MATHEMATICAL METHODS IN THE APPLIED SCIENCES
Math. Meth. Appl. Sci. 2005; **28**:101–126
Published online 5 November 2004 in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/mma.560
MOS subject classification: 15 A 66; 51 M 15; 58 D 15; 44 A 12

A concise quaternion geometry of rotations

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Communicated by W. Sprößig

SUMMARY

This communication compiles propositions concerning the spherical geometry of rotations when represented by unit quaternions. The propositions are thought to establish a two-way correspondence between geometrical objects in the space of real unit quaternions representing rotations and geometrical objects constituted by directions in the three-dimensional space subjected to these rotations. In this way a purely geometrical proof of the spherical Ásgeirsson's mean value theorem and a geometrical interpretation of integrals related to the spherical Radon transform of a probability density functions of unit quaternions are accomplished. Copyright © 2004 John Wiley & Sons, Ltd.

1. INTRODUCTION

The background of this communication is in crystallography, in particular in patterns of preferred crystallographic orientations of crystals within a polycrystalline specimen. Neglecting crystal symmetry for the sake of simplicity, a crystallographic orientation is a rotation. Thus the focus is on even probability density functions f defined on the sphere[‡] $\mathbb{S}^3 \subset \mathbb{R}^4$ in four-dimensional space $\mathbb{R}^4$ when rotations are represented by unit quaternions. A useful spherical distribution for this purpose is the Bingham distribution and its special cases which provide a characterization of distinct patterns of preferred crystallographic orientation [1,2]. Since a distribution on $\mathbb{S}^3$ is hard to visualize and grasp, it proved helpful to look at the distribution of unit vectors $\mathbf{h} \in \mathbb{S}^2 \subset \mathbb{R}^3$ which have been subjected to random rotations $q \in \mathbb{S}^3$ with a given—say Bingham—distribution f ([3,4]). The distribution of these unit vectors is actually given in terms of the spherical $\mathscr{R}$ Radon transform $\mathscr{R}f$ of the probability density function f.

Let SO(3) denote the special orthogonal group of proper rotations $\boldsymbol{g}$ in $\mathbb{R}^3$. Since in the context of crystallography normal unit vectors of lattice planes are subjected to rota-

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‡Incompatible conventions for the meaning of '*n*-sphere' are used in geometry and topology. We use the topological definition.

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Received 7 January 2004

tions, considerations are confined to the unit sphere $\mathbb{S}^2 \subset \mathbb{R}^3$ in three-dimensional space $\mathbb{R}^3$.

Let $f : \mathrm{SO}(3) \mapsto [0, \infty)$ be a probability density function of a random rotation $\boldsymbol{g} \in \mathrm{SO}(3)$. For any given direction $\mathbf{h} \in \mathbb{S}^2$ the probability density function of coincidence of the random direction $\boldsymbol{g}\mathbf{h} \in \mathbb{S}^2$ with a given direction $\mathbf{r} \in \mathbb{S}^2$ is provided by

$$(\mathscr{R} f)(\mathbf{h}, \mathbf{r}) = \frac{1}{2\pi} \int_{G(\mathbf{h},\mathbf{r})} f(\boldsymbol{g}) \, \mathrm{d}\boldsymbol{g}$$

with fibres

$$G(\mathbf{h}, \mathbf{r}) = \{\boldsymbol{g} \in \mathrm{SO}(3) \,|\, \boldsymbol{g}\,\mathbf{h} = \mathbf{r}\}$$

inducing a double fibration of SO(3).

In practice, the inverse problem arises and may be specified as to which extent and for which assumptions is it possible to determine a reasonable approximation of f globally on SO(3) or locally in a neighbourhood $\mathscr{U}(\boldsymbol{g}_0) \subset \mathrm{SO}(3)$ numerically from data sampled from $(\mathscr{R} f)(\mathbf{h}, \mathbf{r})$.

It is well-known that a rotation $\boldsymbol{g}$ mapping the unit vector $\mathbf{h} \in \mathbb{S}^2$ onto the unit vector $\mathbf{r} \in \mathbb{S}^2$ according to $\boldsymbol{g}\,\mathbf{h} = \mathbf{r}$ may be represented by its corresponding (3×3) orthogonal matrix $M(\boldsymbol{g})$ or by its corresponding real quaternion $q(\boldsymbol{g})$. The quaternion representation has some clear advantages which have been discussed by many authors.

In the present communication we pursue geometry in quaternion space $\mathbb{H}$, in particular we consider geometrical objects in the space of real unit quaternions representing rotations with respect to geometrical objects in three-dimensional space of unit vectors being subjected to these rotations. We show, for instance, that the set of quaternions mapping a unit vector onto another one is a circle, and that the set of quaternions mapping a unit vector onto a small circle is a torus, and more generally that there is a correspondence between objects like circle, sphere, and torus of unit quaternions in $\mathbb{S}^3$ representing rotations and objects like point and circle of unit vectors in $\mathbb{S}^2$.

Our geometrical approach leads to an alternative proof of a spherical variant of Ásgeirsson's mean value theorem [5], and to clarifications of the interpretation of some integrals related to the spherical Radon transform [6] of probability density functions of unit quaternions.

We use the symbol $\square$ to mark the end of proofs.

2. NOTATION

The algebra of real quaternions $\mathbb{H}$ is the tuple of $\mathbb{R}^4$ endowed with the operation of quaternion multiplication; furtheron, $\mathbb{H}$ is referred to as skew-field of real quaternions. Its exposition follows References [7–9].

2.1. *Skew-field of real quaternions*

An arbitrary quaternion $q \in \mathbb{H}$ is composed of its scalar and vector part

$$q = q_0 + \mathbf{q} = \mathrm{Sc}q + \mathrm{Vec}q$$

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with $\mathbf{q} = \sum_{i=1}^{3} q^i e_i = \mathrm{Vec}q$ and $q_0 = \mathrm{Sc}q$, where Vec$q$ denotes the vector part of q, and Scq denotes the scalar part of q. The basis elements $e_i,\ i = 1,2,3$, fulfil the relations

(i) $e_i^2 = -1,\ i = 1,2,3;$
(ii) $e_1 e_2 = e_3,\ e_2 e_3 = e_1,\ e_3 e_1 = e_2;$
(iii) $e_i e_j + e_j e_i = 0,\ i,j = 1,2,3;\ i \neq j.$

If $\mathrm{Sc}q = 0$, then q is called a pure quaternion, the subset of all pure quaternions is denoted $\mathrm{Vec}\mathbb{H}$. For $q \in \mathrm{Vec}\mathbb{H}$, q and $\mathbf{q}$ are identified, i.e. $q = \mathbf{q}$. The subset of all scalars may be denoted $\mathrm{Sc}\mathbb{H}$. In this way $\mathbb{R}$ and $\mathbb{R}^3$ are embedded in $\mathbb{H}$.

Given two quaternions, $p, q \in \mathbb{H}$, their product according to the algebraic rules of multiplications given above is

$$pq = p_0 q_0 - \mathbf{p} \cdot \mathbf{q} + p_0 \mathbf{q} + q_0 \mathbf{p} + \mathbf{p} \times \mathbf{q}$$

where $\mathbf{p} \cdot \mathbf{q}$ and $\mathbf{p} \times \mathbf{q}$ represent the standard inner and cross product in $\mathbb{R}^3$; thus

$$\begin{aligned} \mathrm{Sc}(pq) &= p_0 q_0 - \mathbf{p} \cdot \mathbf{q} \\ \mathrm{Vec}(pq) &= p_0 \mathbf{q} + q_0 \mathbf{p} + \mathbf{p} \times \mathbf{q} \end{aligned} \tag{1}$$

Quaternion multiplication reduces for pure quaternions $p, q \in \mathrm{Vec}\mathbb{H}$ to

$$pq = \mathbf{pq} = -\mathbf{p} \cdot \mathbf{q} + \mathbf{p} \times \mathbf{q} \tag{2}$$

and thus

$$\mathrm{Sc}(pq) = \mathrm{Sc}(\mathbf{pq}) = -\mathbf{p} \cdot \mathbf{q}$$

$$\mathrm{Vec}(pq) = \mathrm{Vec}(\mathbf{pq}) = \mathbf{p} \times \mathbf{q}$$

2.2. Conjugation of a real quaternion

The quaternion $q^* = \mathrm{Sc}q - \mathrm{Vec}q$ is called the conjugate of q. With conjugated quaternions it is possible to represent the scalar and vector part in an algebraic fashion as

$$q_0 = \mathrm{Sc}q = \tfrac{1}{2}(q + q^*) \tag{3}$$

$$\mathbf{q} = \mathrm{Vec}q = \tfrac{1}{2}(q - q^*) \tag{4}$$

Since

$$\mathrm{Vec}q^* = -\mathrm{Vec}q$$

conjugation of pure quaternions $q \in \mathrm{Vec}\mathbb{H}$ means change of sign, i.e. $q^* = \mathbf{q}^* = -\mathbf{q} = -q$. Therefore, for arbitrary pure quaternions we have

$$\mathrm{Sc}(pq^*) = \mathbf{p} \cdot \mathbf{q} = -\frac{1}{2}(pq + qp)$$

$$\mathrm{Vec}(pq^*) = -\mathbf{p} \times \mathbf{q} = -\frac{1}{2}(pq - qp)$$

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2.3. Norm of a real quaternion

It holds that

$$qq^* = q^*q = \|q\|^2 = q_0^2 + (q^1)^2 + (q^2)^2 + (q^3)^2$$

and the number $\|q\|$ is called the norm of q. The norm of quaternions coincides with the Euclidean norm of q regarded as an element of the vector space $\mathbb{R}^4$. The usual Euclidean inner product in the space $\mathbb{R}^4$ corresponds to the scalar part of pq^*, i.e. considering quaternions as vectors in $\mathbb{R}^4$, one gets

$$p \cdot q = \mathrm{Sc}(pq^*)$$

It holds that $(pq)^* = q^* p^*$, and therefore $\|pq\| = \|p\| \, \|q\|$.

A quaternion q with $\|q\| = 1$ is called a unit quaternion. Furthermore, let $\mathbb{S}^2$ denote the unit sphere in $\mathrm{Vec}\mathbb{H} \simeq \mathbb{R}^3$ of all unit vectors, and $\mathbb{S}^3$ the sphere in $\mathbb{H} \simeq \mathbb{R}^4$ of all unit quaternions.

In complete analogy to $\mathbb{S}^3 \subset \mathbb{R}^4$, $\mathrm{Sc}(pq^*)$ provides a canonical measure for the spherical distance of unit quaternions $p, q \in \mathbb{S}^3$ in terms of their enclosed angle.

2.4. Inverse of a real quaternion

Moreover, each non-zero quaternion q has a unique inverse $q^{-1} = q^*/\|q\|^2$ with $\|q^{-1}\| = \|q\|^{-1}$. For unit quaternions it is $q^{-1} = q^*$; for pure unit quaternions it is $q^{-1} = -q$, implying $qq = -1$.

2.5. Orthogonality of real quaternions

Since orthogonality of unit quaternions will provide essential arguments throughout the paper, we shall give its formal definition.

Definition 1
Two quaternions $p, q \in \mathbb{H}$ are said to be orthogonal if pq^* is a pure quaternion. If p, q are orthogonal unit quaternions, they are called orthonormal quaternions.

The condition of orthogonality means that $pq^* \in \mathrm{Vec}\mathbb{H}$, or due to Equation (3)

$$\mathrm{Sc}(pq^*) = \tfrac{1}{2}(pq^* + qp^*) = 0$$

It is emphasized that pure quaternions with orthogonal vector parts are orthogonal, but that the inverse is not generally true. Orthogonality of two quaternions does not imply orthogonality of their vector parts unless they are pure quaternions.

If the pure quaternions p, q are orthogonal, then their multiplication simplifies further to

$$pq = \mathbf{p} \times \mathbf{q}$$

Proposition 1
Two unit quaternions $p, q \in \mathbb{S}^3$ are orthogonal, if and only if $p = vq$, where v is a pure unit quaternion.

Proof
If p and q are orthogonal, then pq^* is a pure quaternion, say v, for some $\mathbf{v} \in \mathbb{S}^2$. Hence, $p = vq \in \mathbb{S}^2 q$. The inverse is evident. □

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2.6. Representation of real quaternions

An arbitrary quaternion $q \neq 0$ permits the representation

$$q = \|q\| \left(\frac{q_0}{\|q\|} + \frac{\mathbf{q}}{\|\mathbf{q}\|} \frac{\|\mathbf{q}\|}{\|q\|} \right) = \|q\| \left(\cos \frac{\omega}{2} + \frac{\mathbf{q}}{\|\mathbf{q}\|} \sin \frac{\omega}{2} \right)$$

with $\omega = 2 \arccos(q_0/\|q\|)$, and $\|\mathbf{q}\|^2 = \mathbf{q}\mathbf{q}^*$ considering $\mathbf{q}$ as a pure quaternion. For an arbitrary unit quaternion the representation

$$q = \cos \frac{\omega}{2} + \mathbf{n} \sin \frac{\omega}{2} \tag{5}$$

with the normalized vector part $\mathbf{n} = \mathbf{q}/\|\mathbf{q}\| \in \mathbb{S}^2$ will often be applied in the context of rotations, where $\mathbf{n} \in \mathbb{S}^2$ denotes the axis and ω the angle of a counter-clockwise rotation about $\mathbf{n}$.

2.7. Quaternion representation of rotations in $\mathbb{R}^3$

Any active rotation $\boldsymbol{g} \in \mathrm{SO}(3)$ mapping the unit vector $\mathbf{h} \in \mathbb{S}^2$ onto the unit vector $\mathbf{r} \in \mathbb{S}^2$ according to

$$\boldsymbol{g}\,\mathbf{h} = \mathbf{r}$$

can be written in terms of its quaternion representation $q \in \mathbb{H}$ as

$$q(\boldsymbol{g})\mathbf{h}\, q^{-1}(\boldsymbol{g}) = \mathbf{r} \tag{6}$$

equivalent to $q(\boldsymbol{g})\,\mathbf{h} - \mathbf{r}q(\boldsymbol{g}) = 0$, where quaternion multiplication applies. To perform quaternion multiplication, $\mathbf{h}$ and $\mathbf{r}$ must be read as pure quaternions, i.e. they must be augmented with a zero scalar quaternion part; then Equation (6) reads

$$qhq^{-1} = r \tag{7}$$

Moreover, for $q \in \mathbb{S}^3$ the previous expression becomes

$$qhq^* = r$$

which explicitly reads then [7]

$$\mathbf{r} = \mathbf{h} \cos \omega + (\mathbf{n} \times \mathbf{h}) \sin \omega + (\mathbf{n} \cdot \mathbf{h})\mathbf{n}(1 - \cos \omega) \tag{8}$$

where the representation of Equation (5) has been applied.[§]

The unit quaternion $q \in \mathbb{S}^3$ represents the rotation about the unit axis $\mathbf{q}/\|\mathbf{q}\|, \mathbf{q} \neq 0$, by the angle $\omega = 2 \arccos(q_0)$. Therefore, each unit quaternion $q \in \mathbb{S}^3$ can be seen as a representation of a rotation in $\mathbb{R}^3$, i.e. $\mathbb{S}^3$ stands for a double covering of the group SO(3). It is emphasized that $\mathbb{S}^2 \subset \mathrm{Vec}\mathbb{H}$ consists of all quaternions representing rotations by the angle π about arbitrary axes, as every unit vector $\mathbf{q}$ can be considered as the pure quaternion $q = \cos(\pi/2) + \mathbf{q} \sin(\pi/2)$.

[§]Nice proofs that Equation (7) actually represents a rotation can be found, for instance, at http://www.cs.berkeley.edu/ laura/cs184/quat/quatproof.html.

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The unit quaternion q^* represents the inverse rotation $\boldsymbol{g}^{-1}\mathbf{r} = \mathbf{h}$, either by the angle $2\pi - \omega$ or by the angle $-\omega$, respectively, and the axis $\mathbf{n}$, or by the angle ω and the axis $-\mathbf{n}$.

Proposition 2
Let $p, q \in \mathbb{S}^3$ be arbitrary unit quaternions, where q represents the rotation about the axis $\mathbf{n}$ by the angle ω according to Equation (5). Then the quaternion $pqp^* \in \mathbb{S}^3$ represents the rotation about the rotated axes $p\,\mathbf{n}\,p^* \in \mathbb{S}^2$ by the same angle ω.

Proof
It simply holds that

$$pqp^* = p\left(\cos\frac{\omega}{2} + \mathbf{n}\sin\frac{\omega}{2}\right)p^* = \cos\frac{\omega}{2} + p\mathbf{n}p^*\sin\frac{\omega}{2} \tag{9}$$

□

The left-hand side of Equation (9) is referred to as representing the conjugation of rotations.

In terms of passive rotations, $q\mathbf{h}q^{-1}$ provides the coordinate transformation of a unique vector $\mathbf{h}_{K_{\mathscr{C}}}$ with respect to the (crystal) co-ordinate system $K_{\mathscr{C}}$ and $\mathbf{r} = \mathbf{h}_{K_{\mathscr{S}}}$ with respect to the (specimen) coordinate system $K_{\mathscr{S}}$ if the coordinate systems are related to each other by $\boldsymbol{g} : K_{\mathscr{S}} \mapsto K_{\mathscr{C}}$.

Henceforward, no distinction will be made between the rotation $\boldsymbol{g}$ and its (up to the sign) unique quaternion representation q. In the same way, a unit vector $\mathbf{x} \in \mathbb{S}^2 \subset \mathrm{Vec}\mathbb{H}$ is identified with its corresponding pure unit quaternion $x \in \mathbb{S}^3 \subset \mathbb{H}$, for which the rules of quaternion multiplication apply.

3. CORRESPONDENCE OF GEOMETRICAL OBJECTS OF $\mathbb{S}^3 \subset \mathbb{H}$ AND GEOMETRICAL OBJECTS OF $\mathbb{S}^2 \subset \mathbb{R}^3$ IN TERMS OF ROTATIONS

3.1. Mapping a given vector onto another one

We shall start with the geometric interpretation of the well-known problem to find all rotations which map a given unit vector onto another one. This problem arises in different areas of applied sciences like crystallography, robotic, photogrammetry, navigation, calibration of measurement equipment, image recognition, computer games, etc. Many authors tackled the problem using features of their application. A review of three methods of solution: an algebraic method, a geometric method, and the method of conditional extrema is given, for instance, in Reference [10]. Here, we pursue the geometric approach to the problem based on the orthogonality of quaternions.

We begin with the following definition.

Definition 2
Let q_1 and q_2 be two orthogonal unit quaternions. The set of quaternions

$$q(t) = q_1\cos t + q_2\sin t, \quad t \in [0, 2\pi) \tag{10}$$

is called a circle in the space of quaternions and is denoted $C(q_1, q_2)$.

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Obviously, the circle $C(q_1,q_2)$ is the intersection of the plane $E(q_1,q_2)=\langle q_1,q_2\rangle \subset \mathbb{H}$ spanned by q_1,q_2 and passing through the origin $\mathcal{O}$ with the unit sphere $\mathbb{S}^3 \subset \mathbb{H}$, i.e. $C(q_1,q_2)=E(q_1,q_2)\cap \mathbb{S}^3$.

Proposition 3
Given a pair of unit vectors $(\mathbf{h},\mathbf{r})\in\mathbb{S}^2\times\mathbb{S}^2$ with $\mathbf{h}\times\mathbf{r}\neq 0$, the set $G(\mathbf{h},\mathbf{r})\subset \mathrm{SO}(3)$ of all rotations with $\boldsymbol{g}\,\mathbf{h}=\mathbf{r}$ may be represented as a circle $C(q_1,q_2)$ of unit quaternions such that

$$q\mathbf{h}q^*=\mathbf{r},\ \ \forall\ q\in C(q_1,q_2) \tag{11}$$

with orthogonal quaternions

$$q_1 := \frac{1}{\|1-rh\|}(1-rh)=\cos\frac{\eta}{2}+\frac{\mathbf{h}\times\mathbf{r}}{\|\mathbf{h}\times\mathbf{r}\|}\sin\frac{\eta}{2} \tag{12}$$

$$q_2 := \frac{1}{\|h+r\|}(h+r)=0+\frac{\mathbf{h}+\mathbf{r}}{\|\mathbf{h}+\mathbf{r}\|} \tag{13}$$

where η denotes the angle between $\mathbf{h}$ and $\mathbf{r}$, and

$$\|1-rh\|=\sqrt{2(1+\cos\eta)}=2\cos\frac{\eta}{2} \tag{14}$$

$$\|h+r\|=2\cos\frac{\eta}{2} \tag{15}$$

Proof
By geometrical reasoning (see Figure 1) it can be seen that the axis of any rotation $\boldsymbol{g}\mathbf{h}=\mathbf{r}$ is in the plane spanned by

$$\mathbf{n}_1 := \frac{\mathbf{h}\times\mathbf{r}}{\|\mathbf{h}\times\mathbf{r}\|}=\frac{1}{\sin\eta}(\mathbf{h}\times\mathbf{r}) \tag{16}$$

$$\mathbf{n}_2 := \frac{\mathbf{h}+\mathbf{r}}{\|\mathbf{h}+\mathbf{r}\|}=\frac{1}{2\cos(\eta/2)}(\mathbf{h}+\mathbf{r}) \tag{17}$$

The plane $E(\mathbf{n}_1,\mathbf{n}_2)=\langle\mathbf{n}_1,\mathbf{n}_2\rangle\subset\mathbb{R}^3$ of rotation axes is uniquely given by its unit normal

$$\mathbf{n}_1\times\mathbf{n}_2=\frac{1}{2\sin(\eta/2)}(\mathbf{r}-\mathbf{h}) \tag{18}$$

The angles of rotations about the axes $\mathbf{n}_1$ and $\mathbf{n}_2$ are η and π, respectively. The quaternions representing these rotations are

$$\begin{aligned} q_1 &= \cos\frac{\eta}{2}+\mathbf{n}_1\sin\frac{\eta}{2}\\ q_2 &= \mathbf{n}_2 \end{aligned} \tag{19}$$

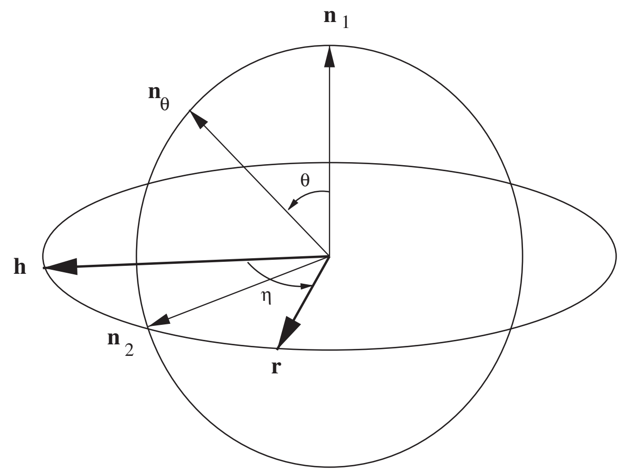

Figure 1. Axes of rotations $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_\theta$.

respectively. Clearly, q_1 and q_2 are orthogonal quaternions, as their vector parts are orthogonal and the scalar part of q_2 is zero.

The normalized axis $\mathbf{n}_\theta$ of any rotation $\boldsymbol{g}\mathbf{h} = \mathbf{r}$, i.e. the normalized vector part of a unit quaternion q with $q\mathbf{h}q^* = \mathbf{r}$, is an element of the circle $C(\mathbf{n}_1, \mathbf{n}_2) = E(\mathbf{n}_1, \mathbf{n}_2) \cap \mathbb{S}^2$. The corresponding angle ω_θ of rotation varies between η and $2\pi - \eta$. Thus

$$G(\mathbf{h}, \mathbf{r}) = \{\boldsymbol{g}_\theta \in \mathrm{SO}(3); \boldsymbol{g}_\theta = \boldsymbol{g}(\omega_\theta, \mathbf{n}_\theta)\} \tag{20}$$

where the axis of rotation $\mathbf{n}_\theta$ is

$$\mathbf{n}_\theta = \mathbf{n}_1 \cos\,\theta + \mathbf{n}_2 \sin\,\theta, \quad \theta \in [0, 2\pi) \tag{21}$$

and θ is the angle between the axis $\mathbf{n}_\theta$ and $\mathbf{n}_1$, i.e. $\cos\,\theta = \mathbf{n}_\theta \cdot \mathbf{n}_1$, see Figure 1.

The angle of rotation ω_θ is related to $\mathbf{n}_\theta$ [11] by

$$\tan\,\frac{\omega_\theta}{2} = \frac{\sin(\eta/2)}{\cos\,\theta\,\cos(\eta/2)} \tag{22}$$

Then the set of unit quaternions $q(\theta)$ defined as

$$q(\theta) = \cos\,\frac{\omega_\theta}{2} + \mathbf{n}_\theta \sin\,\frac{\omega_\theta}{2} \tag{23}$$

represents the set of all required rotations.

Let us show now that $q(\theta) \in C(q_1, q_2)$. Indeed, based on the trigonometric relations for an arbitrary φ

$$\tan\,\varphi = \frac{a}{b}; \;\; \sin\,\varphi = \frac{a}{\sqrt{a^2 + b^2}}; \;\; \cos\,\varphi = \frac{b}{\sqrt{a^2 + b^2}}$$

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with signs of $\sin\varphi$ and $\cos\varphi$ depending on φ, due to (22) we can write

$$\begin{aligned}\sin\frac{\omega_\theta}{2} &= \frac{\sin(\eta/2)}{(\sin^2(\eta/2)+\cos^2(\eta/2)\cos^2\theta)^{1/2}}\\ \cos\frac{\omega_\theta}{2} &= \frac{\cos\theta\cos(\eta/2)}{(\sin^2(\eta/2)+\cos^2(\eta/2)\cos^2\theta)^{1/2}}\end{aligned} \tag{24}$$

Substituting (21) and (24) in (23) and rearrangement gives

$$\begin{aligned}q(\theta) &= \left(\cos\frac{\eta}{2}+\mathbf{n}_1\sin\frac{\eta}{2}\right)\frac{\cos\theta}{(\sin^2(\eta/2)+\cos^2(\eta/2)\cos^2\theta)^{1/2}}\\ &\quad +\mathbf{n}_2\frac{\sin\theta\sin(\eta/2)}{(\sin^2(\eta/2)+\cos^2(\eta/2)\cos^2\theta)^{1/2}}\\ &= q_1 a_1(\theta)+q_2 a_2(\theta)\end{aligned} \tag{25}$$

Direct calculations give $a_1^2(\theta)+a_2^2(\theta)=1$ for every θ, hence we can introduce a new parameter $t\in[0,2\pi)$ such that $\cos t=a_1(\theta)$ and $\sin t=a_2(\theta)$ and rewrite Equation (25) as follows

$$q(t)=q_1\cos t+q_2\sin t,\quad t\in[0,2\pi). \tag{26}$$

Thus we conclude that the circle $C(q_1,q_2)$ corresponding to Equation (26) represents all rotations mapping $\mathbf{h}$ on $\mathbf{r}$, and obviously $q(0)=q_1$ and $q(\pi/2)=q_2$.

The case $\mathbf{r}=-\mathbf{h}$ must be considered separately. All rotations q with $q\mathbf{h}q^*=-\mathbf{h}$ are provided by rotations with their axes in the orthogonal complement $\mathbf{h}^\perp\cap\mathbb{S}^2$ of $\mathbf{h}$, which again represents a circle, and their angles constantly equal to π. □

Some useful equalities follow. Since r and h are pure unit quaternions, we get

$$r(1-rh)=(1-rh)h=h+r,$$

and obviously, $\|1-rh\|=\|h+r\|$. Then with Equation (12) and Equation (13)

$$rq_1=q_1h=q_2, \tag{27}$$

i.e. rq_1 and q_1h also represent rotations mapping $\mathbf{h}$ onto $\mathbf{r}$. Moreover, it should be noted that Equation (27) implies

$$q_2^*rq_1=1 \tag{28}$$

$$q_1hq_2^*=1 \tag{29}$$

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which may be interpreted as a remarkable 'factorization' of 1. It follows also from Equation (27) that

$$h = q_1^* q_2 \tag{30}$$

$$r = q_2 q_1^* \tag{31}$$

It can be easily proved by straightforward quaternion calculations that if an arbitrary quaternion $q \in C(q_1, q_2)$ is given, then rq and qh also represent rotations mapping $\mathbf{h}$ onto $\mathbf{r}$, and so does rqh, too. Moreover, with the unit quaternions

$$h(t) := \cos\frac{t}{2} + \mathbf{h}\sin\frac{t}{2}, \quad t \in [0, 2\pi) \tag{32}$$

$$r(t) := \cos\frac{t}{2} + \mathbf{r}\sin\frac{t}{2}, \quad t \in [0, 2\pi) \tag{33}$$

the elements of circle $C(q_1, q_2)$ can obviously be factorized by virtue of

$$C(q_1, q_2) = \{qh(t); q \in C(q_1, q_2), t \in [0, 2\pi)\} \tag{34}$$

$$C(q_1, q_2) = \{r(t)q; q \in C(q_1, q_2), t \in [0, 2\pi)\} \tag{35}$$

This factorization will prove useful for a unique specification of a rotation mapping $\mathbf{h}$ onto $\mathbf{r}$ as required in an advanced visualization approach suggested in References [3,4].

More generally, a quaternion $q(t) \in C(q_1, q_2)$ can be represented by

$$q(t) = p_2 v(t) p_1, \quad t \in [0, 2\pi) \tag{36}$$

where (i) $p_1 \in \mathbb{S}^3$ is any fixed quaternion such that $p_1 \mathbf{h} p_1^* = \mathbf{v}$ with an arbitrarily given unit vector $\mathbf{v} \in \mathbb{S}^2$, (ii) $v(t) := \cos t/2 + \mathbf{v}\sin t/2 \in \mathbb{S}^3$ such that $v(t)\mathbf{v}v^*(t) = \mathbf{v}$, and (iii) $p_2 \in \mathbb{S}^3$ is any fixed quaternion such that $p_2 \mathbf{v} p_2^* = \mathbf{r}$.

The inverse assertion to Proposition 3 is also true.

Proposition 4

Let $C(q_1, q_2)$ denote the circle with centre $\mathcal{O}$ in the plane $E(q_1, q_2) \subset \mathbb{H}$ spanned by the orthonormal quaternions $q_1, q_2 \in \mathbb{S}^3$. Then there exists a pair of unit vectors $(\mathbf{h}, \mathbf{r}) \in \mathbb{S}^2 \times \mathbb{S}^2$ such that

$$q\mathbf{h}q^* = \mathbf{r} \ \forall \ q \in C(q_1, q_2) \tag{37}$$

and $C(q_1, q_2)$ is the set of all rotations mapping $\mathbf{h}$ to $\mathbf{r}$. The pair of unit vectors is unique up to the common sign of $\mathbf{h}$ and $\mathbf{r}$, because $q(-\mathbf{h})q^* = -\mathbf{r}$ if and only if $q\mathbf{h}q^* = \mathbf{r}$.

Proof

The circle $C(q_1, q_2)$ with the centre $\mathcal{O}$ is given by Equation (26). Since q_1 and q_2 are orthogonal quaternions, $\mathrm{Sc}(q_1 q_2^*) = \mathrm{Sc}(q_2 q_1^*) = 0$. Then, the circle $C(q_1, q_2)$ represents the set of all

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rotations mapping the vector $\mathbf{h} = q_1^* q_2$ on the vector $\mathbf{r} = q_2 q_1^*$. In fact, for every $q(t) \in C(q_1, q_2)$ it holds $\|q(t)\|^2 = q^*(t)q(t) = 1$ and

$$\begin{aligned} q(t)hq^*(t) &= (q_1 \cos t + q_2 \sin t)q_1^* q_2 (q_1^* \cos t + q_2^* \sin t) \\ &= q_2 q_1^* \cos^2 t + q_2 q_1^* q_2 q_1^* \sin t \cos t + \sin t \cos t + q_2 q_1^* \sin^2 t \\ &= q_2 q_1^* = r \end{aligned}$$

Here we used that for orthogonal quaternions $q_2 q_1^* = -q_1 q_2^*$ holds, hence $q_2 q_1^* q_2 q_1^* = -1$. □

It should be noted that a one-to-one relationship exists between a circle $C = E \cap \mathbb{S}^3$ and a pair $\mathbf{h}, \mathbf{r}$ of unit vectors. However, since the circle may be represented as being spanned by a different pair of unit quaternions in the plane E, different pairs of spanning quaternions may be related to the same pair of unit vectors $\mathbf{h}, \mathbf{r}$.

Even though the sets $G(\mathbf{h}, \mathbf{r})$ and $G(\mathbf{r}, \mathbf{h})$ have the same set of rotation axes and the same interval of rotation angles in common, they are not equal because the association of axes and angles is reversed. Therefore, $C(q_1, q_2)$ representing $G(\mathbf{h}, \mathbf{r})$ is not equal to $C(q_1^*, q_2^*) = C^*(q_1, q_2)$ representing $G(\mathbf{r}, \mathbf{h})$.

Proposition 5

The two circles $C(q_1, q_2)$ and $C(q_3, q_4)$ representing the sets of rotations $G(\mathbf{h}, \mathbf{r})$ and $G(-\mathbf{h}, \mathbf{r})$, respectively, are orthonormal to one another.

Proof

It was shown above in Proposition 3 that q_1 and q_2 are defined by Equation (19), and the circle $C(q_3, q_4)$ represents all rotations mapping $-\mathbf{h}$ into $\mathbf{r}$ with

$$\begin{aligned} q_3 &:= \frac{1 + rh}{\|1 + rh\|} = \cos \frac{\pi - \eta}{2} + \mathbf{n}_3 \sin \frac{\pi - \eta}{2} \\ q_4 &:= \frac{-h + r}{\| -h + r\|} = \mathbf{n}_4 \end{aligned} \tag{38}$$

From geometrical reasons, it is clear that

$$\begin{aligned} \mathbf{n}_3 &:= \frac{-\mathbf{h} \times \mathbf{r}}{\| -\mathbf{h} \times \mathbf{r}\|} = -\mathbf{n}_1 \\ \mathbf{n}_4 &:= \frac{\mathbf{r} - \mathbf{h}}{\|\mathbf{r} - \mathbf{h}\|} = \frac{1}{2 \sin(\eta/2)}(\mathbf{r} - \mathbf{h}) = \mathbf{n}_1 \times \mathbf{n}_2 \end{aligned} \tag{39}$$

The two circles $C(\mathbf{n}_1, \mathbf{n}_2) \subset \mathbb{S}^2$ and $C(\mathbf{n}_3, \mathbf{n}_4) \subset \mathbb{S}^2$ are orthogonal to one another.

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Now, let $q \in C(q_1, q_2)$ and $p \in C(q_3, q_4)$ be arbitrary unit quaternions

$$\begin{aligned} q &= q_1 \cos t + q_2 \sin t \\ p &= q_3 \cos t + q_4 \sin t \end{aligned} \tag{40}$$

Substituting expressions for q_1, q_2, q_3, q_4, i.e. Equations (19), (38), and (39) in Equation (40) we get

$$\begin{aligned} q &= \cos \frac{\eta}{2} \cos t + \mathbf{n}_1 \sin \frac{\eta}{2} \cos t + \mathbf{n}_2 \sin t \\ p &= \cos \frac{\pi - \eta}{2} \cos t + \mathbf{n}_3 \sin \frac{\pi - \eta}{2} \cos t + \mathbf{n}_4 \sin t \\ &= \sin \frac{\eta}{2} \cos t - \mathbf{n}_1 \cos \frac{\eta}{2} \cos t + (\mathbf{n}_1 \times \mathbf{n}_2) \sin t \end{aligned}$$

Now, ordinary quaternion multiplication yields

$$\begin{aligned} \mathrm{Sc}(q p^*) = {} & \cos \frac{\eta}{2} \cos t \sin \frac{\eta}{2} \cos t \\ & + \left(\mathbf{n}_1 \sin \frac{\eta}{2} \cos t + \mathbf{n}_2 \sin t\right) \cdot \left(-\mathbf{n}_1 \cos \frac{\eta}{2} \cos t + \mathbf{n}_1 \times \mathbf{n}_2 \sin t\right) = 0 \end{aligned}$$

Thus, the two circles $C(q_1, q_2) \subset \mathbb{S}^3$ and $C(q_3, q_4) \subset \mathbb{S}^3$ are orthonormal to one another. □

Remark
Obviously, $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_4$ provide a right-handed orthonormal basis of $\mathrm{Vec}\mathbb{H} \simeq \mathbb{R}^3$, and $q_i, i = 1, \ldots, 4$, provide a right-handed orthonormal basis of $\mathbb{H}$.

Corollary 1
Eventually, it holds that

(i) given $\mathbf{h}_0$, it holds that $G(\mathbf{h}_0, \mathbf{r}_1) \cap G(\mathbf{h}_0, \mathbf{r}_2) = \emptyset$ if $\mathbf{r}_1 \neq \mathbf{r}_2$, and, analogously, given $\mathbf{r}_0$, it holds that $G(\mathbf{h}_1, \mathbf{r}_0) \cap G(\mathbf{h}_2, \mathbf{r}_0) = \emptyset$ if $\mathbf{h}_1 \neq \mathbf{h}_2$;

(ii) $$\bigcup_{\mathbf{r} \in \mathbb{S}^2} G(\mathbf{h}_0, \mathbf{r}) = \bigcup_{\mathbf{h} \in \mathbb{S}^2} G(\mathbf{h}, \mathbf{r}_0) = \mathrm{SO}(3)$$

(iii) given $\boldsymbol{g} \in \mathrm{SO}(3)$ and $\mathbf{h}_0$, there exists a vector $\mathbf{r}$ such that $\boldsymbol{g} \in G(\mathbf{h}_0, \mathbf{r})$, and, analogously, given $\boldsymbol{g} \in \mathrm{SO}(3)$ and $\mathbf{r}_0$, there exists a vector $\mathbf{h}$ such that $\boldsymbol{g} \in G(\mathbf{h}, \mathbf{r}_0)$.

The major property of the circle $C(q_1, q_2)$ is that it consists of all quaternions $q(t), t \in [0, 2\pi)$, with $q(t)\mathbf{h}q^*(t) = \mathbf{r}$ for all $t \in [0, 2\pi)$, and that it is uniquely characterized by the pair $\mathbf{h}, \mathbf{r} \in \mathbb{S}^2$. For any other $\mathbf{h}' \in \mathbb{S}^2$ with $\mathbf{h} \cdot \mathbf{h}' = \cos \rho$ the vector $q(t)\mathbf{h}'q^*(t) =: \mathbf{r}'(t) \in \mathbb{S}^2$ is not a constant unit vector, but it encloses the same angle ρ with $\mathbf{r}$ for every t

$$\mathbf{r} \cdot \mathbf{r}'(t) = (q(t)\mathbf{h}q^*(t)) \cdot (q(t)\mathbf{h}'q^*(t)) = \mathbf{h} \cdot \mathbf{h}' = \cos \rho \tag{41}$$

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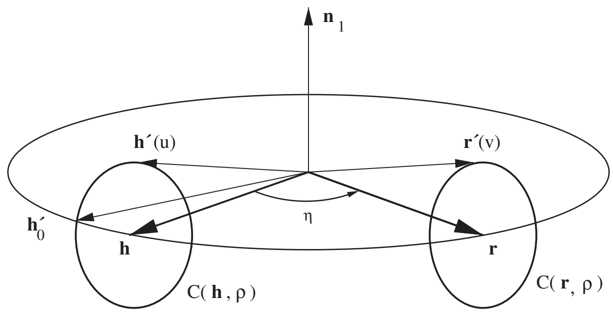

Figure 2. Circles $C(\mathbf{h},\rho)$ and $C(\mathbf{r},\rho)$.

Next, it is shown that $\mathbf{r}'(t)$ actually represents the small circle with centre $\mathbf{r}$ and angle ρ of $\mathbb{S}^2$. To this end we define the small circle $C(\mathbf{r},\rho)\subset\mathbb{S}^2$ properly by

$$C(\mathbf{r},\rho)=\{\mathbf{r}'\in\mathbb{S}^2|\mathbf{r}\cdot\mathbf{r}'=\cos\rho\} \tag{42}$$

and observe that it can be parametrized by virtue of Equation (33) and represented as

$$\mathbf{r}'(t)=r(t)\mathbf{r}'_0 r^*(t) \tag{43}$$

with $\mathbf{r}'_0\in\mathbb{S}^2$ in the plane spanned by $\mathbf{h}$ and $\mathbf{r}$ with $\mathbf{h}\cdot\mathbf{r}'_0=\cos(\eta-\rho)$. In this way the small circle $C(\mathbf{r},\rho)$ is seen as the result of all rotations of the vector $\mathbf{r}'_0$ about the axis $\mathbf{r}$, see Figure 2. Analogously, the small circle $C(\mathbf{h},\rho)$ can be represented as

$$\mathbf{h}'(t)=h(t)\mathbf{h}'_0 h^*(t) \tag{44}$$

with $\mathbf{h}'_0\in\mathbb{S}^2$ in the plane spanned by $\mathbf{h}$ and $\mathbf{r}$ with $\mathbf{h}'_0\cdot\mathbf{r}=\cos(\eta+\rho)$.

Proposition 6
The circle $C(q_1,q_2)$ represents rotations mapping the small circle $C(\mathbf{h},\rho)$ onto the small circle $C(\mathbf{r},\rho)$; i.e. for every $\mathbf{h}'(u)\in C(\mathbf{h},\rho)$ and $q(t)\in C(q_1,q_2)$

$$q(t)\mathbf{h}'(u)q^*(t)=\mathbf{r}'(u+2t),\quad t,u\in[0,2\pi) \tag{45}$$

holds.

Proof
Let us consider the vector $\mathbf{r}'_0=q_1\mathbf{h}'_0 q_1^*$. Since rotations preserve angles, the angle between $\mathbf{r}'_0$ and $\mathbf{r}$ is ρ as the angle between $\mathbf{h}'_0$ and $\mathbf{h}$. Then

$$\begin{aligned} q(t)\mathbf{h}'(u)q^*(t) &= q(t)h(u)\mathbf{h}'_0 h^*(u)q^*(t) \\ &= (q(t)h(u)q_1^*)(q_1\mathbf{h}'_0 q_1^*)(q_1 h^*(u)q^*(t)) \\ &= (q(t)h(u)q_1^*)\mathbf{r}'_0(q_1 h^*(u)q^*(t)) \end{aligned} \tag{46}$$

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Substituting Equations (32) and (26) yields

$$
\begin{aligned}
q(t)h(u)q_1^* &= (q_1 \cos t + q_2 \sin t)\left(\cos \frac{u}{2} + \mathbf{h} \sin \frac{u}{2}\right) q_1^* \\
&= \cos t \cos \frac{u}{2} + q_2 q_1^* \sin t \cos \frac{u}{2} \\
&\quad + q_1 \mathbf{h} q_1^* \cos t \sin \frac{u}{2} + q_2 \mathbf{h} q_1^* \sin t \sin \frac{u}{2}
\end{aligned} \tag{47}
$$

It follows from Equation (29) that $q_2 \mathbf{h} q_1^* = -1$. With this substitution in Equation (47) and with Equation (31) in mind, we accomplish

$$
\begin{aligned}
q(t)h(u)q_1^* &= \cos t \cos \frac{u}{2} - \sin t \sin \frac{u}{2} + \mathbf{r}\left(\sin t \cos \frac{u}{2} + \cos t \sin \frac{u}{2}\right) \\
&= \cos \frac{u+2t}{2} + \mathbf{r} \sin \frac{u+2t}{2}
\end{aligned} \tag{48}
$$

Thus, for every t the vector $q(t)\mathbf{h}'(u)q^*(t)$ is the result of the rotation of $\mathbf{r}_0'$ about $\mathbf{r}$ by the angle $u+2t$. This completes the proof. □

Corollary 2

Let $p(u)$ be a quaternion mapping $\mathbf{h}$ onto $\mathbf{h}'(u) \in C(\mathbf{h}, \rho)$, then for every $q(t) \in C(q_1, q_2)$ the quaternion $q(t)p(u)q^*(t)$ is mapping $\mathbf{r}$ onto $\mathbf{r}'(v) \in C(\mathbf{r}, \rho), v = u + 2t$.

It should be noted that $C(q_1, q_2)$ does not represent all rotations mapping an element of $C(\mathbf{h}, \rho)$ onto an element of $C(\mathbf{r}, \rho)$. In fact, the rotation about $(\mathbf{h}_0' + \mathbf{r}_0')/\|\mathbf{h}_0' + \mathbf{r}_0'\|$ by π mapping $\mathbf{h}_0' \in C(\mathbf{h}, \rho)$ on $\mathbf{r}_0' \in C(\mathbf{r}, \rho)$ cannot be represented by any element of $C(q_1, q_2)$ as the pure unit quaternion $(\mathbf{h}_0' + \mathbf{r}_0')/\|\mathbf{h}_0' + \mathbf{r}_0'\| \notin C(q_1, q_2)$.

Slightly generalizing the notation of Proposition 3, the set $\bigcup_{u \in [0,2\pi)} \bigcup_{v \in [0,2\pi)} G(\mathbf{h}'(u), \mathbf{r}'(v))$ of all rotations mapping $C(\mathbf{h}, \rho)$ onto $C(\mathbf{r}, \rho)$ is represented by the union of all circles $\bigcup_{u \in [0,2\pi)} \bigcup_{v \in [0,2\pi)} C(q_1(\mathbf{h}'(u), \mathbf{r}'(v)), q_2(\mathbf{h}'(u), \mathbf{r}'(v))$ representing rotations $\mathbf{g}\mathbf{h}'(u) = \mathbf{r}'(v)$. Rewriting Equation (45) as

$$
q\left(\frac{v-u}{2}\right)\mathbf{h}'(u)q^*\left(\frac{v-u}{2}\right) = \mathbf{r}'(v) \text{ for all } u, v \in [0, 2\pi)
$$

leads to

$$
\bigcap_{v-u=2t} C(q_1(\mathbf{h}'(u), \mathbf{r}'(v)), q_2(\mathbf{h}'(u), \mathbf{r}'(v)) = \{q(t; \mathbf{h}, \mathbf{r})\}
$$

and furthermore to

$$
\begin{aligned}
\bigcup_{t \in [0,2\pi)} \bigcap_{v-u=2t} C(q_1(\mathbf{h}'(u), \mathbf{r}'(v)), q_2(\mathbf{h}'(u), \mathbf{r}'(v)) &= \bigcup_{t \in [0,2\pi)} \{q(t; \mathbf{h}, \mathbf{r})\} \\
&= C(q_1(\mathbf{h}, \mathbf{r}), q_2(\mathbf{h}, \mathbf{r}))
\end{aligned}
$$

With respect to small circles another proposition holds.

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Proposition 7
The set of all rotations mapping $\mathbf{h}$ on $C(\mathbf{r},\rho)$ is equal to the set of all rotations mapping $C(\mathbf{h},\rho)$ onto $\mathbf{r}$, i.e.

$$\bigcup_{\mathbf{r}'\in C(\mathbf{r},\rho)} G(\mathbf{h},\mathbf{r}') = \bigcup_{\mathbf{h}'\in C(\mathbf{h},\rho)} G(\mathbf{h}',\mathbf{r})$$

or equivalently

$$\bigcup_{v\in[0,2\pi)} G(\mathbf{h},\mathbf{r}'(v)) = \bigcup_{u\in[0,2\pi)} G(\mathbf{h}'(u),\mathbf{r})$$

employing the parametric representation, Equations (43) and (44), respectively.

Proof
The set of rotations $G(\mathbf{h},\mathbf{r}'(v))$, $v\in[0,2\pi)$, is represented by the circle

$$C(q_1(\mathbf{h},\mathbf{r}'(v)),q_2(\mathbf{h},\mathbf{r}'(v))) = \{q(t;\mathbf{h},\mathbf{r}'(v)),\ \ t,v\in[0,2\pi)\} \tag{49}$$

such that

$$q(t;\mathbf{h},\mathbf{r}'(v))\mathbf{h}q^*(t;\mathbf{h},\mathbf{r}'(v)) = \mathbf{r}'(v),\ \ \forall\ \ t,v\in[0,2\pi),$$

Applying Proposition 6 implies that $q(t;\mathbf{h},\mathbf{r}'(v))$ of Equation (49) maps $\mathbf{h}'(u)$ for arbitrary $t,u\in[0,2\pi)$ onto the circle $C(\mathbf{r}'(v),\rho)$, i.e.

$$q(t;\mathbf{h},\mathbf{r}'(v))\mathbf{h}'(u)q^*(t;\mathbf{h},\mathbf{r}'(v)) = \mathbf{r}''(u+2t)\in C(\mathbf{r}'(v),\rho)$$

where

$$\mathbf{r}''(v) = r'(v)\mathbf{r}_0''r'^*(v)$$

with $\mathbf{r}_0''\in\mathbb{S}^2$ in the plane spanned by $\mathbf{h}$ and $\mathbf{r}'(v)$ with $\mathbf{h}\cdot\mathbf{r}_0'' = \cos(\eta'(v)-\rho)$ with $\cos\eta'(v) = \mathbf{h}\cdot\mathbf{r}'(v)$. Since $\mathbf{r}\in C(\mathbf{r}'(v),\rho)$, it holds that $t_0\in[0,2\pi)$ exists such that $q(t_0;\mathbf{h},\mathbf{r}'(v))\mathbf{h}'(u)q^*(t_0;\mathbf{h},\mathbf{r}'(v)) = \mathbf{r}$. Thus, $q(t_0;\mathbf{h},\mathbf{r}'(v))$ represents a rotation g_0 such that $g_0\mathbf{h} = \mathbf{r}'(v)$ and also $g_0\mathbf{h}'(u) = \mathbf{r}$.

The same argument applies analogously in the other direction.

Let us find an explicit form of these rotations. Considering the sequence of rotations

$$\mathbf{h}'(u)\xrightarrow{p^*(u)}\mathbf{h}\xrightarrow{q(t)}\mathbf{r} \tag{50}$$

where $p(u)$ is a rotation mapping $\mathbf{h}$ onto $\mathbf{h}'(u)$ with its axis orthogonal to the plane spanned by the vectors $\mathbf{h}$ and $\mathbf{h}'(u)$, and where therefore $p^*(u)$ is the inverse rotation mapping $\mathbf{h}'(u)$ onto $\mathbf{h}$, we get that $q(t)p^*(u)$ is the resulting quaternion mapping $\mathbf{h}'(u)$ onto $\mathbf{r}$. On the other side, due to Corollary 2, the sequence of rotations

$$\mathbf{h}\xrightarrow{q(t)}\mathbf{r}\xrightarrow{q(t)pq(t)^*}\mathbf{r}'(v) \tag{51}$$

gives us the resulting quaternion $q(t)p(u)$ mapping $\mathbf{h}$ onto $\mathbf{r}'(u+2t) = \mathbf{r}'(v)$. Let us show that $\{q(t)p(u);u\in[0,2\pi)\} = \{q(t)p^*(u);u\in[0,2\pi)\}$. Indeed, since $C(\mathbf{h},\rho)$ is a circle, it contains

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points $\mathbf{h}'(u)$ and $\mathbf{h}'(u+\pi)$ which are symmetric with respect to $\mathbf{h}$ for every u and all three vectors $\mathbf{h}'(u), \mathbf{h}$ and $\mathbf{h}'(u+\pi)$ are lying in the same plane. Then the quaternion $p^*(u)$ is mapping $\mathbf{h}$ onto $\mathbf{h}'(u+\pi)$. Hence, the set of all quaternions mapping $\mathbf{h}$ onto $\mathbf{h}'(u), u \in [0, 2\pi)$ can be represented by

$$\{p(u); u \in [0, 2\pi)\} = \{p(u); u \in [0, \pi)\} \cup \{p^*(u); u \in [0, \pi)\} \tag{52}$$

It gives us immediately that $\{p(u); u \in [0, 2\pi)\} = \{p^*(u); u \in [0, 2\pi)\}$, and therefore $\{q(t)p(u); u \in [0, 2\pi)\} = \{q(t)p^*(u); u \in [0, 2\pi)\}$. Thus,

$$\bigcup_{v \in [0,2\pi)} G(\mathbf{h}, \mathbf{r}'(v)) = \bigcup_{u \in [0,2\pi)} G(\mathbf{h}'(u), \mathbf{r}) \tag{53}$$

This completes the proof. □

Corollary 3
The set of all rotations mapping $\mathbf{h}$ on the spherical cap $\bigcup_{\varrho \in [0,\rho]} C(\mathbf{r}, \rho)$ is equal to the set of all rotations mapping the spherical cap $\bigcup_{\varrho \in [0,\rho]} C(\mathbf{h}, \rho)$ onto $\mathbf{r}$.

It should be noted that Proposition 7 leads to a completely geometrical proof of Ásgeirsson's mean value theorem [5,6,12–14] for Radon transforms $\mathscr{R}f$ of even functions defined on $\mathbb{S}^3$.

3.2. Mapping a pair of given vectors onto another pair

Now we consider the problem with two pairs of given unit vectors $(\mathbf{h}, \mathbf{r})$ and $(\mathbf{h}_1, \mathbf{r}_1)$ to be mapped onto each other by the same rotation. It is possible to solve the problem by a conditional extremum approach looking for the rotation which minimizes $\|\mathbf{h} - \mathbf{r}\|^2 + \|\mathbf{h}_1 - \mathbf{r}_1\|^2$ subject to the constraint $\mathbf{h} \cdot \mathbf{h}_1 = \mathbf{r} \cdot \mathbf{r}_1$. However, we shall continue the geometric approach to find an exact solution.

Proposition 8
Given two pairs of unit vectors $(\mathbf{h}, \mathbf{r}), (\mathbf{h}_1, \mathbf{r}_1) \in \mathbb{S}^2 \times \mathbb{S}^2$ such that $(\mathbf{h} \times \mathbf{r}) \times (\mathbf{h}_1 \times \mathbf{r}_1) \neq 0$. Then there exists a unique quaternion $q \in \mathbb{S}^3$ such that

$$q\mathbf{h}q^* = \mathbf{r} \text{ and } q\mathbf{h}_1 q^* = \mathbf{r}_1 \tag{54}$$

provided that $\mathbf{h} \cdot \mathbf{h}_1 = \mathbf{r} \cdot \mathbf{r}_1$, as rotations preserve the geodetic distance of unit vectors.

Proof
Algebraically, q is given as the solution of the system of the two equations

$$q\mathbf{h} - \mathbf{r}q = 0 \tag{55}$$

$$q\mathbf{h}_1 - \mathbf{r}_1 q = 0 \tag{56}$$

subject to $\mathbf{h} \cdot \mathbf{h}_1 = \mathbf{r} \cdot \mathbf{r}_1$. By geometrical reasoning the solution is given as follows. The axis $\mathbf{q}$ of the rotation q is given by the intersection of the two planes of rotation axes corresponding to the circle Equation (55) and the circle Equation (56), respectively. The intersection of two

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planes is provided by the vector product of their normals, thus

$$\mathbf{q} = \left[\left(\frac{\mathbf{h}\times\mathbf{r}}{\|\mathbf{h}\times\mathbf{r}\|}\right)\times\left(\frac{\mathbf{h}+\mathbf{r}}{\|\mathbf{h}+\mathbf{r}\|}\right)\right]\times\left[\left(\frac{\mathbf{h}_1\times\mathbf{r}_1}{\|\mathbf{h}_1\times\mathbf{r}_1\|}\right)\times\left(\frac{\mathbf{h}_1+\mathbf{r}_1}{\|\mathbf{h}_1+\mathbf{r}_1\|}\right)\right]$$
$$= \frac{\mathbf{h}-\mathbf{r}}{\|\mathbf{h}-\mathbf{r}\|}\times\frac{\mathbf{h}_1-\mathbf{r}_1}{\|\mathbf{h}_1-\mathbf{r}_1\|} \tag{57}$$

If the vectors $\mathbf{h}-\mathbf{r}$ and $\mathbf{h}_1-\mathbf{r}_1$ are not collinear, Equation (57) yields the unique axis of the required rotation. The angle ω of the rotation q is provided by Equation (22). The required quaternion of rotation is

$$q = \cos\frac{\omega}{2} + \frac{\mathbf{q}}{\|\mathbf{q}\|}\sin\frac{\omega}{2} \tag{58}$$

If the vectors $\mathbf{h}-\mathbf{r}$ and $\mathbf{h}_1-\mathbf{r}_1$ are collinear, two possibilities arise.

In the first case $\mathbf{h} = -\mathbf{h}_1$. Then it follows that all vectors $\mathbf{h},\mathbf{r},\mathbf{h}_1,\mathbf{r}_1$ are lying in the same plane. The axis of rotation coincides with the vector $(\mathbf{h}\times\mathbf{r})/\|\mathbf{h}\times\mathbf{r}\|$ and the angle of rotation ω is equal to the angle η between $\mathbf{h}$ and $\mathbf{r}$.

In the second case $\mathbf{h} \neq -\mathbf{h}_1$. Then, due to symmetry, the axis of rotation coincides with the line of intersection of two planes: the plane spanned by the vectors $\mathbf{h},\mathbf{h}_1$ and the plane spanned by the vectors $\mathbf{r},\mathbf{r}_1$, i.e. it is the vector product of two normals

$$\mathbf{q} = \frac{\mathbf{h}\times\mathbf{h}_1}{\|\mathbf{h}\times\mathbf{h}_1\|}\times\frac{\mathbf{r}\times\mathbf{r}_1}{\|\mathbf{r}\times\mathbf{r}_1\|} \tag{59}$$

and the angle of rotation ω is again given by Equation (22). □

Remark

The condition of collinearity has a simple quaternion analogue. Two arbitrary vectors $\mathbf{h},\mathbf{r}$ are collinear if the corresponding pure quaternions h,r are commutative, i.e. $hr - rh = 0$.

Next, the factorization, Equation (34), is applied to control the degree of freedom when specifying and representing a particular rotation mapping $\mathbf{h}$ onto $\mathbf{r}$. Instead of using two pairs of unit vectors mapped onto each other, the condition now is that we have two unit vectors in the tangential plane of the radius vector $\mathbf{r}\in\mathbb{S}^2$—one of them arbitrarily given, the other one subjected to a rotation $r(t)\in\mathbb{S}^3$ about $\mathbf{r}$ by $t\in[0,2\pi)$—enclose a given angle, say t_0.

Let q be the quaternion defined in Equation (58), i.e $q\mathbf{h}q^* = \mathbf{r}$ and $q\mathbf{h}_1q^* = \mathbf{r}_1$. Defining the orthogonal projection $(\mathbf{v})_T$ of an arbitrary unit vector $\mathbf{v}\in\mathbb{S}^2$ onto the tangential plane of the radius vector $\mathbf{r}$ (see Figure 3)

$$(\mathbf{v})_T(\mathbf{r}) = \mathbf{v} - (\mathbf{v}\cdot\mathbf{r})\ \mathbf{r}$$

we get

$$(\mathbf{r}_1)_T(\mathbf{r}) = \mathbf{r}_1 - (\mathbf{r}_1\cdot\mathbf{r})\mathbf{r} = q\mathbf{h}_1q^* - (q\mathbf{h}_1q^*\cdot\mathbf{r})\ \mathbf{r}$$

where the latter yields

$$(\mathbf{r}_1)_T(\mathbf{r}) = q\mathbf{h}_1q^* - (q\mathbf{h}_1q^*\cdot q\mathbf{h}q^*)q\mathbf{h}q^*$$

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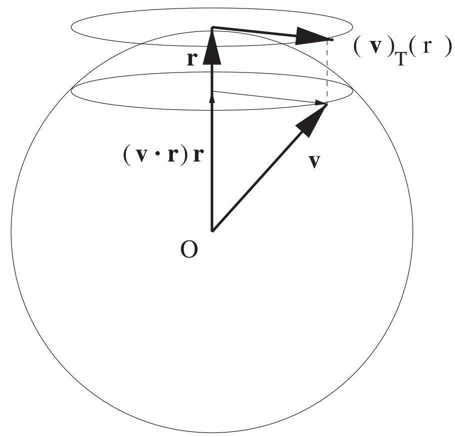

Figure 3. Projection $(\mathbf{v})_T$.

$$= q\mathbf{h}_1 q^* - (\mathbf{h}_1 \cdot \mathbf{h}) q\mathbf{h} q^*$$

$$= q(\mathbf{h}_1 - (\mathbf{h}_1 \cdot \mathbf{h})\mathbf{h}) q^* = q(\mathbf{h}_1)_T(\mathbf{h}) q^*$$

Then the projection $(\mathbf{v})_T(\mathbf{r})$ of an arbitrary vector $\mathbf{v}$ may be thought of as the result of a rotation of $(\mathbf{r}_1)_T(\mathbf{r})$ about $\mathbf{r}$ by the angle $\alpha = \arccos((\mathbf{v})_T \cdot (\mathbf{r}_1)_T)$.

Proposition 9
Given a pair of unit vectors $(\mathbf{h}, \mathbf{r}) \in \mathbb{S}^2 \times \mathbb{S}^2$, and two additional unit vectors $\mathbf{h}_1, \mathbf{v} \in \mathbb{S}^2$. Then there exists a unique quaternion $q \in \mathbb{S}^3$ such that

$$q\mathbf{h}q^* = \mathbf{r} \text{ and } (\mathbf{v})_T(\mathbf{r}) \cdot (q\mathbf{h}_1 q^*)_T(\mathbf{r}) = \cos t_0 \tag{60}$$

where $t_0 \in [0, 2\pi)$ denotes the angle between the orthogonal projection of $\mathbf{v}$ and the orthogonal projection of $q\mathbf{h}_1 q^*$ onto the tangential plane of $\mathbf{r}$.

Proof
Let p be a quaternion obtained like in Proposition 8 such that

$$p\mathbf{h} p^* = \mathbf{r}$$

$$p\mathbf{h}_1 p^* = \mathbf{v}$$

When a vector is rotating about the vector $\mathbf{r}$ by the angle t_0, its projection on the tangential plane of $\mathbf{r}$ is also rotating about $\mathbf{r}$ by the same angle by definition.

Now, the quaternion we are looking for is $q = r(t_0) p$, where $r(t_0) = \cos(t_0/2) + \mathbf{r} \sin(t_0/2)$. Indeed,

$$q\mathbf{h}q^* = r(t_0) p\mathbf{h} p^* r^*(t_0) = r(t_0)\mathbf{r} r^*(t_0) = \mathbf{r} \tag{61}$$

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as a rotation of a vector about itself does not change the vector, and

$$q\mathbf{h}_1 q^* = r(t_0) p\mathbf{h}_1 p^* r^*(t_0) = r(t_0)\mathbf{v}r^*(t_0) \tag{62}$$

The angle between $(\mathbf{v})_T(\mathbf{r})$ and $(r(t_0)\mathbf{v}r^*(t_0))_T(\mathbf{r})$ is just t_0. □

For mutually orthogonal unit quaternions $q, p_1, p_2, p_3 \in \mathbb{S}^3$ let $S(p_1, p_2, p_3)$ denote the orthogonally complementary sphere of a given quaternion $q \in \mathbb{S}^3$, i.e. $S(p_1, p_2, p_3) := q^\perp \cap \mathbb{S}^3$. Due to Proposition 1 we can write

$$S(p_1, p_2, p_3) = \mathbb{S}^2 q \tag{63}$$

Since $\mathbb{S}^2$ consists of all pure unit quaternions, Equation (63) means that the orthogonal complement of q consists of all quaternions representing rotations composed of a first rotation represented by q and a second rotation by the angle π about an arbitrary axes in $\mathbb{S}^2$.

Moreover, for every quaternion $q \in C(q_1, q_2)$, the circle $C(q_3, q_4) \subset q^\perp$, i.e. if $q\mathbf{h}q^* = \mathbf{r}$, then the set of all rotations $p\mathbf{h}p^* = -\mathbf{r}$ is completely contained in the sphere $q^\perp$.

Proposition 10

Given an arbitrary quaternion $q_0 \in \mathbb{S}^3$ and denote $S(p_1, p_2, p_3)$ the orthogonally complementary sphere of q_0. For each choice of $p_3 \in q_0^\perp$ there exists a unique pair of unit vectors $(\mathbf{h}, \mathbf{r}) \in \mathbb{S}^2 \times \mathbb{S}^2$ such that

$$q\mathbf{h}q^* = \mathbf{r}, \ \ \forall \ q \in C(p_1, p_2) \tag{64}$$

Proof

Of course, the statement holds true for

$$\mathbf{h} = \mathrm{Vec}(p_1^* p_2)$$

$$\mathbf{r} = \mathrm{Vec}(p_2 p_1^*)$$

because of Proposition 4. However, here we would like to find $\mathbf{h}$ and $\mathbf{r}$ in terms of q_0 and p_3.

First, remember that $q_0^\perp = \mathbb{S}^2 q_0$. Then, because of Proposition 1 every three mutually orthonormal quaternions $p_1, p_2, p_3 \in q_0^\perp \cap \mathbb{S}^3$, which are assumed to build a right-handed system in this order, can always be written as

$$p_i = \mathbf{v}_i q_0$$

where $\mathbf{v}_i = p_i q_0^* \in \mathbb{S}^2, \ \ i = 1, 2, 3$. Hence

$$p_i p_j^* = v_i q_0 q_0^* v_j^* = \mathbf{v}_i \cdot \mathbf{v}_j - \mathbf{v}_i \times \mathbf{v}_j$$

The orthonormality of p_1, p_2, p_3 implies for the associated vectors that $\mathrm{Sc}(p_i p_j^*) = \mathbf{v}_i \cdot \mathbf{v}_j = 0$, i.e. the vectors $\mathbf{v}_i, i = 1, 2, 3$, build an orthonormal basis with no handedness assigned yet. Furthermore, using Equation (4) we get

$$2(\mathbf{v}_i \cdot \mathbf{v}_j) = v_i v_j + v_j v_i = 0$$

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thus $v_i v_j = -v_j v_i$. A (right) handedness is assigned to $\mathbf{v}_i, i = 1,2,3$, by setting

$$v_3 = v_1 v_2 = -v_2 v_1$$

Now, we define h as following

$$h = p_1^* p_2 = q_0^* v_1^* v_2 q_0 = -q_0^* v_1 v_2 q_0 = -q_0^* v_3 q_0 = q_0^* v_3^* q_0 = p_3^* q_0$$

and

$$r = p_2 p_1^* = v_2 q_0 q_0^* v_1^* = -v_2 v_1 = v_3 = p_3 q_0^*$$

Thus, a quaternion $q(t) = p_1 \cos t + p_2 \sin t \in C(p_1, p_2)$ maps the vector $\mathbf{h} = q_0^* p_3$ on the vector $\mathbf{r} = q_0 p_3^*$. To check the result one can use the quaternion multiplication $q(t) h q^*(t)$. □

The parametrization of $C(p_1, p_2)$ in terms of q_0, p_3 proves instrumental in integration, e.g. as with respect to spherical Radon transforms of order 1, 2 [14]. Moreover, this parametrization implies that each circle contained in $q_0^\perp$ refers to a different unique pair of unit vectors related to one another by the corresponding rotations.

Corollary 4
Let $C(q_1, q_2)$ and $C(q_3, q_4)$ be defined like in Proposition 5. If $q_0 \in C(q_1, q_2)$, then $C(q_3, q_4)$ is the only circle representing all rotations acting on $\mathbf{h}$ which is completely contained in $q_0^\perp$.

Thus, the major property of the sphere $q_0^\perp = \mathbb{S}^2 q_0 \subset \mathbb{S}^3 \subset \mathbb{H}$ is that it contains the circle representing all rotations mapping $\mathbf{h}$ on $-\mathbf{r}$ and that it does not contain any other circle representing all rotations mapping $\mathbf{h}$ on a direction different of $-\mathbf{r}$.

Proposition 11
Given a pair of unit vectors $(\mathbf{h}, \mathbf{r}) \in \mathbb{S}^2 \times \mathbb{S}^2$, there exists a pair of orthogonal unit quaternions $p, q \in \mathbb{S}^3$ such that

$$q\mathbf{h}q^* = \mathbf{r} \text{ and } p\mathbf{h}p^* \in \mathbf{r}^\perp \cap \mathbb{S}^2. \tag{65}$$

Proof
Let $q \in \mathbb{S}^3$ be an arbitrary unit quaternion such that $q\mathbf{h}q^* = \mathbf{r}$. For any $p \in \mathbb{S}^3$ it holds

$$p\mathbf{h}p^* = pq^* q\mathbf{h}q^* q p^* = pq^* \mathbf{r} (pq^*)^*$$

Thus, $p \in \mathbb{S}^3$ has to be constructed to satisfy the orthogonality condition $\mathrm{Sc}(pq^*) = 0$ and it has to be

$$pq^* \mathbf{r} (pq^*)^* = \mathbf{r}_1 \in \mathbf{r}^\perp \cap \mathbb{S}^2$$

Hence, for any $\mathbf{r}_1 \in \mathbf{r}^\perp \cap \mathbb{S}^2$ we get

$$\mathrm{Vec}(pq^*) = \frac{\mathbf{r} + \mathbf{r}_1}{\|\mathbf{r} + \mathbf{r}_1\|}$$

and the angle of rotation is π. Thus

$$pq^* = 0 + \frac{\mathbf{r} + \mathbf{r}_1}{\|\mathbf{r} + \mathbf{r}_1\|}$$

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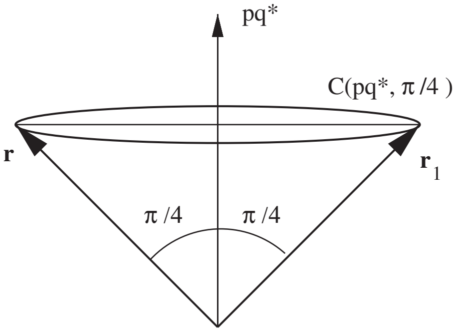

Figure 4. Rotation of $\mathbf{r}$ by pq^*.

Eventually the quaternion we are looking for is

$$p = \frac{\mathbf{r}+\mathbf{r}_1}{\|\mathbf{r}+\mathbf{r}_1\|}\, q \tag{66}$$

If $\mathbf{r}_1 \in \mathbf{r}^{\perp} \cap \mathbb{S}^2$ and $q \in \mathbb{S}^3$ are fixed, then p is uniquely defined by Equation (66). Since the set $G(\mathbf{h}, \mathbf{r})$ is represented by the circle $C(q_1, q_2)$ of Proposition 3 spanned by two linearly independent quaternions $q_1, q_2 \in \mathbb{S}^3$, there are also two linearly independent solutions $p_i = (\mathbf{r}+\mathbf{r}_1)/(\|\mathbf{r}+\mathbf{r}_1\|)q_i,\ i = 1, 2$, of Equation (66). □

The inverse assertion holds also.

Proposition 12
Given a pair of unit orthonormal quaternions $p, q \in \mathbb{S}^3$, there exists a pair of unit vectors $(\mathbf{h}, \mathbf{r}) \in \mathbb{S}^2 \times \mathbb{S}^2$ such that

$$q\mathbf{h}q^* = \mathbf{r} \ \text{and} \ p\mathbf{h}p^* \in \mathbf{r}^{\perp} \cap \mathbb{S}^2 \tag{67}$$

Proof
Since p and q are assumed to be orthonormal, $\mathrm{Sc}(pq^*) = 0$. Thus, $pq^* \in \mathbb{S}^2$ is a pure quaternion. Choosing $\mathbf{r}$ as a unit vector of the small circle $C(pq^*, \pi/4)$ with centre pq^* and $(pq^*) \cdot \mathbf{r} = \cos \pi/4$, it holds that $(pq^*)\mathbf{r}(pq^*)^* = \mathbf{r}_1$ is a vector orthonormal to $\mathbf{r}$, i.e. $\mathbf{r}_1 \in \mathbf{r}^{\perp}$, since pq^* represents a rotation about $pq^* \in \mathbb{S}^2$ by the angle π, see Figure 4. Next, defining $\mathbf{h} = q^*\mathbf{r}q$, we get, obviously, $q\mathbf{h}q^* = \mathbf{r}$ and

$$p\mathbf{h}p^* = pq^*\mathbf{r}qp^* = (pq^*)\mathbf{r}(pq^*)^* = \mathbf{r}_1 \in \mathbf{r}^{\perp} \tag{68}$$

If $\mathbf{r}_1 \in \mathbf{r}^{\perp} \cap \mathbb{S}^2$ is fixed, then $\mathbf{h}$ is uniquely defined by Equation (68). □

The propositions proved above lead to the following final result.

Proposition 13
Let q_1, q_2, q_3, q_4 denote four mutually orthonormal quaternions; let $C(q_1, q_2)$ denote the circle of quaternions $q(s), s \in [0, 2\pi)$, representing the rotations $\boldsymbol{g} \in G(\mathbf{h}, \mathbf{r})$, and $C(q_3, q_4)$ the circle $q(t), t \in [0, 2\pi)$, representing the rotations $\boldsymbol{g} \in G(-\mathbf{h}, \mathbf{r})$. Then the spherical torus

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$T(q_1, q_2, q_3, q_4; \Theta) \subset S^3$ defined as the set of quaternions

$$q(s,t;\Theta) = (q_1 \cos s + q_2 \sin s)\cos\Theta + (q_3 \cos t + q_4 \sin t)\sin\Theta$$
$$s,t \in [0,2\pi), \quad \Theta \in [0,\pi/2]$$

represents all rotations mapping $\mathbf{h}$ on the small circle $C(\mathbf{r}, 2\Theta) \subset \mathbb{S}^2$.

In particular, $q(s,-s;\Theta)$ maps $\mathbf{h}$ for all $s \in [0,2\pi)$ onto $\mathbf{r}'_0$ in the plane spanned by $\mathbf{h}$ and $\mathbf{r}$ with $\mathbf{h} \cdot \mathbf{r}'_0 = \cos(\eta - 2\Theta)$,

$$q(s,-s;\Theta)\mathbf{h}q^*(s,-s;\Theta) = \mathbf{r}'_0 \text{ for all } s \in [0,2\pi)$$

Moreover, for an arbitrary $s_0 \in [0,2\pi)$, $q(s_0, t-s_0;\Theta)$ (or $q(s_0+t, -s_0;\Theta)$, respectively,) maps $\mathbf{h}$ on $\mathbf{r}' \in C(\mathbf{r}, 2\Theta)$ which results from a positive (counter-clockwise) rotation of $\mathbf{r}'_0$ about $\mathbf{r}$ by the angle $t \in [0,2\pi)$,

$$q(s_0, t-s_0;\Theta)\mathbf{h}q^*(s_0, t-s_0;\Theta) = r(t)\mathbf{r}'_0 r^*(t), \text{ for all } s \in [0,2\pi).$$

Proof

It can be shown by using Equation (27) and straightforward quaternion multiplication that

$$q_1\mathbf{h}q_2^* = -q_2\mathbf{h}q_1^* = 1$$
$$q_1\mathbf{h}q_3^* = -q_3\mathbf{h}q_1^* = -\mathbf{n}_1 \times \mathbf{r}$$
$$q_1\mathbf{h}q_4^* = -q_4\mathbf{h}q_1^* = -\mathbf{n}_1$$
$$q_2\mathbf{h}q_3^* = -q_3\mathbf{h}q_2^* = -\mathbf{n}_1$$
$$q_2\mathbf{h}q_4^* = -q_4\mathbf{h}q_2^* = \mathbf{n}_1 \times \mathbf{r}$$
$$q_3\mathbf{h}q_4^* = -q_4\mathbf{h}q_3^* = -1$$

where $\mathbf{n}_1$ is defined in Equation (16). Appropriate substitution of terms in the expression for $q(s,t;\Theta)$ results in

$$\begin{aligned}\mathbf{r}' &= q(s,t;\Theta)\mathbf{h}q^*(s,t;\Theta)\\ &= \mathbf{r}\cos 2\Theta - (\mathbf{n}_1 \times \mathbf{r})\sin 2\Theta \cos(s+t) - \mathbf{n}_1 \sin 2\Theta \sin(s+t)\end{aligned} \tag{69}$$

Since $\mathbf{r}$ is orthogonal to $\mathbf{n}_1 \times \mathbf{r}$ and $\mathbf{n}_1$, the angle between the vectors $\mathbf{r}$ and $\mathbf{r}'$ is 2Θ (up to the sign) for every s and t. It means that the quaternion $q(s,t;\Theta)$ maps the vector $\mathbf{h}$ onto the small circle $C(\mathbf{r}, 2\Theta)$.

In particular, for $t = -s$ Equation (69) simplifies to

$$q(s,-s;\Theta)\mathbf{h}q^*(s,-s;\Theta) = \mathbf{r}\cos 2\Theta - (\mathbf{n}_1 \times \mathbf{r})\sin 2\Theta = \mathbf{r}'_0 \tag{70}$$

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where the right-hand side can be seen to be equal to $\mathbf{r}'_0$ by simple trigonometry, as $\mathbf{r}'_0$ can be decomposed into the sum of its corresponding orthogonal projections. Hence, we can assume $s_0 = 0$. Since the small circle may be thought of as the result of rotating $\mathbf{r}'_0$ about $\mathbf{r}$ by the angle $t \in [0, 2\pi)$, it can be written

$$q(0,t;\Theta)\mathbf{h}q^*(0,t;\Theta) = r(t)\mathbf{r}'_0 r^*(t) \tag{71}$$

which is easily verified using Equations (8) and (70).

Conversely, if $q \in \mathbb{S}^3$ maps $\mathbf{h}$ on $\mathbf{r}' \in C(\mathbf{r}, 2\Theta)$, then its distance from the circle $C(q_1, q_2) = \{q(s) | s \in [0, 2\pi)\}$ representing all rotations mapping $\mathbf{h}$ on $\mathbf{r}$ is $d(q, C) = \inf_{s \in [0,2\pi)} \arccos(\mathrm{Sc}(qq^*(s)) = \frac{1}{2} \arccos((qhq^*) \cdot r) = \Theta$ [15], which implies that q is an element of the torus $T(q_1, q_2, q_3, q_4, \Theta)$.

This completes the proof. □

Concludingly, the torus $T(q_1, q_2, q_3, q_4; \Theta)$ consisting of all quaternions with distance Θ from $C(q_1, q_2)$ essentially consists of all circles with distance Θ from $C(q_1, q_2)$ representing all rotations $\bigcup_{\mathbf{r}' \in C(\mathbf{r},2\Theta)} G(\mathbf{h}, \mathbf{r}')$ mapping $\mathbf{h}$ on $C(\mathbf{r}, 2\Theta)$, which was shown to be equal to $\bigcup_{\mathbf{h}' \in C(\mathbf{h},2\Theta)} G(\mathbf{h}', \mathbf{r})$ mapping $C(\mathbf{h}, 2\Theta)$ on $\mathbf{r}$ in Proposition 7, i.e.

$$\begin{aligned} T(q_1, q_2, q_3, q_4; \Theta) &= \bigcup_{\mathbf{r}' \in C(\mathbf{r},2\Theta)} C(q_1(\mathbf{h}, \mathbf{r}'), q_2(\mathbf{h}, \mathbf{r}')) \\ &= \bigcup_{\mathbf{h}' \in C(\mathbf{h},2\Theta)} C(q_1(\mathbf{h}', \mathbf{r}), q_2(\mathbf{h}', \mathbf{r})) \end{aligned}$$

which is essential to the inversion of the spherical Radon transform [6].

Corollary 5

All unit quaternions $q(s, t; \pi/4)$ with the same distance (of $\pi/4$) to $C(q_1, q_2)$ and $C(q_3, q_4)$ map $\mathbf{h}$ on the great circle $\mathbf{r}^\perp \subset \mathbb{S}^2$.

Obviously, for the special choice of $\Theta = \pi/4$ it holds

$$q\left(s, t - s; \frac{\pi}{4}\right) = \frac{1}{\sqrt{2}}(q_1 \cos s + q_2 \sin s + q_3 \cos(t - s) + q_4 \sin(t - s))$$

$$q(0, t; \frac{\pi}{4}) = \frac{1}{\sqrt{2}}(q_1 + q_3 \cos t + q_4 \sin t)$$

and in particular

$$q(0, 0; \frac{\pi}{4}) = \frac{1}{\sqrt{2}}(q_1 + q_3) =: p_1$$

$$q\left(\frac{\pi}{2}, 0; \frac{\pi}{4}\right) = \frac{1}{\sqrt{2}}(q_2 + q_3) =: p_2$$

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$$q\left(0,\frac{\pi}{2};\frac{\pi}{4}\right)=\frac{1}{\sqrt{2}}(q_1+q_4)=:p_3$$

$$q\left(\frac{\pi}{2},\frac{\pi}{2};\frac{\pi}{4}\right)=\frac{1}{\sqrt{2}}(q_2+q_4)=:p_4$$

Any three out of the four unit quaternions p_i are linearly independent, e.g. $p_2+p_3-p_1=p_4$.

Eventually, the set of all circles $C(p_1,p_2)\subset\mathbb{S}^3$ with a fixed distance Θ of a given $q\in\mathbb{S}^3$ is characterized by

$$\Theta=d(q,C(p_1,p_2))=\frac{1}{2}\arccos(q\mathbf{h}q^*\cdot\mathbf{r})$$

where $\mathbf{r}\in\mathbb{S}^2$ is uniquely defined in terms of $\mathbf{h}$ and p_1,p_2 by $\mathbf{r}:=p(t)\mathbf{h}p^*(t)$ for all $p(t)\in C(p_1,p_2)$ and any arbitrary $\mathbf{h}\in\mathbb{S}^2$, i.e. each circle represents all rotations mapping some $\mathbf{h}\in\mathbb{S}^2$ onto an element of the small circle $C(q\mathbf{h}q^*,2\Theta)$. Thus, for each $q\in\mathbb{S}^3$ and $\Theta\in[0,\pi)$

$$\{C(p_1,p_2)|d(q,C(p_1,p_2))=\Theta\}=\bigcup_{\mathbf{h}\in\mathbb{S}^2}\bigcup_{\mathbf{r}\in C(q\mathbf{h}q^*,2\Theta)}C(p_1(\mathbf{h},\mathbf{r}),p_2(\mathbf{h},\mathbf{r}))$$

4. APPLICATIONS

Let $f:\mathbb{S}^3\mapsto[0,\infty)$ be an even probability density function of random unit quaternions representing random rotations. For any given direction $\mathbf{h}\in\mathbb{S}^2$ the probability density function of the random direction $q\mathbf{h}q^*\in\mathbb{S}^2$ is provided by the spherical Radon transform $(\mathscr{R}f):\mathbb{S}^2\times\mathbb{S}^2\mapsto[0,\infty)$ defined as

$$(\mathscr{R}f)(\mathbf{h},\mathbf{r})=\frac{1}{2\pi}\int_{C(q_1,q_2)}f(q)\,\mathrm{d}q=\frac{1}{2\pi}\int_0^{2\pi}f(q(t))\,\mathrm{d}t$$

Then Propositions 7 and 13 amount to

$$\begin{aligned}\int_{C(\mathbf{h},2\Theta)}(\mathscr{R}f)(\mathbf{h}',\mathbf{r})\,\mathrm{d}\mathbf{h}'&=\int_{C(\mathbf{r},2\Theta)}(\mathscr{R}f)(\mathbf{h},\mathbf{r}')\,\mathrm{d}\mathbf{r}'\\&=\int_{C(\mathbf{r},2\Theta)}\int_{C(q_1(\mathbf{h},\mathbf{r}'),q_2(\mathbf{h},\mathbf{r}'))}f(q)\,\mathrm{d}q\,\mathrm{d}\mathbf{r}' \qquad (72)\\&=\int_{T(q_1,q_2,q_3,q_4;\Theta)}f(q)\,\mathrm{d}q\\&=\int_{d(q,C(q_1(\mathbf{h},\mathbf{r}),q_2(\mathbf{h},\mathbf{r})))=\Theta}f(q)\,\mathrm{d}q \qquad (73)\end{aligned}$$

where Equation (72) is an Ásgeirsson-type mean value theorem, and where Equation (73) is instrumental to the inversion of the spherical Radon transform as given by Helgason [6,16]

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and its relationship with the inversion formula as derived in texture analysis [17–19]. Details will be elaborated on in a forthcoming paper [20].

5. CONCLUSIONS

We have considered relations between geometrical objects—circles, spheres and tori—of unit quaternions representing rotations and geometrical objects—points, pairs of points, small and great circles—of unit vectors in three-dimensional space which have been subjected to these rotations. The geometrical approach to the description of some particular sets of quaternions is very useful with respect to Radon transforms of real-valued functions defined for rotations.

In a companion paper [3] the quaternion geometry will be applied to characterize the different cases of the Bingham distribution for $\mathbb{S}^3$, in particular it will be shown that all cases of ideal orientation patterns (cf. [21]) except for cone and ring fibre textures can be represented as special cases of the Bingham distribution.

In spite of the crystallographic background of our results, their featured geometrical approach may prove useful in other fields when one has to deal with rotations of spherical objects in three-dimensional space.

ACKNOWLEDGEMENTS

The author H.S. would like to thank Gerald van den Boogaart, now with the Mathematics Department of Greifswald University, Germany, for many helpful and clarifying discussions on the subject of quaternions.

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