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Quaternions in Classical Mechanics

The invention of the calculus of quaternions is a step towards the knowledge of quantities related to space which can only be compared for its importance, with the invention of triple coordinates by Descartes. The ideas of this calculus, as distinguished from its operations and symbols, are fitted to be of the greatest in all parts of science.
- J. C. Maxwell (1869). *Proceedings of the London Mathematical Society* **3**, p. 226.[1]

Quaternions come from Hamilton after his really good work had been done; and, though beautifully ingenious, have been an unmixed evil to those who have touched them in any way, including Clerk Maxwell.
- Lord Kelvin (1892). *Letter to Hayward* quoted by S. P. Thompson (1910), *The life of William Thompson, Baron Kelvin of Largs*. Macmillan, London, vol. II, p. 1070.[2]

Quaternions were invented by Sir William Rowan Hamilton as an extension to the complex numbers. Hamilton tried for ten years to create an analog of the complex numbers that had two distinct values, i and j, that were both roots of negative one.[3] Finally, while he was on a walk with his wife, he realized that he needed to have not two but three distinct imaginary units. Upon making this discovery he carved his result on the Broom Bridge in Dublin, which today is immortalized by a commemorative plaque.[4] Hamilton's defining relation is most succinctly written as:

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

Soon after discovering quaternions, Hamilton was able to find connections between this new algebra and spatial rotations. Although Hamilton derived his work independently, it had in fact been discovered earlier in a nearly identical form by a mostly unknown mathematician by the name of Olinde Rodrigues. Rodrigues in fact had a much stronger grasp on the algebra of rotations and even had the beginnings of what would later become Lie algebra.[5]

Compared to the calculus of vectors, quaternions have slipped into the realm of obscurity. They do however still find use in the computation of rotations. Many physical laws in classical, relativistic, and quantum mechanics can be written nicely using quaternions. Some physicists hope they will find deeper understanding of the universe by restating basic principles in terms of quaternion algebra.[6]

The unit quaternions form a group that is isomorphic to the group SU(2) and is a double cover of SO(3), the group of 3 dimensional rotations.[7] As such they are useful for representing rotations in both quantum and classical mechanics. Under these isomorphisms the quaternion multiplication operation corresponds to the composition operation of rotations.

1 S. L. Altmann, Rotations, Quaternions, and Double Groups, 1986, page 201
2 Altmann, page 9
3 Altmann, page 12
4 http://en.wikipedia.org/wiki/Quaternion
5 Altman, page 20-21
6 http://www.theworld.com/~sweetser/quaternions/qindex/qindex.html
7 http://en.wikipedia.org/wiki/Quaternion

Construction of quaternions from the complex numbers

The complex numbers can be constructed as an extension of the reals by introducing a quantity i with the property $i * i = -1$. Every complex number can then be written as $C = R_1 + i * R_2$ where R_1 and R_2 are real numbers. The quaternions can be constructed from the complex numbers in the same way. A new quantity j is defined such that $j * j = -1$ and the two imaginary units are assumed to anticommute so that $ij = -ji$. With this new unit a quaternion can be written as $Q = C_1 + j * C_2$ where C_1 and C_2 are complex numbers. This sequence can be repeated to generate higher order groups but something is lost each time. Quaternions are not commutative and the next step, the Cayley numbers, are not associative. The next group after the Cayley numbers is no longer a division ring (not every number has a multiplicative inverse).[8]

Quaternion arithmetic

Every quaternion can be written in terms of its basis components

$$Q = [q_0, q_1, q_2, q_3] = q_0 + iq_1 + jq_2 + kq_3,$$

with addition defined pairwise and multiplication defined by the following rules:

$$i^2 = j^2 = k^2 = -1$$
$$ij = -ji = k$$
$$jk = -kj = i$$
$$ki = -ik = j.$$ [9]

Quaternions may also be written as an ordered pair of a scalar and a vector

$$Q = [q_0, \vec{q}].$$

A quaternion with only a scalar part is called a *real quaternion* and a quaternion with only a vector part is called a *pure quaternion*.[10] It is customary to use a shorthand notation for writing a quaternion that has only a scalar or vector component as if it was simply just a scalar or a vector:

$q_0 \equiv [q_0, \vec{0}]$, $\vec{q} \equiv [0, \vec{q}]$, and $q_0 + \vec{q} = [q_0, \vec{q}]$.

In this ordered pair notation the multiplication law can be rewritten as

$$PQ = [p_0 q_0 - \vec{p} \cdot \vec{q}, p_0 \vec{q} + q_0 \vec{p} + \vec{p} \times \vec{q}].$$ [11]

This can be split into a symmetric and an antisymmetric product

$\frac{PQ+QP}{2} = [p_0 q_0 - \vec{p} \cdot \vec{q}, p_0 \vec{q} + q_0 \vec{p}]$ and

$$\frac{PQ-QP}{2} = [0, \vec{p} \times \vec{q}].$$ [12]

The complex conjugate of a quaternion is $Q^* = [q_0, -\vec{q}]$ and has the property $(PQ)^* = Q^* P^*$.[13]

The norm is $|Q| = \sqrt{Q^* Q} = \sqrt{q_0^2 + \vec{q}^2}$ and the multiplicative inverse is $Q^{-1} = \frac{Q^*}{|Q|^2}$.[14] Quaternions with norm 1 are called *unit quaternions*.

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8 R. Gilmore, Lie Groups, Lie Algebras, and Some of Their Applications, 2002, page 17-18
9 J. B. Kuipers, Quaternions and Rotation Sequences, 1999, page 104-106
10 Altmann, page 203
11 Kuipers, page 108
12 http://en.wikipedia.org/wiki/Quaternion
13 Kuipers, page 110
14 Kuipers, page 111-112

If $n=[0,\hat{n}]$ is a unit quaternion with zero real part then it is easy to see from the multiplication rule that $n^2=-1$. From this it follows that the units 1 and n form a group isomorphic to the complex plane. In particular, Euler's relation holds:

$$e^{\theta n}=cos(\theta)+\hat{n}sin(\theta).$$ [15]

The standard rules of arithmetic can be used to extend this result to arbitrary quaternions:

$$e^{Q}=e^{q_0}e^{|\vec{q}|\hat{q}}=e^{q_0}[cos(|\vec{q}|)+\hat{q}sin(|\vec{q}|)].$$

Quaternions as a Lie algebra

The quaternions form a continuous group and therefore can be represented by a Lie algebra. Any general quaternion can then be formed from the generators of the Lie algebra via exponentiation.[16] To make the discussion easier we will temporarily change our notation and use the basis elements $\lambda_0,\lambda_1,\lambda_2,\lambda_3$ instead of $1,i,j,k$. The quaternions in the vicinity of identity can then be written

$$1\lambda_0+\delta q=(1+\tfrac{1}{2}\delta\theta^0)\lambda_0+\sum_{i=1}^{3}\frac{1}{2}\delta\theta^i\lambda_i$$

where $\delta\theta^i$ are infinitesimal constants and the factor of $\frac{1}{2}$ has been introduced to make the commutators appear the way we want. The Lie generators are therefore

$$X_i=\tfrac{1}{2}\lambda_i$$

and the commutators (the Lie algebra) are

$$[X_0,X_i]=0$$

$$[X_i,X_j]=\epsilon_{ijk}X_k.$$ [17]

The subgroup of unit quaternions is given by setting $\delta\theta^0=0$. In this case the X_0 generator is not used and the Lie algebra is given by $[X_i,X_j]=\epsilon_{ijk}X_k$ which is exactly the same Lie algebra as that for three dimensional rotation.[18] The group of unit quaternions is therefore isomorphic to the group of three dimensional rotations.

The Lie group is computed from the Lie algebra via exponentiation, so a general group element is given by $e^{\theta^i X_i}$. Using Euler's formula and the fact that the λ_i are pure unit quaternions, this can be written as

$$e^{\theta^i X_i}=e^{\frac{\theta^i}{2}\lambda_i}=cos(\tfrac{\theta}{2})+\hat{\theta}^i\lambda_i sin(\tfrac{\theta}{2}).$$

Using the isomorphism between unit quaternions and three dimensional rotations shows that a rotation by the angle θ about the axis $\hat{\theta}$ is represented by the quaternion $cos(\frac{\theta}{2})+\hat{\theta}^i\lambda_i sin(\frac{\theta}{2})$, which is known as the Rodrigues quaternion. In this context the quaternion parameters are known as Euler-Rodrigues parameters.[19] The conjugate of the quaternion then gives the inverse rotation, as can be seen by negating $\vec{\theta}$.

Using quaternions to rotate vectors

The group of unit quaternions have the same algebra as the three dimensional rotations so it is reasonable to assume that they can somehow be used to rotate vectors. This cannot be done with the tools that have so far been developed because we can compose rotations (via quaternion multiplication) but we have not yet devised a way for a quaternion to operate upon a vector. The way to solve this problem is to turn the vector into a rotation. Each unit vector can be considered as an axis of rotation and the quaternion that represents rotation about that axis can be associated with the vector. For

15 http://en.wikipedia.org/wiki/Quaternion
16 Goldstein, Poole, Safko, Classical Mehanics Third Edition, 2002, page 612
17 Gilmore, page 121
18 Gilmore, page 121-124
19 Altmann, page 20

simplicity we take the angle of rotation to be π. We therefore have a map between vectors and rotations (unit quaternions) defined as

$$\hat{v} \mapsto R(\hat{v}, \pi) = [0, \hat{v}],$$

where the last term is a quaternion.[20]

To rotate this vector we need to devise a scheme for turning a rotation about one axis into a rotation about another axis. This is accomplished by the similarity transform $v' = QvQ^*$. This transform serves as a change of coordinates so that rotation about the $\hat{v}$ axis becomes rotation about the $\hat{v}'$ axis. We have thus accomplished the goal of rotating the vector $\hat{v}$.[21] Since real numbers always commute with quaternions, the same equation can also be used for vectors that are not of unit length. The general rotation equation is then

$$Q = cos(\tfrac{\theta}{2}) + \hat{\theta}^i \lambda_i sin(\tfrac{\theta}{2})$$
$$[0, \vec{v}'] = Q[0, \vec{v}]Q^*.$$

This quaternion representation of rotations has advantages over the competing methods of Euler angles and orthogonal matrices. Given a rotation in quaternion notation it is easy to find the angle and axis of rotation, which is difficult to do with Euler angles or matrices. In fact, the easiest way to create a rotation matrix from an axis and angle is to use quaternions. Quaternions also avoid the gimbal lock (discontinuities) of Euler angles. Unlike matrices, quaternions always represent orthogonal transformations even in the face of numeric instability. For these reasons, quaternions are widely used in computer graphics and navigation systems.[22]

In addition to rotations, quaternions can be used to compute reflections. If $\hat{n}$ is a unit vector then the reflection of a vector $\vec{v}$ across the plane normal to $\hat{n}$ is given by $[0, \hat{n}][0, \vec{v}][0, \hat{n}]$. Two reflections in sequence define a rotation and this rotation is computed as

$$[0, \hat{n}][0, \hat{m}] = [-\hat{n} \cdot \hat{m}, -\hat{n} \times \hat{m}] = -[cos(\theta), sin(\theta)\frac{\hat{n} \times \hat{m}}{|\hat{n} \times \hat{m}|}]$$

where θ is the angle between $\hat{n}$ and $\hat{m}$. The composition of reflections is therefore equal to a rotation by an angle 2θ about the axis $\hat{n} \times \hat{m}$.[23]

The topology of quaternion rotations

The group of unit quaternions has the same Lie algebra as the group of 3-dimensional rotations (also known as SO(3)) but there is a fundamental difference: each element of SO(3) corresponds to two unit quaternions, Q and -Q. This can be seen by taking a look at the rotation recipe

$$\vec{v}' = Q\vec{v}Q^* = (-Q)\vec{v}(-Q)^*.$$

This equivalence is expressed by saying that the unit quaternion group is a double cover of SO(3).[24] The resulting difference in topology explains why quaternions don't suffer from the gimbal lock of Euler angles and other representations.

To visualize the topology of rotations imagine a solid ball of radius π. The points in this ball each correspond to a rotation with the direction from the origin representing the axis of rotation and the distance from the origin representing the angle of rotation. Since a rotation by π and a rotation by $-\pi$ are equivalent, the antipodes of the surface of the ball need to be identified with each other. The ball we have set up therefore does not depict rotation in a continuous way – the antipodal points of the ball are considered to be the same even though they are far apart in our representation.[25] This lack of continuity is the source of the gimbal lock of Euler angles and the axis-angle representation.

The problem can be fixed be considering a second ball superimposed upon the first with

20 Altmann, page 214-215
21 Altmann page 214-215
22 http://en.wikipedia.org/wiki/Quaternions_and_spatial_rotation
23 W. B. Heard, Rigid Body Mechanics, 2006, page 25
24 Heard, page 35
25 http://en.wikipedia.org/wiki/Rotation_group#Topology

coordinates that are a mirror image of the first. The two surfaces are glued together so that a rotation by π on the one ball is connected to the corresponding rotation by $-\pi$ on the other. This object is equivalent to S^3, the three-dimensional sphere (in the same way that two discs glued together form the two-dimensional sphere S^2). The topology is now represented by a simply connected and continuous shape in four parameters ($S^3 = \{x \in \Re^4 | x \cdot x = 1\}$)[26] but the price paid is that there are now two points corresponding to each rotation. This is the topology of the unit quaternions and of SU(2), the 2x2 special unitary matrices.

Despite its more elegant structure (S^3 instead of a strangely connected hemisphere of S^3), there is a very nonintuitive property of unit quaternions – namely the fact that the quaternion representing rotation by $360°$ is -1 as can be seen by substituting 2π into our previously derived formula:

$$Q = cos(\frac{2\pi}{2}) + \hat{\theta}^i \lambda_i sin(\frac{2\pi}{2}) = -1.$$

In order to get back to 1 we need a rotation by $720°$.[27] This double valued nature of unit quaternions is in a strange way related to certain unwinding problems. For example, consider a coffee cup attached to the walls by an elastic band. When the coffee cup is rotated by $360°$ the elastic bands will get wrapped up. They can be untangled but no matter what is done there will always be a twist in the bands. If the cup is now rotated another $360°$ in the same direction it will be possible to completely untangle the bands with no remaining twist.[28] This is just one of many examples where a rotation by $720°$ is needed to get back to the identity. Similar issues arise in quantum mechanics in regard to the electron spin.

The matrix representation of the quaternion group

Quaternions can be represented in the form of 2x2 complex or 4x4 real matrices in such a way that matrix multiplication corresponds to quaternion multiplication. The 2x2 complex representation is

$$Q = q_0 + q_1 i + q_2 j + q_3 k = \begin{pmatrix} q_0 + iq_3 & iq_1 - q_2 \\ iq_1 + q_2 & q_0 - iq_3 \end{pmatrix},$$

which can be conveniently written as

$$Q = q_0 I + q_1(i\sigma_1) + q_2(i\sigma_2) + q_3(i\sigma_3)$$

where I is the identity matrix and the σ_j are the Pauli spin matrices.[29] In this form the determinant of the matrix is equal to the square of the norm of the quaternion and the matrix transpose corresponds to quaternion conjugation.[30] The four components of this matrix are called the Cayley-Klein parameters $\alpha, \beta, \gamma, \delta$:[31]

$$Q = \begin{pmatrix} q_0 + iq_3 & iq_1 - q_2 \\ iq_1 + q_2 & q_0 - iq_3 \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix}$$

The Cayley-Klein parameters satisfy the relation $\beta = -\gamma^*$ and $\delta = \alpha^*$. In this context the group of unit quaternions is called SU(2), the 2x2 special unitary matrices.

The representation as a 4x4 real matrix is

$$Q = \begin{pmatrix} q_0 & -q_1 & -q_2 & -q_3 \\ q_1 & q_0 & -q_3 & q_2 \\ q_2 & q_3 & q_0 & -q_1 \\ q_3 & -q_2 & q_1 & q_0 \end{pmatrix},$$

which is a useful way to compute quaternion products:

26 Heard, page 35
27 Altmann, page 22-24
28 http://en.wikipedia.org/wiki/Orientation_entanglement
29 Gilmore, page 17
30 http://en.wikipedia.org/wiki/Quaternion
31 Heard, page 31

$$QP = \begin{pmatrix} q_0 & -q_1 & -q_2 & -q_3 \\ q_1 & q_0 & -q_3 & q_2 \\ q_2 & q_3 & q_0 & -q_1 \\ q_3 & -q_2 & q_1 & q_0 \end{pmatrix} \begin{pmatrix} p_0 \\ p_1 \\ p_2 \\ p_3 \end{pmatrix}.$$ [32]

The rotation operator $R(\vec{v}) = Q[0, \vec{v}]Q*$ can be represented as the 3x3 real matrix

$$R = \begin{pmatrix} q_0^2 + q_1^2 - q_2^2 - q_3^2 & 2(q_1 q_2 - q_0 q_3) & 2(q_1 q_3 + q_0 q_2) \\ 2(q_2 q_1 + q_0 q_3) & q_0^2 - q_1^2 + q_2^2 - q_3^2 & 2(q_2 q_3 - q_0 q_1) \\ 2(q_3 q_1 - q_0 q_2) & 2(q_3 q_2 + q_0 q_1) & q_0^2 - q_1^2 - q_2^2 + q_3^2 \end{pmatrix}.$$ [33]

This is a convenient way to generate a rotation matrix from an axis/angle representation. Notice that Q and $-Q$ both correspond to the same rotation matrix R. This is due to the fact that the group of quaternions is a double cover of SO(3), the group of special orthogonal matrices.

The mechanics of quaternion rotations

Suppose the that orientation of a body is represented as a quaternion rotation so that $\vec{v}' = Q\vec{v}Q^*$ where $\vec{v}'$ is a vector in fixed space coordinates and $\vec{v}$ is a vector in body coordinates. It is then possible to compute the angular velocity in terms of the quaternion parameters. The derivative of $\vec{v}'$ is (assuming $\vec{v}$ is constant)

$$\dot{\vec{v}}' = \dot{Q}\vec{v}Q^* + Q\vec{v}\dot{Q}^*.$$

Substituting to express this in terms of fixed coordinates gives

$$\dot{\vec{v}}' = \dot{Q}(Q^*Q)\vec{v}(Q^*Q)Q^* + Q(Q^*Q)\vec{v}(Q^*Q)\dot{Q}^*,$$
$$\dot{\vec{v}}' = \dot{Q}Q^*\vec{v}' + \vec{v}'Q\dot{Q}^*.$$

The scalar part of $\dot{Q}Q^*$ happens to be zero because Q is a unit quaternion, so

$$\dot{Q}Q^* = -(\dot{Q}Q^*)^* = -Q\dot{Q}^*.$$

Substituting this into the above gives

$$\dot{\vec{v}}' = \dot{Q}Q^*\vec{v}' - \vec{v}'\dot{Q}Q^*$$

which is just the antisymmetric product of $\dot{Q}Q^*$ and $\vec{v}'$. As shown above, the antisymmetric product is just the vector cross product, so $\dot{\vec{v}}' = 2\vec{w} \times \vec{v}'$ where $[0, \vec{w}] = \dot{Q}Q^*$. Comparing this to the expression for angular velocity $\dot{\vec{v}}' = \vec{\omega} \times x$ it is clear that $\vec{\omega} = 2\vec{w}$ so that

$$[0, \vec{\omega}] = 2\dot{Q}Q^*.$$ [34]

In terms of components the relation is

$$\begin{pmatrix} 0 \\ \omega \end{pmatrix} = 2 \begin{pmatrix} q_0 & q_1 & q_2 & q_3 \\ -q_1 & q_0 & -q_3 & q_2 \\ -q_2 & q_3 & q_0 & -q_1 \\ -q_3 & -q_2 & q_1 & q_0 \end{pmatrix} \begin{pmatrix} \dot{q_0} \\ \dot{q_1} \\ \dot{q_2} \\ \dot{q_3} \end{pmatrix}.$$ [35]

In terms of the Cayley-Klein parameters this is written as

$$\omega_1 + i\omega_2 = 2i(\beta\dot{\delta} - \dot{\beta}\delta)$$
$$\omega_1 - i\omega_2 = 2i(\gamma\dot{\alpha} - \dot{\gamma}\alpha)$$
$$\omega_3 = 2i(\alpha\dot{\delta} - \dot{\beta}\gamma) = 2i(\beta\dot{\gamma} - \dot{\alpha}\delta).$$ [36]

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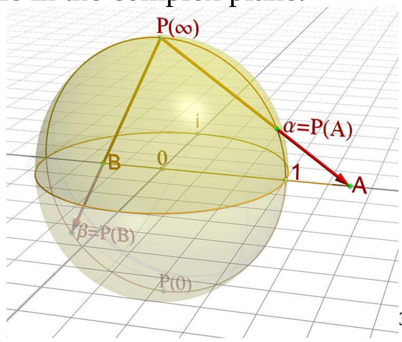
32 Heard, page 22
33 Heard, page 24
34 http://audiophile.tam.cornell.edu/~als93/quaternion.pdf
35 Heard, page 49
36 A.I. Lurie, Analytical Mechanics, 2002, page 139

Another way to rotate – Möbius transformations

There is one more way to represent rotations of 3-dimensional unit vectors. The unit vectors sit on the surface of the Riemann sphere, which is a unit sphere centered on the origin of the complex plane. The points on the sphere are identified with the points on the complex plane through stereographic projection. A line is drawn from the north pole to each point on the sphere. The point where the line intersects the complex plane is identified with the point where the line intersects the sphere. Under this mapping the north pole corresponds to ∞, the south pole corresponds to 0, and the equator corresponds to the unit circle in the complex plane.[37]



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When the sphere is rotated the image of the sphere will be transformed in the complex plane. Since the axis of rotation consists of two points on the sphere that do not move, their image in the complex plane will not move either. The orbits of rotation are circles on the sphere and they are circles on the complex plane also.[39] After a bit of algebra it can be shown that the rotation transforms points in the complex plane as

$$z' = f(z) = \frac{\alpha z+\beta}{-\beta^* z+\alpha^*},$$

where α, β, γ, and δ are the Cayley-Klein parameters.[40] There is a one-to-one correspondence between these Möbius transformations and the matrices in SU(2)

$$\begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix} \leftrightarrow \frac{\alpha z+\beta}{-\beta^* z+\alpha^*}$$

such that matrix multiplication in SU(2) corresponds to composition of functions in the complex plane: if $A \leftrightarrow z' = f(z), B \leftrightarrow z' = g(z)$ then $AB \leftrightarrow z' = f(g(z))$.[41]

Conclusion

Quaternions appear to be in most cases much clumsier than vectors but they do seem to have advantages in the calculation of rotations. Goldstein's Classical Mechanics said that the Cayley-Klein parameters were of great use in the calculation of gyroscopic motion but I was not able to find any examples of complete physical problems solved in terms of quaternions - the reference given in Goldstein was the only example I could find and it was written in German. The formula for angular momentum was rather elegant in my opinion and in principle it could be used to form the kinetic energy term in the Lagrangian. I suspect though that by the time it was converted to the body coordinates and put into a quadratic form it would no longer be so elegant. On the other hand, Euler angles are not too friendly in this context either. Mainly what I got from doing this project was a greater appreciation of the algebra of rotations.

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37 Heard, page 31
38 http://en.wikipedia.org/wiki/Riemann_sphere
39 Heard, page 32
40 Heard, page 34
41 Heard, page 35

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