe that the trace of R_q is given by

$$\mathrm{tr}(R_q) = 3a^2 - b^2 - c^2 - d^2,$$

but since $a^2 + b^2 + c^2 + d^2 = 1$, we get $\mathrm{tr}(R_q) = 4a^2 - 1$, so

$$a^2 = \frac{\mathrm{tr}(R_q) + 1}{4}.$$

If $R \in \mathbf{SO}(3)$ is any rotation matrix and if we write

$$R = \begin{pmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33}, \end{pmatrix}$$

we are looking for a unit quaternion $q \in \mathbf{SU}(2)$ such that $R_q = R$. Therefore, we must have

$$a^2 = \frac{\mathrm{tr}(R) + 1}{4}.$$

We also know that

$$\mathrm{tr}(R) = 1 + 2\cos\theta,$$

where $\theta \in [0, \pi]$ is the angle of the rotation R, so we get

$$a^2 = \frac{\cos\theta + 1}{2} = \cos^2\left(\frac{\theta}{2}\right),$$

which implies that

$$|a| = \cos\left(\frac{\theta}{2}\right) \quad (0 \le \theta \le \pi).$$

Note that we may assume that $\theta \in [0, \pi]$, because if $\pi \le \theta \le 2\pi$, then $\theta - 2\pi \in [-\pi, 0]$, and then the rotation of angle $\theta - 2\pi$ and axis determined by the vector (b, c, d) is the same as the rotation of angle $2\pi - \theta \in [0, \pi]$ and axis determined by the vector $-(b, c, d)$. There are two cases.

Case 1. $\mathrm{tr}(R) \neq -1$, or equivalently $\theta \neq \pi$. In this case $a \neq 0$. Pick

$$a = \frac{\sqrt{\mathrm{tr}(R) + 1}}{2}.$$

Then by equating $R - R^\top$ and $R_q - R_q^\top$, we get

$$\begin{aligned} 4ab &= r_{32} - r_{23} \\ 4ac &= r_{13} - r_{31} \\ 4ad &= r_{21} - r_{12}, \end{aligned}$$

which yields
$$b = \frac{r_{32} - r_{23}}{4a}, \quad c = \frac{r_{13} - r_{31}}{4a}, \quad d = \frac{r_{21} - r_{12}}{4a}.$$

Case 2. $\mathrm{tr}(R) = -1$, or equivalently $\theta = \pi$. In this case $a = 0$. By equating $R + R^\top$ and $R_q + R_q^\top$, we get

$$\begin{aligned} 4bc &= r_{21} + r_{12} \\ 4bd &= r_{13} + r_{31} \\ 4cd &= r_{32} + r_{23}. \end{aligned}$$

By equating the diagonal terms of R and R_q, we also get

$$\begin{aligned} b^2 &= \frac{1 + r_{11}}{2} \\ c^2 &= \frac{1 + r_{22}}{2} \\ d^2 &= \frac{1 + r_{33}}{2}. \end{aligned}$$

Since $q \neq 0$ and $a = 0$, at least one of b, c, d is nonzero.

If $b \neq 0$, let
$$b = \frac{\sqrt{1 + r_{11}}}{\sqrt{2}},$$
and determine c, d using

$$\begin{aligned} 4bc &= r_{21} + r_{12} \\ 4bd &= r_{13} + r_{31}. \end{aligned}$$

If $c \neq 0$, let
$$c = \frac{\sqrt{1 + r_{22}}}{\sqrt{2}},$$
and determine b, d using

$$\begin{aligned} 4bc &= r_{21} + r_{12} \\ 4cd &= r_{32} + r_{23}. \end{aligned}$$

If $d \neq 0$, let
$$d = \frac{\sqrt{1 + r_{33}}}{\sqrt{2}},$$
and determine b, c using

$$\begin{aligned} 4bd &= r_{13} + r_{31} \\ 4cd &= r_{32} + r_{23}. \end{aligned}$$

It is easy to check that whenever we computed a square root, if we had chosen a negative sign instead of a positive sign, we would obtain the quaternion $-q$. However, both q and $-q$ determine the same rotation r_q.

The above discussion involving the cases $\mathrm{tr}(R) \neq -1$ and $\mathrm{tr}(R) = -1$ is reminiscent of the procedure for finding a logarithm of a rotation matrix using the Rodrigues formula (see Section 12.7). This is not surprising, because if

$$B = \begin{pmatrix} 0 & -u_3 & u_2 \\ u_3 & 0 & -u_1 \\ -u_2 & u_1 & 0 \end{pmatrix}$$

and if we write $\theta = \sqrt{u_1^2 + u_2^2 + u_3^2}$ (with $0 \leq \theta \leq 2\pi$), then the Rodrigues formula says that

$$e^B = I + \frac{\sin\theta}{\theta} B + \frac{(1-\cos\theta)}{\theta^2} B^2, \quad \theta \neq 0,$$

with $e^0 = I$. It is easy to check that $\mathrm{tr}(e^B) = 1 + 2\cos\theta$. Then it is an easy exercise to check that the quaternion q corresponding to the rotation $R = e^B$ (with $B \neq 0$) is given by

$$q = \left[\cos\left(\frac{\theta}{2}\right), \sin\left(\frac{\theta}{2}\right)\left(\frac{u_1}{\theta}, \frac{u_2}{\theta}, \frac{u_3}{\theta}\right)\right].$$

So the method for finding the logarithm of a rotation R is essentially the same as the method for finding a quaternion defining R.

Remark: Geometrically, the group $\mathbf{SU}(2)$ is homeomorphic to the 3-sphere S^3 in $\mathbb{R}^4$,

$$S^3 = \{(x, y, z, t) \in \mathbb{R}^4 \mid x^2 + y^2 + z^2 + t^2 = 1\}.$$

However, since the kernel of the surjective homomorphism $r\colon \mathbf{SU}(2) \to \mathbf{SO}(3)$ is $\{I, -I\}$, as a topological space, $\mathbf{SO}(3)$ is homeomorphic to the quotient of S^3 obtained by identifying antipodal points (x, y, z, t) and $-(x, y, z, t)$. This quotient space is the (real) projective space $\mathbb{RP}^3$, and it is more complicated than S^3. The space S^3 is simply-connected, but $\mathbb{RP}^3$ is not.

16.5 The Exponential Map $\exp\colon \mathfrak{su}(2) \to \mathbf{SU}(2)$

Given any matrix $A \in \mathfrak{su}(2)$, with

$$A = \begin{pmatrix} iu_1 & u_2 + iu_3 \\ -u_2 + iu_3 & -iu_1 \end{pmatrix},$$

it is easy to check that

$$A^2 = -\theta^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

with $\theta = \sqrt{u_1^2 + u_2^2 + u_3^2}$. Then we have the following formula whose proof is very similar to the proof of the formula given in Proposition 9.22.

Proposition 16.7. *For every matrix $A \in \mathfrak{su}(2)$, with*

$$A = \begin{pmatrix} iu_1 & u_2 + iu_3 \\ -u_2 + iu_3 & -iu_1 \end{pmatrix},$$

if we write $\theta = \sqrt{u_1^2 + u_2^2 + u_3^2}$, then

$$e^A = \cos\theta I + \frac{\sin\theta}{\theta} A, \quad \theta \neq 0,$$

and $e^0 = I$.

Therefore, by the discussion at the end of the previous section, e^A is a unit quaternion representing the rotation of angle 2θ and axis (u_1, u_2, u_3) (or I when $\theta = k\pi$, $k \in \mathbb{Z}$). The above formula shows that we may assume that $0 \leq \theta \leq \pi$. Proposition 16.7 shows that the exponential yields a map $\exp\colon \mathfrak{su}(2) \to \mathbf{SU}(2)$. It is an analog of the exponential map $\exp\colon \mathfrak{so}(3) \to \mathbf{SO}(3)$.

Remark: Because $\mathfrak{so}(3)$ and $\mathfrak{su}(2)$ are real vector spaces of dimension 3, they are isomorphic, and it is easy to construct an isomorphism. In fact, $\mathfrak{so}(3)$ and $\mathfrak{su}(2)$ are isomorphic as Lie algebras, which means that there is a linear isomorphism preserving the the Lie bracket $[A, B] = AB - BA$. However, as observed earlier, the groups $\mathbf{SU}(2)$ and $\mathbf{SO}(3)$ are *not isomorphic*.

An equivalent, but often more convenient, formula is obtained by assuming that $u = (u_1, u_2, u_3)$ is a unit vector, equivalently $\det(A) = 1$, in which case $A^2 = -I$, so we have

$$e^{\theta A} = \cos\theta I + \sin\theta A.$$

Using the quaternion notation, this is read as

$$e^{\theta A} = [\cos\theta, \sin\theta\, u].$$

Proposition 16.8. *The exponential map* $\exp\colon \mathfrak{su}(2) \to \mathbf{SU}(2)$ *is surjective*

Proof. We give an algorithm to find the logarithm $A \in \mathfrak{su}(2)$ of a unit quaternion

$$q = \begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix}$$

with $\alpha = a + bi$ and $\beta = c + id$.

If $q = I$ (*i.e.* $a = 1$), then $A = 0$. If $q = -I$ (*i.e.* $a = -1$), then

$$A = \pm\pi \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}.$$

Otherwise, $a \neq \pm 1$ and $(b, c, d) \neq (0, 0, 0)$, and we are seeking some $A = \theta B \in \mathfrak{su}(2)$ with $\det(B) = 1$ and $0 < \theta < \pi$, such that, by Proposition 16.7,

$$q = e^{\theta B} = \cos\theta I + \sin\theta B.$$

Let

$$B = \begin{pmatrix} iu_1 & u_2 + iu_3 \\ -u_2 + iu_3 & -iu_1 \end{pmatrix},$$

with $u = (u_1, u_2, u_3)$ a unit vector. We must have

$$a = \cos\theta, \quad e^{\theta B} - (e^{\theta B})^* = q - q^*.$$

Since $0 < \theta < \pi$, we have $\sin\theta \neq 0$, and

$$2\sin\theta \begin{pmatrix} iu_1 & u_2 + iu_3 \\ -u_2 + iu_3 & -iu_1 \end{pmatrix} = \begin{pmatrix} \alpha - \overline{\alpha} & 2\beta \\ -2\overline{\beta} & \overline{\alpha} - \alpha \end{pmatrix}.$$

Thus, we get

$$u_1 = \frac{1}{\sin\theta} b, \quad u_2 + iu_3 = \frac{1}{\sin\theta}(c + id);$$

that is,

$$\begin{aligned} \cos\theta &= a \qquad (0 < \theta < \pi) \\ (u_1, u_2, u_3) &= \frac{1}{\sin\theta}(b, c, d). \end{aligned}$$

Since $a^2+b^2+c^2+d^2 = 1$ and $a = \cos\theta$, the vector $(b, c, d)/\sin\theta$ is a unit vector. Furthermore if the quaternion q is of the form $q = [\cos\theta, \sin\theta u]$ where $u = (u_1, u_2, u_3)$ is a unit vector (with $0 < \theta < \pi$), then

$$A = \theta \begin{pmatrix} iu_1 & u_2 + iu_3 \\ -u_2 + iu_3 & -iu_1 \end{pmatrix} \tag{$*_{\log}$}$$

is a logarithm of q. $\square$

Observe that not only is the exponential map $\exp\colon \mathfrak{su}(2) \to \mathbf{SU}(2)$ surjective, but the above proof shows that it is injective on the open ball

$$\{\theta B \in \mathfrak{su}(2) \mid \det(B) = 1, 0 \leq \theta < \pi\}.$$

Also, unlike the situation where in computing the logarithm of a rotation matrix $R \in \mathbf{SO}(3)$ we needed to treat the case where $\mathrm{tr}(R) = -1$ (the angle of the rotation is π) in a special way, computing the logarithm of a quaternion (other than $\pm I$) does not require any case analysis; no special case is needed when the angle of rotation is π.

16.6 Quaternion Interpolation ⊛

We are now going to derive a formula for interpolating between two quaternions. This formula is due to Ken Shoemake, once a Penn student and my TA! Since rotations in $\mathbf{SO}(3)$ can be defined by quaternions, this has applications to computer graphics, robotics, and computer vision.

First we observe that multiplication of quaternions can be expressed in terms of the inner product and the cross-product in $\mathbb{R}^3$. Indeed, if $q_1 = [a, u_1]$ and $q_2 = [a_2, u_2]$, it can be verified that

$$q_1 q_2 = [a_1, u_1][a_2, u_2] = [a_1 a_2 - u_1 \cdot u_2,\ a_1 u_2 + a_2 u_1 + u_1 \times u_2]. \tag{$*_{\text{mult}}$}$$

We will also need the identity

$$u \times (u \times v) = (u \cdot v)u - (u \cdot u)v.$$

Given a quaternion q expressed as $q = [\cos\theta, \sin\theta\, u]$, where u is a unit vector, we can interpolate between I and q by finding the logs of I and q, interpolating in $\mathfrak{su}(2)$, and then exponentiating. We have

$$A = \log(I) = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad B = \log(q) = \theta \begin{pmatrix} iu_1 & u_2 + iu_3 \\ -u_2 + iu_3 & -iu_1 \end{pmatrix},$$

and so $q = e^B$. Since $\mathbf{SU}(2)$ is a compact Lie group and since the inner product on $\mathfrak{su}(2)$ given by

$$\langle X, Y \rangle = \mathrm{tr}(X^\top Y)$$

is $\mathrm{Ad}(\mathbf{SU}(2))$-invariant, it induces a biinvariant Riemannian metric on $\mathbf{SU}(2)$, and the curve

$$\lambda \mapsto e^{\lambda B}, \quad \lambda \in [0, 1]$$

is a geodesic from I to q in $\mathbf{SU}(2)$. We write $q^\lambda = e^{\lambda B}$. Given two quaternions q_1 and q_2, because the metric is left invariant, the curve

$$\lambda \mapsto Z(\lambda) = q_1(q_1^{-1} q_2)^\lambda, \quad \lambda \in [0, 1]$$

is a geodesic from q_1 to q_2. Remarkably, there is a closed-form formula for the interpolant $Z(\lambda)$.

Say $q_1 = [\cos\theta, \sin\theta\, u]$ and $q_2 = [\cos\varphi, \sin\varphi\, v]$, and assume that $q_1 \neq q_2$ and $q_1 \neq -q_2$. First, we compute $q^{-1} q_2$. Since $q^{-1} = [\cos\theta, -\sin\theta\, u]$, we have

$$q^{-1} q_2 = [\cos\theta\cos\varphi + \sin\theta\sin\varphi(u \cdot v),\ -\sin\theta\cos\varphi\, u + \cos\theta\sin\varphi\, v - \sin\theta\sin\varphi(u \times v)].$$

Define Ω by

$$\cos\Omega = \cos\theta\cos\varphi + \sin\theta\sin\varphi(u \cdot v). \tag{$*_\Omega$}$$

Since $q_1 \neq q_2$ and $q_1 \neq -q_2$, we have $0 < \Omega < \pi$, so we get

$$q_1^{-1}q_2 = \left[\cos\Omega,\ \sin\Omega\,\frac{(-\sin\theta\cos\varphi\, u + \cos\theta\sin\varphi\, v - \sin\theta\sin\varphi(u \times v)}{\sin\Omega}\right],$$

where the term multiplying $\sin\Omega$ is a unit vector because q_1 and q_2 are unit quaternions, so $q_1^{-1}q_2$ is also a unit quaternion. By $(*_{\log})$, we have

$$(q_1^{-1}q_2)^\lambda = \left[\cos\lambda\Omega,\ \sin\lambda\Omega\,\frac{(-\sin\theta\cos\varphi\, u + \cos\theta\sin\varphi\, v - \sin\theta\sin\varphi(u \times v)}{\sin\Omega}\right].$$

Next we need to compute $q_1(q_1^{-1}q_2)^\lambda$. The scalar part of this product is

$$\begin{aligned} s = \cos\theta\cos\lambda\Omega + \frac{\sin\lambda\Omega}{\sin\Omega}\sin^2\theta\cos\varphi(u\cdot u) - \frac{\sin\lambda\Omega}{\sin\Omega}\sin\theta\sin\varphi\cos\theta(u\cdot v)& \\ + \frac{\sin\lambda\Omega}{\sin\Omega}\sin^2\theta\sin\varphi(u\cdot(u\times v)).& \end{aligned}$$

Since $u\cdot(u\times v) = 0$, the last term is zero, and since $u\cdot u = 1$ and

$$\sin\theta\sin\varphi(u\cdot v) = \cos\Omega - \cos\theta\cos\varphi,$$

we get

$$\begin{aligned} s &= \cos\theta\cos\lambda\Omega + \frac{\sin\lambda\Omega}{\sin\Omega}\sin^2\theta\cos\varphi - \frac{\sin\lambda\Omega}{\sin\Omega}\cos\theta(\cos\Omega - \cos\theta\cos\varphi) \\ &= \cos\theta\cos\lambda\Omega + \frac{\sin\lambda\Omega}{\sin\Omega}(\sin^2\theta + \cos^2\theta)\cos\varphi - \frac{\sin\lambda\Omega}{\sin\Omega}\cos\theta\cos\Omega \\ &= \frac{(\cos\lambda\Omega\sin\Omega - \sin\lambda\Omega\cos\Omega)\cos\theta}{\sin\Omega} + \frac{\sin\lambda\Omega}{\sin\Omega}\cos\varphi \\ &= \frac{\sin(1-\lambda)\Omega}{\sin\Omega}\cos\theta + \frac{\sin\lambda\Omega}{\sin\Omega}\cos\varphi. \end{aligned}$$

The vector part of the product $q_1(q_1^{-1}q_2)^\lambda$ is given by

$$\begin{aligned} \nu = -\frac{\sin\lambda\Omega}{\sin\Omega}\cos\theta\sin\theta\cos\varphi\, u + \frac{\sin\lambda\Omega}{\sin\Omega}\cos^2\theta\sin\varphi\, v - \frac{\sin\lambda\Omega}{\sin\Omega}\cos\theta\sin\theta\sin\varphi(u\times v)& \\ + \cos\lambda\Omega\sin\theta\, u - \frac{\sin\lambda\Omega}{\sin\Omega}\sin^2\theta\cos\varphi(u\times u) + \frac{\sin\lambda\Omega}{\sin\Omega}\cos\theta\sin\theta\sin\varphi(u\times v)& \\ - \frac{\sin\lambda\Omega}{\sin\Omega}\sin^2\theta\sin\varphi(u\times(u\times v)).& \end{aligned}$$

We have $u\times u = 0$, the two terms involving $u\times v$ cancel out,

$$u\times(u\times v) = (u\cdot v)u - (u\cdot u)v,$$

and $u \cdot u = 1$, so we get

$$\nu = -\frac{\sin\lambda\Omega}{\sin\Omega}\cos\theta\sin\theta\cos\varphi\, u + \cos\lambda\Omega\sin\theta\, u + \frac{\sin\lambda\Omega}{\sin\Omega}\cos^2\theta\sin\varphi\, v + \frac{\sin\lambda\Omega}{\sin\Omega}\sin^2\theta\sin\varphi\, v - \frac{\sin\lambda\Omega}{\sin\Omega}\sin^2\theta\sin\varphi(u\cdot v)u.$$

Using

$$\sin\theta\sin\varphi(u\cdot v) = \cos\Omega - \cos\theta\cos\varphi,$$

we get

$$\begin{aligned}
\nu &= -\frac{\sin\lambda\Omega}{\sin\Omega}\cos\theta\sin\theta\cos\varphi\, u + \cos\lambda\Omega\sin\theta\, u + \frac{\sin\lambda\Omega}{\sin\Omega}\sin\varphi\, v \\
&\quad - \frac{\sin\lambda\Omega}{\sin\Omega}\sin\theta(\cos\Omega - \cos\theta\cos\varphi)u \\
&= \cos\lambda\Omega\sin\theta\, u + \frac{\sin\lambda\Omega}{\sin\Omega}\sin\varphi\, v - \frac{\sin\lambda\Omega}{\sin\Omega}\sin\theta\cos\Omega\, u \\
&= \frac{(\cos\lambda\Omega\sin\Omega - \sin\lambda\Omega\cos\Omega)}{\sin\Omega}\sin\theta\, u + \frac{\sin\lambda\Omega}{\sin\Omega}\sin\varphi\, v \\
&= \frac{\sin(1-\lambda)\Omega}{\sin\Omega}\sin\theta\, u + \frac{\sin\lambda\Omega}{\sin\Omega}\sin\varphi\, v.
\end{aligned}$$

Putting the scalar part and the vector part together, we obtain

$$\begin{aligned}
q_1(q_1^{-1}q_2)^\lambda &= \left[\frac{\sin(1-\lambda)\Omega}{\sin\Omega}\cos\theta + \frac{\sin\lambda\Omega}{\sin\Omega}\cos\varphi,\ \frac{\sin(1-\lambda)\Omega}{\sin\Omega}\sin\theta\, u + \frac{\sin\lambda\Omega}{\sin\Omega}\sin\varphi\, v\right], \\
&= \frac{\sin(1-\lambda)\Omega}{\sin\Omega}[\cos\theta,\ \sin\theta\, u] + \frac{\sin\lambda\Omega}{\sin\Omega}[\cos\varphi,\ \sin\varphi\, v].
\end{aligned}$$

This yields the celebrated *slerp interpolation formula*

$$Z(\lambda) = q_1(q_1^{-1}q_2)^\lambda = \frac{\sin(1-\lambda)\Omega}{\sin\Omega}q_1 + \frac{\sin\lambda\Omega}{\sin\Omega}q_2,$$

with

$$\cos\Omega = \cos\theta\cos\varphi + \sin\theta\sin\varphi(u\cdot v).$$

16.7 Nonexistence of a "Nice" Section from $\mathbf{SO}(3)$ to $\mathbf{SU}(2)$

We conclude by discussing the problem of a consistent choice of sign for the quaternion q representing a rotation $R = \rho_q \in \mathbf{SO}(3)$. We are looking for a "nice" section $s\colon \mathbf{SO}(3) \to \mathbf{SU}(2)$, that is, a function s satisfying the condition

$$\rho\circ s = \mathrm{id},$$

where ρ is the surjective homomorphism $\rho\colon \mathbf{SU}(2) \to \mathbf{SO}(3)$.

Proposition 16.9. *Any section* $s\colon \mathbf{SO}(3) \to \mathbf{SU}(2)$ *of* ρ *is neither a homomorphism nor continuous.*

Intuitively, this means that there is no “nice and simple ” way to pick the sign of the quaternion representing a rotation.

The following proof is due to Marcel Berger.

Proof. Let Γ be the subgroup of $\mathbf{SU}(2)$ consisting of all quaternions of the form $q = [a,(b,0,0)]$. Then, using the formula for the rotation matrix R_q corresponding to q (and the fact that $a^2 + b^2 = 1$), we get

$$R_q = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2a^2 - 1 & -2ab \\ 0 & 2ab & 2a^2 - 1 \end{pmatrix}.$$

Since $a^2 + b^2 = 1$, we may write $a = \cos\theta, b = \sin\theta$, and we see that

$$R_q = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos 2\theta & -\sin 2\theta \\ 0 & \sin 2\theta & \cos 2\theta \end{pmatrix},$$

a rotation of angle 2θ around the x-axis. Thus, both Γ and its image are isomorphic to $\mathbf{SO}(2)$, which is also isomorphic to $\mathbf{U}(1) = \{w \in \mathbb{C} \mid |w| = 1\}$. By identifying $\mathbf{i}$ and i, and identifying Γ and its image to $\mathbf{U}(1)$, if we write $w = \cos\theta + i\sin\theta \in \Gamma$, the restriction of the map ρ to Γ is given by $\rho(w) = w^2$.

We claim that any section s of ρ is not a homomorphism. Consider the restriction of s to $\mathbf{U}(1)$. Then since $\rho \circ s = \mathrm{id}$ and $\rho(w) = w^2$, for $-1 \in \rho(\Gamma) \approx \mathbf{U}(1)$, we have

$$-1 = \rho(s(-1)) = (s(-1))^2.$$

On the other hand, if s is a homomorphism, then

$$(s(-1))^2 = s((-1)^2) = s(1) = 1,$$

contradicting $(s(-1))^2 = -1$.

We also claim that s is not continuous. Assume that $s(1) = 1$, the case where $s(1) = -1$ being analogous. Then s is a bijection inverting ρ on Γ whose restriction to $\mathbf{U}(1)$ must be given by

$$s(\cos\theta + i\sin\theta) = \cos(\theta/2) + \mathbf{i}\sin(\theta/2), \quad -\pi \leq \theta < \pi.$$

If θ tends to π, that is $z = \cos\theta + i\sin\theta$ tends to -1 in the upper-half plane, then $s(z)$ tends to $\mathbf{i}$, but if θ tends to $-\pi$, that is z tends to -1 in the lower-half plane, then $s(z)$ tends to $-\mathbf{i}$, which shows that s is not continuous. ∎

Another way (due to Jean Dieudonné) to prove that a section s of ρ is not a homomorphism is to prove that any unit quaternion is the product of two unit pure quaternions. Indeed, if $q = [a, u]$ is a unit quaternion, if we let $q_1 = [0, u_1]$, where u_1 is any unit vector orthogonal to u, then

$$q_1 q = [-u_1 \cdot u, au_1 + u_1 \times u] = [0, au_1 + u_1 \times u] = q_2$$

is a nonzero unit pure quaternion. This is because if $a \neq 0$ then $au_1 + u_1 \times u \neq 0$ (since $u_1 \times u$ is orthogonal to $au_1 \neq 0$), and if $a = 0$ then $u \neq 0$, so $u_1 \times u \neq 0$ (since u_1 is orthogonal to u). But then, $q_1^{-1} = [0, -u_1]$ is a unit pure quaternion and we have

$$q = q_1^{-1} q_2,$$

a product of two pure unit quaternions.

We also observe that for any two pure quaternions q_1, q_2, there is some unit quaternion q such that

$$q_2 = q q_1 q^{-1}.$$

This is just a restatement of the fact that the group $\mathbf{SO}(3)$ is transitive. Since the kernel of $\rho\colon \mathbf{SU}(2) \to \mathbf{SO}(3)$ is $\{I, -I\}$, the subgroup $s(\mathbf{SO}(3))$ would be a normal subgroup of index 2 in $\mathbf{SU}(2)$. Then we would have a surjective homomorphism η from $\mathbf{SU}(2)$ onto the quotient group $\mathbf{SU}(2)/s(\mathbf{SO}(3))$, which is isomorphic to $\{1, -1\}$. Now, since any two pure quaternions are conjugate of each other, η would have a constant value on the unit pure quaternions. Since $\mathbf{k} = \mathbf{ij}$, we would have

$$\eta(\mathbf{k}) = \eta(\mathbf{ij}) = (\eta(\mathbf{i}))^2 = 1.$$

Consequently, η would map all pure unit quaternions to 1. But since every unit quaternion is the product of two pure quaternions, η would map every unit quaternion to 1, contradicting the fact that it is surjective onto $\{-1, 1\}$.

16.8 Summary

The main concepts and results of this chapter are listed below:

- The group $\mathbf{SU}(2)$ of unit quaternions.
- The skew field $\mathbb{H}$ of quaternions.
- Hamilton's identities.
- The (real) vector space $\mathfrak{su}(2)$ of 2×2 skew Hermitian matrices with zero trace.
- The adjoint representation of $\mathbf{SU}(2)$.

- The (real) vector space $\mathfrak{su}(2)$ of 2×2 Hermitian matrices with zero trace.
- The group homomorphism $r\colon \mathbf{SU}(2) \to \mathbf{SO}(3)$; $\mathrm{Ker}\,(r) = \{+I, -I\}$.
- The matrix representation R_q of the rotation r_q induced by a unit quaternion q.
- Surjectivity of the homomorphism $r\colon \mathbf{SU}(2) \to \mathbf{SO}(3)$.
- The exponential map $\exp\colon \mathfrak{su}(2) \to \mathbf{SU}(2)$.
- Surjectivity of the exponential map $\exp\colon \mathfrak{su}(2) \to \mathbf{SU}(2)$.
- Finding a logarithm of a quaternion.
- Quaternion interpolation.
- Shoemake's slerp interpolation formula.
- Sections $s\colon \mathbf{SO}(3) \to \mathbf{SU}(2)$ of $r\colon \mathbf{SU}(2) \to \mathbf{SO}(3)$.

16.9 Problems

Problem 16.1. Verify the quaternion identities

$$\begin{aligned}
&\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = \mathbf{ijk} = -\mathbf{1},\\
&\mathbf{ij} = -\mathbf{ji} = \mathbf{k},\\
&\mathbf{jk} = -\mathbf{kj} = \mathbf{i},\\
&\mathbf{ki} = -\mathbf{ik} = \mathbf{j}.
\end{aligned}$$

Problem 16.2. Check that for every quaternion $X = a\mathbf{1} + b\mathbf{i} + c\mathbf{j} + d\mathbf{k}$, we have

$$XX^* = X^*X = (a^2 + b^2 + c^2 + d^2)\mathbf{1}.$$

Conclude that if $X \neq 0$, then X is invertible and its inverse is given by

$$X^{-1} = (a^2 + b^2 + c^2 + d^2)^{-1}X^*.$$

Problem 16.3. Given any two quaternions $X = a\mathbf{1}+b\mathbf{i}+c\mathbf{j}+d\mathbf{k}$ and $Y = a'\mathbf{1}+b'\mathbf{i}+c'\mathbf{j}+d'\mathbf{k}$, prove that

$$\begin{aligned}
XY = {} & (aa' - bb' - cc' - dd')\mathbf{1} + (ab' + ba' + cd' - dc')\mathbf{i}\\
& + (ac' + ca' + db' - bd')\mathbf{j} + (ad' + da' + bc' - cb')\mathbf{k}.
\end{aligned}$$

Also prove that if $X = [a, U]$ and $Y = [a', U']$, the quaternion product XY can be expressed as

$$XY = [aa' - U \cdot U',\ aU' + a'U + U \times U'].$$