Applications of Quaternions in 3D Rotation

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To what extent can quaternions supersede rotation matrices and Euler angles in representing 3D rotation?

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1 Introduction

In the modern day, digital entertainment industries aim to replicate and extend the appearance of our 3D world for artistic effects. Extensive use of 3D computer graphics is made in films through CGI (computer generated imagery), or in video games through real-time rendering on the player's device. Every day, scientists conduct simulation research in three dimensional spaces, i.e. in the fields of aerodynamic modeling, astrophysics, weather modelling and computational chemistry. In all of these use cases, there is a need for a rigorous mathematical framework to represent and manipulate the 3D world.

1.1 Three Dimensional Objects

In the real world, matter is composed of atoms which move on a microscopic level. Any interaction with objects results in the collective transformation of these atoms, perceived by us as something moving. In the simulated world, it is not practical to simulate the granular motion of the billions of atoms in a single object, hence the need for simplification of the way objects are represented.

The conventional approach to creating a three dimensional world is to split it into intuitive chunks, called "3D models". For example, in a scene with a teapot resting on a wooden table, it would make sense to split the teapot and the table into separate 3D models, to perform calculations on each of them individually. For example, one may wish to move just the teapot, without moving the table.

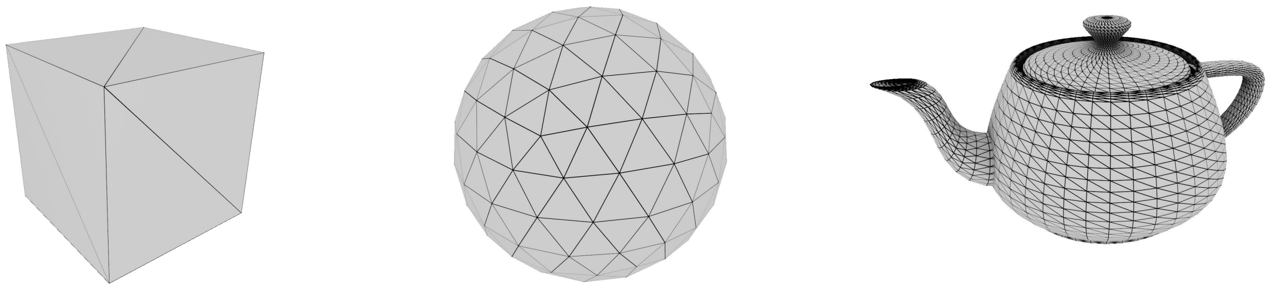
1.1.1 Vertices

Every object can be represented with a set of three-dimensional points along its surface (called "vertices") which define its shape. For maximum detail, vertices are usually placed where the shape of the object changes most, like on the object's edges or corners. Increasing the number of vertices increases the detail of the 3D model's shape.

1.1.2 Edges & Faces

Edges are three dimensional straight lines connecting three vertices together, forming a "wireframe" of the object. Faces are filled planes between three edges, in total connected to three vertices. In this way, an object with a complex shape is approximated to a certain precision with a number of faces proportional to the desired precision.

Using this method, nearly every three dimensional object one wants to represent can be approximated with a finite number of vertices, edges and faces.



(a) Cube (b) Sphere (c) Teapot

Figure 1: Wireframe view of various 3D objects

1.2 3D Transformations

In the real world, objects are not static. They move, rotate and change shape through time. In the simulated world, it is necessary to be able to perform similar transformations on the 3D models. A valuable property of the vertex-edge-face object representation is that transformations on a whole object are a product of smaller transformations on its comprising vertices.

1.2.1 Translation

Translation is the simplest transformation, and is defined as the movement of an object along a vector. For example, if an object is translated by the vector $(1, 2, 3)$, it will move by 1 unit along the x axis, 2 units along the y axis and 3 units along the z axis. In order to translate an object, one would simply add the vector to the co-ordinates of each of its vertices.

1.2.2 Scale

Scaling is the dilation of an object by a factor along each of the three axes. For example, if an object is scaled by a factor of 2 along the x axis, it will be twice as wide as before. In order to scale an object, one would simply multiply the co-ordinates of each of its vertices by the scale factor. A uniform scale refers to dilating an object by all three of the axes equally, which would make the object bigger or smaller, but maintain its proportions.

1.2.3 Rotation

Rotation is one of the more complex transformations. It is defined as the movement of an object's vertices in such a way so that the object appears to rotate, while its shape remains unchanged. However, the concept of rotation could be ambiguous in that it is not clear how exactly the object should rotate. One could rotate the object around the origin, or around its center of mass, or in fact around any arbitrary point of reference in 3D space.

Due to its complexity, there have been many different ways of defining and implementing rotation in three dimensions by many different mathematicians such as Leonard Euler, William Rowan Hamilton and Olinde Rodrigues.

Currently, there are three main methods of describing rotation in 3D space: Euler angles, rotation matrices and quaternions. In this investigation, we will compare and contrast these different rotational methods in order to draw conclusions about the usefulness and applicability of quaternions in 3D computer graphics and scientific simulations.

2 Rotation Matrices

2.1 Object & world axes

Any object transformation can be represented by where its three axes "end up" after the transformation. The direction of each axis is represented as a 3D vector of norm one, which "points" in the desired direction. However, the meaning of the "object's axes" is ambigous here. It is important to make the distinction between the "world axes" which represent the axes of the surrounding 3D scene, and the "object axes", which describe it in its own space, as if it were the only object in a scene. The useful property of this abstraction is that the object axes do not necessary have to be oriented the same as the world axes, and this can be leveraged for transformation.

The three object X,Y,Z axes can be represented by the vectors $\vec{x}$, $\vec{y}$, $\vec{z}$:

$$\vec{x} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad \vec{y} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad \vec{z} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

This orientation of the axes is called the "identity". It describes a space where all three axes are perpendicular, and are aligned with the world axes.

2.2 Rotating points

Whenever a point $\vec{p}$ has to be rotated, its X,Y and Z components (p_x, p_y and p_z respectively) can be multiplied by their respective object axis.

$$\vec{a} = \vec{x}p_x \quad \vec{b} = \vec{y}p_y \quad \vec{c} = \vec{z}p_z$$

The resulting vectors are then added together for the final position of the transformed point $\vec{r}$.

$$\vec{r} = \vec{a} + \vec{b} + \vec{c}$$

2.2.1 3×3 Matrix form

The process of transforming $\vec{p} \to \vec{r}$ is highly reminiscent of matrix multiplication. It is useful to represent $\vec{x}$, $\vec{y}$, $\vec{z}$ as a single 3×3 matrix of their components M of the form

$$M = \begin{bmatrix} \vec{x}_x & \vec{y}_x & \vec{z}_x \\ \vec{x}_y & \vec{y}_y & \vec{z}_y \\ \vec{x}_z & \vec{y}_z & \vec{z}_z \end{bmatrix}$$

The transformation of $\vec{p}$ to $\vec{r}$ can then be described by $M\vec{p}$ because of the properties of matrix multiplication, in that

$$M\vec{p} = \vec{M}_1 p_x + \vec{M}_2 p_y + \vec{M}_3 p_z \quad \text{where } M_n \text{ represents the } n\text{th column of } M.$$

Since the columns $\vec{M}_1$, $\vec{M}_2$, $\vec{M}_3$ correspond to the object axes X, Y and Z respectively, this is equivalent to the rotation equation shown in Section 2.2.

In this form, the identity axes are represented by the matrix $I = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$.

2.3 Construction from Euler angles

2.3.1 Concept

In real life, it is practical to represent rotations with easily measurable metrics, like angles. Aircraft and watercraft make extensive use of yaw, pitch and roll angles in instrumentation to aid their pilots in judging the orientation of the craft.

Euler angles are based around this concept. A set of Euler angles is a 3D vector containing the yaw, pitch and roll of an object from a reference frame. In the example of aircraft, the reference frame is usually the surface of the Earth. In space, it is usually a prominent constellation or celestial object.

It is possible to construct rotation matrices for a rotation of θ around each axis.

2.3.2 Deriving rotation matrices for each angle

Consider rotating the identity axes by θ around the X axis. Let the rotation matrix that describes this transformation be R_x.

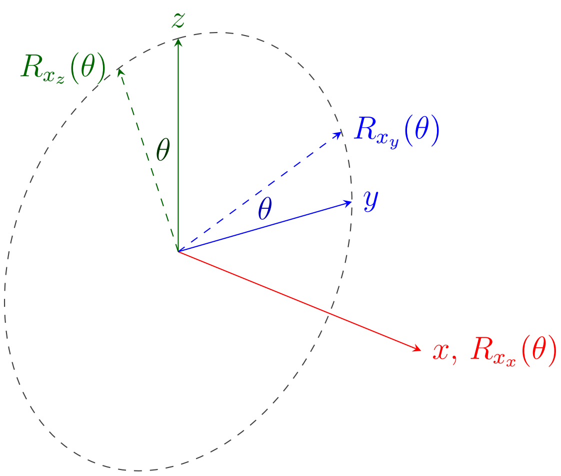


Figure 2: Rotation around the X-axis by angle θ. R_{x_x}, R_{x_y} and R_{x_z} represent the object axes after the transformation by $R_x(\theta)$ where $x \rightarrow R_{x_x}, y \rightarrow R_{x_y}$ and $z \rightarrow R_{x_z}$

From Figure 2 it becomes apparent that points that lie along the identity X-axis do not move at all. Hence, for the first column R_{x_x} representing the object X-axis post-transform,

$$R_{x_x}(\theta) = x = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

Points that lie along the Y axis get transformed against a circle of radius one along the YZ plane, meaning its coordinates are described by the trigonometric functions sine and cosine. Hence,

$$R_{x_y}(\theta) = \begin{bmatrix} 0 \\ \cos\theta \\ \sin\theta \end{bmatrix}$$

The Z-axis corresponds to the circle's Y-axis on a cartesian plane (along the 3D YZ plane), so it is as if the Z-axis was rotated by a right angle, then by θ. Hence,

$$R_{x_z}(\theta) = \begin{bmatrix} 0 \\ \cos\left(\theta + \frac{\pi}{2}\right) \\ \sin\left(\theta + \frac{\pi}{2}\right) \end{bmatrix} = \begin{bmatrix} 0 \\ -\sin\theta \\ \cos\theta \end{bmatrix}$$

.

Finally, combining R_{x_x}, R_{x_y} and R_{x_z},

$$R_x(\theta) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix}$$

A very similar process can be followed for the rotation matrices by the Y (R_y) and Z (R_z) axes, so it has been omitted for brevity. The only thing that changes in the process is that the plane of the circle follows the two axes perpendicular to the rotation axis.

$$R_y(\theta) = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix} \qquad R_z(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

2.3.3 Multiplication

For the Euler angles α, β and γ representing yaw, pitch and roll respectively, it is now possible to compute a general rotation matrix by first constructing each individual matrix, then multiplying them.

$$\begin{aligned} R(\alpha,\beta,\gamma) &= R_z(\gamma)R_y(\beta)R_x(\alpha) \\ &= \begin{bmatrix} \cos\gamma & -\sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & -\sin\alpha \\ 0 & \sin\alpha & \cos\alpha \end{bmatrix} \\ &= \begin{bmatrix} \cos\beta\cos\gamma & \sin\alpha\sin\beta\cos\gamma - \cos\alpha\sin\gamma & \cos\alpha\sin\beta\cos\gamma + \sin\alpha\sin\gamma \\ \cos\beta\sin\gamma & \sin\alpha\sin\beta\sin\gamma + \cos\alpha\cos\gamma & \cos\alpha\sin\beta\sin\gamma - \sin\alpha\cos\gamma \\ -\sin\beta & \sin\alpha\cos\beta & \cos\alpha\cos\beta \end{bmatrix} \end{aligned}$$

As matrix multiplication does not commute, it is not always the case that rotating by an axis A, then rotating by B would be the same as rotating first by axis B, then by A. Hence, it is important to note that the order of multiplication of R_z, R_y and R_x produces a unique final rotation. For the rest of the investigation, the $z \to y \to x$ rotation order seen above will be used. This is alternatively called the ZYX Tait-Bryan order.

2.4 The gimball lock problem

There is one large problem with constructing rotation matrices from Euler angles. Suppose you rotated an object with the Euler angles α, β and γ, where $\beta = \frac{\pi}{2}$

$$
\begin{aligned}
R(\alpha, \frac{\pi}{2}, \gamma) &= \begin{bmatrix} \cos\frac{\pi}{2}\cos\gamma & \sin\alpha\sin\frac{\pi}{2}\cos\gamma - \cos\alpha\sin\gamma & \cos\alpha\sin\frac{\pi}{2}\cos\gamma + \sin\alpha\sin\gamma \\ \cos\frac{\pi}{2}\sin\gamma & \sin\alpha\sin\frac{\pi}{2}\sin\gamma + \cos\alpha\cos\gamma & \cos\alpha\sin\frac{\pi}{2}\sin\gamma - \sin\alpha\cos\gamma \\ -\sin\frac{\pi}{2} & \sin\alpha\cos\frac{\pi}{2} & \cos\alpha\cos\frac{\pi}{2} \end{bmatrix} \\
&= \begin{bmatrix} 0 & \sin\alpha\cos\gamma - \cos\alpha\sin\gamma & \cos\alpha\cos\gamma + \sin\alpha\sin\gamma \\ 0 & \sin\alpha\sin\gamma + \cos\alpha\cos\gamma & \cos\alpha\sin\gamma - \sin\alpha\cos\gamma \\ -1 & 0 & 0 \end{bmatrix} \\
&= \begin{bmatrix} 0 & \sin(\alpha-\gamma) & \cos(\alpha-\gamma) \\ 0 & \cos(\alpha-\gamma) & -\sin(\alpha-\gamma) \\ -1 & 0 & 0 \end{bmatrix}
\end{aligned}
$$

Notice how in the above matrix, changing the value of both α and γ would result in a rotation around the world Z-axis as

$$
R_1 = \begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix}
$$

Hence, one degree of freedom is lost here - it is not possible to rotate the object by any other axis than the Z world axis, by changing either α or γ. This problem specifically occurs whenever you rotate around an axis by 90 degrees, and "align" it with another.

This fundamental flaw with Euler angles demonstrates how despite their simplicity and intuitiveness, they are not always the best choice for representing rotations.

In the Apollo 11 mission, (talk about gimball lock)

2.5 The spherical linear interpolation problem

3 Quaternions

3.1 Axis-angle

Another interesting way to represent the rotation of an object

3.2 Standard Form

Quaternions, like complex numbers, are defined with "real" and "imaginary" parts, and are essentially an extension of the complex numbers to four dimensions. The set of all quaternions is known as $\mathbb{H}$, named after the last initial of the Irish mathematician William Rowan Hamilton. Algebraically, a quaternion q can be defined in terms of the coefficients of its terms:

$$q = a + bi + cj + dk \quad a, b, c, d \in \mathbb{R}$$

i, j and k, called "basic quaternions", do not have an explicit definition of their value but are rather defined expressly in terms of the way they interact with each other in that they must satisfy the equality

$$i^2 = j^2 = k^2 = ijk = -1$$

3.3 Basic Quaternions

3.3.1 Multiplying by Real Numbers

For any $n \in \mathbb{R}$, it is defined that $in = ni$, $jn = nj$ and $kn = nk$. Hence, for any $q \in \mathbb{H}$, $qn = nq$. Quaternion multiplication by real numbers does, in fact, commute.

3.3.2 Multiplication by other basic quaternions

Hamilton's quaternion definition can then be used to derive the multiplicative interactions between i, j and k:

$$\begin{aligned} ijk &= k^2 \\ ijk^2 &= k^2k \\ ij(-1) &= (-1)k \\ ij &= k \end{aligned} \qquad \begin{aligned} ijk &= i^2 \\ i^2jk &= i \cdot i^2 \\ (-1)jk &= i(-1) \\ jk &= i \end{aligned}$$

$$\begin{aligned} i &= jk \\ ji &= j^2k \\ ji &= -k \end{aligned} \qquad \begin{aligned} k &= ij \\ kj &= ij^2 \\ kj &= -i \end{aligned}$$

$$\begin{aligned} ij &= k \\ kij &= k^2 \\ kij^2 &= k^2j \\ ki(-1) &= (-1)j \\ ki &= j \end{aligned} \qquad \begin{aligned} k &= ij \\ ik &= i^2j \\ ik &= -j \end{aligned}$$

An important concept becomes apparent from the above calculations - quaternion multiplication by other quaternions is not commutative, that is, it can be the case that $q_1q_2 \neq q_2q_1$ where $q_1, q_2 \in \mathbb{H}$. For example, it is seen above that while $ij = k$, $ji = -k$.

The multiplication table of basic quaternions is hence formed:

$\times$	i	j	k
i	-1	$-k$	j
j	k	-1	$-i$
k	$-j$	i	-1

Table 1: Basic quaternion noncommutative multiplication table

3.3.3 Associativity

Quaternion multiplication is associative in that $(q_1q_2)q_3 = q_1(q_2q_3)$ where $q_1, q_2, q_3 \in \mathbb{H}$. The same property applies for addition, $(q_1 + q_2) + q_3 = q_1 + (q_2 + q_3)$ where $q_1, q_2, q_3 \in \mathbb{H}$.

This associativity allows for application of useful algebraic techniques like the distributive law.

3.4 Quaternion Operations

3.4.1 Multiplication of non-basic quaternions

Let $q_1 = a_1 + b_1i + c_1j + d_1k$ and $q_2 = a_2 + b_2i + c_2j + d_2k$ where $a_1, b_1, c_1, d_1, a_2, b_2, c_2, d_2 \in \mathbb{R}$. The multiplication q_1q_2 can be computed using the distrivutive law.

$$\begin{aligned}
q_1q_2 &= (a_1 + b_1i + c_1j + d_1k)(a_2 + b_2i + c_2j + d_2k) \\
&= a_1a_2 + a_1b_2i + a_1c_2j + a_1d_2k \\
&+ b_1a_2i + b_1b_2i^2 + b_1c_2ij + b_1d_2ik \\
&+ c_1a_2j + c_1b_2ji + c_1c_2j^2 + c_1d_2jk \\
&+ d_1a_2k + d_1b_2ki + d_1c_2kj + d_1d_2k^2 \\
&\text{Applying the basic quaternion rules then} \\
&\text{factoring out the real part and } i,\ j, \text{ and } k, \\
&= a_1a_2 - b_1b_2 - c_1c_2 - d_1d_2 \\
&+ (a_1b_2 + b_1a_2 + c_1d_2 - d_1c_2)i \\
&+ (a_1c_2 - b_1d_2 + c_1a_2 + d_1b_2)j \\
&+ (a_1d_2 + b_1c_2 - c_1b_2 + d_1a_2)k
\end{aligned}$$

3.4.2 Conjugation

For any quaternion $q = a + bi + cj + dk \quad a, b, c, d \in \mathbb{R}$, its conjugate q^* is defined as $q^* = a - bi - cj - dk$.

3.4.3 Multiplication by Conjugate

Suppose one was to multiply a quaternion q by its conjugate q^*,

$$
\begin{aligned}
qq^* &= (a + bi + cj + dk)(a - bi - cj - dk) \\
&= a^2 - abi - acj - adk \\
&+ bia - (bi)^2 - bicj - bidk \\
&+ cja - cjbi - (cj)^2 - cjdk \\
&+ dka - dkbi - dkcj - (dk)^2 \\
&\text{Reordering real coefficients and expanding} \\
&= a^2 - abi - acj - adk \\
&+ abi - b^2i^2 - bcij - bdik \\
&+ acj - bcji - c^2j^2 - cdjk \\
&+ adk - bdki - cdkj - d^2k^2 \\
&\text{Applying basic quaternion rules} \\
&= a^2 - abi - acj - adk \\
&+ abi + b^2 - bck + bdj \\
&+ acj + bck + c^2 - cdi \\
&+ adk - bdj + cdi + d^2 \\
& \\
&a, b, c, d \in \mathbb{R} \\
&\therefore a^2 + b^2 + c^2 + d^2 \in \mathbb{R}
\end{aligned}
$$

Hence, if you multiply a quaternion by its conjugate, the result will always be a real number and equal to the sum of the squares of its coefficients.

3.4.4 Inverse

The inverse q^{-1} of a quaternion $q = a + bi + cj + dk$ exists such that $qq^{-1} = 1$, effectively "undoing" any multiplication caused by q. The inverse of a quaternion can be computed using the previosuly established rules.

$$
\begin{aligned}
&qq^{-1} = 1 \Rightarrow q^{-1} = \frac{1}{q} \\
&\frac{1}{q} \cdot \frac{q^*}{q^*} = \frac{q^*}{qq^*} = \frac{q^*}{a^2 + b^2 + c^2 + d^2}
\end{aligned}
$$

3.5 Proof that qpq^{-1} returns a pure quaternion

Whenever a pure quaternion is multiplied by a rotation quaternion, the transformation inevitably distorts it into the fourth dimension.

$$
\begin{aligned}
qp = {} & (a_q a_p - b_q b_p - c_q c_p - d_q d_p) \\
& + (a_q b_p + b_q a_p + c_q d_p - d_q c_p)i \\
& + (a_q c_p - b_q d_p + c_q a_p + d_q b_p)j \\
& + (a_q d_p + b_q c_p - c_q b_p + d_q a_p)k
\end{aligned}
$$

Let:

$$
\begin{aligned}
a_{qp} &= a_q a_p - b_q b_p - c_q c_p - d_q d_p, \\
b_{qp} &= a_q b_p + b_q a_p + c_q d_p - d_q c_p, \\
c_{qp} &= a_q c_p - b_q d_p + c_q a_p + d_q b_p, \\
d_{qp} &= a_q d_p + b_q c_p - c_q b_p + d_q a_p
\end{aligned}
$$

As q is of norm one, $q^{-1} = q^*$

$$
\begin{aligned}
& \therefore qpq^{-1} = qpq^* \\
& = a_{qp} a_q + b_{qp} b_q + c_{qp} c_q + d_{qp} d_q \\
& + (-a_{qp} b_q + b_{qp} a_q - c_{qp} d_q + d_{qp} c_q)i \\
& + (-a_{qp} c_q + b_{qp} d_q + c_{qp} a_q - d_{qp} b_q)j \\
& + (-a_{qp} d_q - b_{qp} c_q + c_{qp} b_q + d_{qp} a_q)k
\end{aligned}
$$

In order for qpq^* to be pure, its real part must be equal to zero. Let a_{qpq^*} be the real part of qpq^*.

$$
\begin{aligned}
a_{qpq^*} &= a_{qp} a_q + b_{qp} b_q + c_{qp} c_q + d_{qp} d_q \\
&= a_q (a_q a_p - b_q b_p - c_q c_p - d_q d_p) \\
&+ b_q (a_q b_p + b_q a_p + c_q d_p - d_q c_p) \\
&+ c_q (a_q c_p - b_q d_p + c_q a_p + d_q b_p) \\
&+ d_q (a_q d_p + b_q c_p - c_q b_p + d_q a_p) \\
&= a_q^2 a_p - a_q b_q b_p - a_q c_q c_p - a_q d_q d_p \\
&+ b_q a_q b_p + b_q^2 a_p + b_q c_q d_p - b_q d_q c_p \\
&+ c_q a_q c_p - c_q b_q d_p + c_q^2 a_p + c_q d_q b_p \\
&+ d_q a_q d_p + d_q b_q c_p - d_q c_q b_p + d_q^2 a_p \\
&= a_q^2 a_p + b_q^2 a_p + c_q^2 a_p + d_q^2 a_p \\
&= a_p (a_q^2 + b_q^2 + c_q^2 + d_q^2) \\
&= a_p = 0 \\
& \therefore qpq^{-1} \text{ is pure for } ||q||^2 = 1, \mathfrak{Re}(p) = 0
\end{aligned}
$$