

If Hamilton Had Prevailed: Quaternions in Physics

J. Lambek

This is a nostalgic account of how certain key results in modern theoretical physics (prior to World War II) can be expressed concisely in the language of quaternions, thus suggesting how they might have been discovered if Hamilton's views had prevailed. In the first instance, *biquaternions* are used to discuss special relativity and Maxwell's equations. To express Dirac's equation of the electron, we are led to replace the complex number i by the *right regular representation* of the quaternion unit i_1 . Looked at in this way, it is actually equivalent to the relativistic version of Schrödinger's equation. The complex number i reappears as soon as we consider the electron in an electromagnetic field. When expressed in terms of complex matrices, Dirac's equation turns out to be invariant not only under a projective representation of the Lorentz group and under Weyl's gauge transformation but also under a projective representation of $SU(3)$.

The Invention of Quaternions

Bourbaki introduced the following symbols for various species of numbers:

$$\mathbb{N} \subset \mathbb{Z} \subset \mathbb{Q} \subset \mathbb{R} \subset \mathbb{C} \subset \mathbb{H},$$

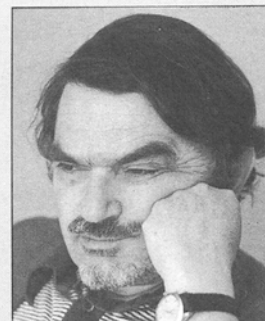
referring to the *naturals*, *integers*, *rationals*, *reals*, *complex numbers*, and *quaternions*, respectively. This sequence expresses a logical development of the number system, but its historical (and pedagogical) development proceeds somewhat differently:

$$\mathbb{N}^+ \subset \mathbb{Q}^+ \subset \mathbb{R}^+ \subset \mathbb{R} \subset \mathbb{C} \subset \mathbb{H},$$

where \mathbb{N}^+ , \mathbb{Q}^+ , and \mathbb{R}^+ refer to the positive naturals, positive rationals, and positive reals, respectively.

Not many mathematicians can claim to have introduced (invented? discovered?) a new kind of number. Although the positive reals had been effectively used by Thales, as ratios of geometric quantities, it was only after the Pythagoreans discovered, to their great discomfort, that the equation $x^2 = 2$ cannot be solved for rational x , that a rigorous definition of the positive reals was given by Eudoxus, essentially by what we now call

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J. Lambek is now retired from active teaching, but McGill University is kindly letting him keep his office. Although primarily a mathematician, he takes an amateur's interest in other matters, such as the ultimate nature of reality. A book on the history and philosophy of mathematics, written in collaboration with Bill Anglin, is just about complete.

Dedekind cuts. As far as we know, the Indian mathematician Brahmagupta was the first to allow zero and negative numbers to be subject to arithmetical operations, thus permitting the transition from \mathbb{R}^+ to \mathbb{R} . Cardano, perhaps better known as a physician than as a mathematician, introduced complex numbers, not just to solve equations such as $x^2 + 1 = 0$, but because they were needed to find real solutions of cubic equations with real coefficients.

After Gauss had proved the fundamental theorem of algebra, there was no longer any need to introduce new numbers to solve equations. It was with a different motivation in mind that quaternions were invented by William Rowan Hamilton and, according to Altmann [1986], independently by Olinde Rodrigues. (He also points out that they were already known to Gauss.)

Hamilton had already made important contributions to mathematical physics, the most celebrated one being his reformulation of the Euler-Lagrange equations in a form in which position and momentum appear on the same footing. He was now looking for numbers of the form $x + iy + jz$, with $i^2 = j^2 = -1$, which would do for space what complex numbers had done for the plane. According to Conway [1951], he may have been influenced by the complex number identity

$$(x + iy)(x - iy) = x^2 + y^2$$

when he looked at

$$(x + iy + jz)(x - iy - jz) = x^2 + y^2 + z^2 - (ij + ji)yz.$$

In 1843 he had the sudden insight to abandon the commutative law of multiplication. (It should be noted that matrix multiplication may have come later.) Writing $ij = k$, he found that

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

Numbers of the form $a + bi + cj + dk$, with $a, b, c, d \in \mathbb{R}$, were called *quaternions*. They were added, subtracted, and multiplied according to the usual laws of arithmetic, except for the commutative law of multiplication.

It will be convenient to replace i, j , and k by i_1, i_2 , and i_3 , respectively, so that any quaternion can be written as

$$a = a_0 + i_1 a_1 + i_2 a_2 + i_3 a_3 = \sum_{\alpha=0}^3 i_{\alpha} a_{\alpha},$$

where $i_0 = 1$. The *conjugate* of a is given by

$$a^{\dagger} = a_0 - i_1 a_1 - i_2 a_2 - i_3 a_3,$$

and one notes that aa^{\dagger} and $a^{\dagger}a$ are both equal to the real number

$$N(a) = a_0^2 + a_1^2 + a_2^2 + a_3^2,$$

called the *norm* of a . When $a \neq 0$, one can define $a^{-1} = a^{\dagger}/N(a)$, so that

$$aa^{-1} = 1 = a^{-1}a.$$

The quaternions form a *skew field* or *division ring*, which is denoted by \mathbb{H} in Hamilton's honour, \mathbb{Q} having been preempted for the field of rationals. Note also that $(ab)^{\dagger} = b^{\dagger}a^{\dagger}$.

As far as we know, Hamilton was the first to look at a noncommutative system of numbers. Had matrices been known to him, Hamilton might have defined

$$i_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad i_2 = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix},$$

where i is the ordinary complex square root of -1 , thus forcing

$$i_3 = i_1 i_2 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}.$$

If these three matrices are multiplied by $-i$, one obtains the so-called *Pauli spin matrices*, which were to play a role in quantum mechanics later. Thus, the quaternion a could have been identified with the complex 2-by-2 matrix

$$\begin{pmatrix} a_0 + ia_3 & a_1 + ia_2 \\ -a_1 + ia_2 & a_0 - ia_3 \end{pmatrix} = \begin{pmatrix} u & v \\ -v^* & u^* \end{pmatrix},$$

where u and v are complex numbers with complex conjugates u^* and v^* . Note that the quaternion conjugate of such a matrix is

$$\begin{pmatrix} u^* & -v \\ v^* & u \end{pmatrix},$$

which is the same as the complex conjugate of the transposed matrix.

Replacing 0, 1, and i in these complex matrices by

$$\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

respectively, one can obtain a representation of quaternions as 4-by-4 real matrices. A more natural way of representing quaternions by real matrices is with the help of linear algebra. Clearly, the mapping $x \mapsto ax$, induced by left multiplication with a , is a linear transformation of the vector space of quaternions x , hence can be represented by a 4-by-4 real matrix $L(a)$. Writing $[x]$ for the column vector associated with the quaternion $x = \sum_{\alpha=0}^3 i_{\alpha} x_{\alpha}$, namely, the transposed of the row vector (x_0, x_1, x_2, x_3) , we thus have

$$[ax] = L(a)[x].$$

We may also represent the linear mapping $x \mapsto xb$, induced by right multiplication with b , by a matrix $R(b)$ such that

$$[xb] = R(b)[x].$$

In view of the associative law

$$(ax)b = a(xb)$$

for quaternions, we have

$$R(b)L(a) = L(a)R(b), \quad L(ax) = L(a)L(x), \\ R(xb) = R(b)R(x).$$

Thus, $L : \mathbb{H} \rightarrow M_4(\mathbb{R})$ and $R : \mathbb{H}^{\text{op}} \rightarrow M_4(\mathbb{R})$ are ring homomorphisms.

Applications to Classical Physics

It seems reasonable to represent a three-dimensional vector (x_1, x_2, x_3) by the headless quaternion

$$\xi = i_1x_1 + i_2x_2 + i_3x_3;$$

but what is the meaning of the fourth coordinate x_0 ? Influenced by the pre-Socratic philosopher Parmenides, who believed that the flow of time is an illusion, Hamilton might have suspected that x_0 stands for time. But what then is the significance of the norm $N(x)$ when $x_0 \neq 0$? (Of course, when $x_0 = 0$, it stands for the square of the distance from the origin.)

If we assume that ξ and

$$\eta = i_1y_1 + i_2y_2 + i_3y_3$$

are pure 3-vectors, then

$$\xi\eta = -(\xi \circ \eta) + \xi \times \eta,$$

where

$$\xi \circ \eta = x_1y_1 + x_2y_2 + x_3y_3$$

and

$$\xi \times \eta = i_1(x_2y_3 - x_3y_2) + i_2(x_3y_1 - x_1y_3) + i_3(x_1y_2 - x_2y_1)$$

came to be called the *scalar product* and *vector product*, respectively. It was these two products which were applied to physics in the vector analysis of Gibbs and Heaviside, rather than the quaternion product. In particular, writing

$$\nabla = i_1 \frac{\partial}{\partial x_1} + i_2 \frac{\partial}{\partial x_2} + i_3 \frac{\partial}{\partial x_3},$$

one usually summarizes Maxwell's equations as follows:

$$\nabla \circ \mathbf{B} = 0, \quad \nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0, \\ \nabla \circ \mathbf{E} = \rho, \quad \nabla \times \mathbf{B} - \frac{\partial \mathbf{E}}{\partial t} = \mathbf{j},$$

where

$$\mathbf{B} = B_1i_1 + B_2i_2 + B_3i_3, \quad \mathbf{E} = E_1i_1 + E_2i_2 + E_3i_3$$

represent the magnetic and electric fields, respectively, ρ is the charge density, and \mathbf{j} is the current density. (Units have been chosen to make c , the velocity of light, equal to one light-second per second.) These laws are usually ascribed to Coulomb, Faraday, Gauss, and Ampère, respectively, although it was Maxwell who added the term $\partial \mathbf{E} / \partial t$ to the last equation. This addition is in fact crucial to what follows.

Using the language of quaternions, albeit quaternions with complex components, known as *biquaternions*, Maxwell's four equations may be combined into a single equation:

$$\left(\frac{\partial}{\partial t} - i\nabla \right) (\mathbf{B} + i\mathbf{E}) + (\rho + i\mathbf{j}) = 0.$$

As far as I know, this was first pointed out independently by Conway [1911] and Silberstein [1912], although it might have been realized by Clerk Maxwell himself, when he said in 1869:

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.

It follows from Maxwell's equations that

$$\frac{\partial \rho}{\partial t} + \nabla \circ \mathbf{j} = 0.$$

This is known as the *equation of continuity*, which asserts that the scalar part of

$$\left(\frac{\partial}{\partial t} + i\nabla \right) (\rho + i\mathbf{j})$$

is zero. Another consequence of Maxwell's equations is the existence of a 4-potential, here denoted by the biquaternion $\varphi + i\mathbf{A}$, such that

$$\mathbf{E} = -\nabla\varphi - \frac{\partial \mathbf{A}}{\partial t}, \quad \mathbf{B} = \nabla \times \mathbf{A}.$$

In quaternion notation, this asserts that the vector part of

$$\left(\frac{\partial}{\partial t} + i\nabla \right) (\varphi + i\mathbf{A})$$

is $\mathbf{B} + i\mathbf{E}$. (Sometimes, the scalar part is put equal to zero.)

If Maxwell had faith in quaternions, other physicists despised them. Thus, Oliver Heaviside, as quoted by Conway [1948], asserted that quaternions are "a positive evil of no inconsiderable magnitude," and William

Thomson, better known as Lord Kelvin, as quoted by Altmann [1986], said that they “have been an unmixed evil to those who touched them in any way, including Clerk Maxwell.” Even Minkowski, who should have known better, rejected quaternions as “too narrow and clumsy.” It may be difficult to understand how a mathematical concept can evoke such strong antagonism; but, even in our day, similar opinions have been expressed about categories, although for different reasons.

Not surprisingly, quaternions never entered the mainstream of physics, yet they had a small but dedicated group of devotees, of whom I shall only mention the few whose articles are cited in the bibliography: Conway, Dirac, Silberstein, Weiss, Gürsey, and Synge. My own interest as a graduate student was raised by the inspiring book by Silberstein [1924] and led to Part I of my thesis, from which, however, all physics was expunged when I realized that my main ideas had been anticipated by Conway [1948].

If we take the quaternion form of Maxwell’s equations seriously, we are led to the study of quaternions with complex components, also called *biquaternions*. Extending the representation of quaternions as 2-by-2 complex matrices to biquaternions, we see that the latter must be represented by matrices of the form

$$\begin{pmatrix} u & v \\ -v^* & u^* \end{pmatrix} + i \begin{pmatrix} u' & v' \\ -v'^* & u'^* \end{pmatrix}.$$

But it is easily seen that any 2-by-2 complex matrix is of this form, as we can solve the four equations

$$\begin{aligned} u + iu' &= p, & v + iv' &= q, \\ -v^* - iv'^* &= r, & u^* + iu'^* &= s \end{aligned}$$

for $u, v, u',$ and v' . For example, writing $u = u_0 + iu_1$, $v = v_0 + iv_1$, and so on, and adding the first and last equations, we see that

$$2u_0 + 2iu'_0 = p + s,$$

so that

$$u_0 = \frac{1}{2} (p_0 + s_0).$$

Thus, the algebra of biquaternions is isomorphic to $M_2(\mathbb{C})$.

The complex conjugate

$$(a + ib)^* = a - ib$$

of a biquaternion is then represented by the conjugate matrix, whereas the quaternion conjugate

$$(a + ib)^\dagger = (a_0 + ib_0) - i_1(a_1 + ib_1) - i_2(a_2 + ib_2) - i_3(a_3 + ib_3)$$

is represented by the transposed matrix.

We may also extend the representation L of quaternions as 4-by-4 real matrices to one of biquaternions as 4-by-4 complex matrices. Using the same letter L for the latter, we see that again

$$L(c^*) = L(c)^*, \quad L(c^\dagger) = L(c)^\dagger$$

are the conjugate and transposed matrices, respectively. For the present, we shall favour this representation and identify the biquaternion c with the matrix $L(c)$ in $M_4(\mathbb{C})$, although later we shall look at a representation of biquaternions in $M_4(\mathbb{R})$.

Applications to Special Relativity

The special theory of relativity requires the invariance of the expression $t^2 - x_1^2 - x_2^2 - x_3^2$ under a coordinate transformation passing from a stationary platform to a moving train. This suggests that position in space and time be joined together in a biquaternion of the form

$$x = x_0 + ii_1x_1 + ii_2x_2 + ii_3x_3 = t + i\mathbf{r},$$

where the x_α are real. These biquaternions are characterized by the property $x^* = x^\dagger$ and have been called *hermitian biquaternions*. In fact, the matrices $L(x)$ and $R(x)$ are then hermitian matrices. The differential operator

$$\frac{d}{dx} = \frac{\partial}{\partial t} - i\nabla$$

is also a hermitian biquaternion, but the so-called *six-vector* $\mathbf{F} = \mathbf{B} + i\mathbf{E}$ satisfies $\mathbf{F}^\dagger = -\mathbf{F}$; it is represented by a skew-symmetric matrix.

We may ask which continuous transformations leave the norm of a hermitian biquaternion invariant. It is easily seen that this is so for

$$\begin{aligned} x &\mapsto x^*, \\ x &\mapsto -x, \\ x &\mapsto qxq^{*\dagger} \quad \text{when } N(q) = 1, \end{aligned}$$

and for no others. (See, e.g., Lambek [1950].) If we ask, more generally, which continuous transformations leave the norm of the difference of two hermitian biquaternions unchanged, we should add also the *translation*

$$x \mapsto x + a.$$

The group generated by all these transformations is called the *Poincaré group*.

We shall rule out the transformation $x \mapsto x^*$ but admit $x \mapsto -x$, thus following Lewis Carroll, who suggested that time is reversed in a mirror. Transformations of the form $x \mapsto qxq^{*\dagger}$ are called (proper) *Lorentz transformations*; they were originally postulated by Lorentz to account for the Michelson–Morley experiment. This *ad hoc* explanation was later justified by Albert Einstein, who

realized that they also described, in addition to rotations, the changes in coordinates when passing from a stationary platform to a uniformly moving train; these are called *boosts* (see Sudbury [1986]) and form the cornerstones of the special theory of relativity.

A Lorentz transformation is given by a biquaternion $q = u + iv$, with $u, v \in \mathbb{H}$, such that $qq^\dagger = 1$, that is,

$$uu^\dagger - vv^\dagger = 1, \quad uv^\dagger + vu^\dagger = 0.$$

q describes a rotation in three-space if $q \in \mathbb{H}$, that is, if $v = 0$; it is a *boost* if it is hermitian, that is, $q^\dagger = u - iv$, which means that u is a scalar and v a 3-vector. It is easily seen that every Lorentz transformation is a rotation followed by a boost. Indeed, let

$$\mu^2 = uu^\dagger = 1 + vv^\dagger \geq 1, \\ r = u\mu^{-1}, \quad s = \mu - iuv^\dagger\mu^{-1};$$

then r is a rotation, s is a boost, and $q = sr$.

The space of hermitian biquaternions is called *Minkowski space*; it is generated by $1, ii_1, ii_2$, and ii_3 . If we put $\lambda_\alpha = i$ when $\alpha > 0$ but $\lambda_0 = 1$, we may write these generators as $\lambda_\alpha i_\alpha$. Any hermitian biquaternion then has the form

$$x = \sum x'_\alpha i_\alpha = \sum x_\alpha \lambda_\alpha i_\alpha,$$

where the $x_\alpha = x'_\alpha \lambda_\alpha^*$ are real. Applying a Lorentz transformation, we obtain another hermitian biquaternion

$$qq^{\dagger*} = \sum_{\alpha, \beta} x'_\alpha \lambda_\alpha^* \Lambda_{\alpha\beta} \lambda_\beta i_\beta,$$

where the $\Lambda_{\alpha\beta}$ are real numbers. Putting

$$\lambda_\alpha^* \Lambda_{\alpha\beta} \lambda_\beta = \Delta_{\alpha\beta},$$

we see that

$$L(q)R(q^{\dagger*})[x] = \Delta^\dagger[x].$$

This being so for all $[x]$, we infer that

$$L(q)R(q^{\dagger*}) = \Delta^\dagger,$$

hence, taking the transposed of each side, that

$$R(q^*)L(q^\dagger) = \Delta.$$

Multiplying this by $[x^*]$, for any hermitian biquaternion x , we obtain

$$q^\dagger x^* q^* = \sum_{\alpha, \beta} i_\alpha \Delta_{\alpha\beta} x'_\beta = \sum_{\alpha, \beta} i_\alpha \lambda_\alpha^* \Lambda_{\alpha\beta} x'_\beta.$$

For later reference, we summarize this observation as follows:

LEMMA 1. *If a Lorentz transformation transforms $\lambda_\alpha i_\alpha$ into $q\lambda_\alpha i_\alpha q^{\dagger*} = \sum_\beta \Lambda_{\alpha\beta} \lambda_\beta i_\beta$, then $q^\dagger \lambda_\beta^* i_\beta q^* = \sum_\alpha i_\alpha \lambda_\alpha^* \Lambda_{\alpha\beta}$.*

Einstein had realized that the mass-momentum $p = m + im\mathbf{v}$ should also transform like x (without using the language of quaternions); hence, he wrote $p = m_0 dx/ds$, where $ds^2 = N(dx)$, and $m_0 = m(dt/ds)^{-1}$ is the *rest mass* of a moving particle, assumed to be invariant. The conservation of momentum is then coupled with the conservation of mass.

Now

$$m = m_0 \frac{dt}{ds} = m_0(1 - v^2)^{-1/2},$$

where $v^2 = \mathbf{v} \circ \mathbf{v}$. If the velocity v of the moving particle is small compared with the velocity $c = 1$ of light,

$$m \doteq m_0 \left(1 + \frac{\frac{1}{2}v^2}{c^2}\right)$$

where we have temporarily restored the symbol c to obtain the famous approximation

$$mc^2 \doteq m_0 c^2 + \frac{1}{2} m_0 v^2.$$

Einstein considered this to be the total energy of the particle, the kinetic energy $\frac{1}{2}m_0 v^2$ being augmented by the atomic energy $m_0 c^2$.

The charge-current density $J = \rho + i\mathbf{j}$ may be thought of as $J = \rho_0 dx/ds$, where $\rho_0 = \rho(dt/ds)^{-1}$ is assumed to be an invariant scalar; hence, J also transforms like x , namely $J \mapsto pJp^{\dagger*}$. In our notation, Maxwell's equations are combined into the single equation $dF/dx + J = 0$. It seems that Henri Poincaré was the first to realize that they are invariant under Lorentz transformations. To see this, we only need $\mathbf{F} \mapsto q^* \mathbf{F} q^{\dagger*}$ and $d/dx \mapsto q(d/dx)q^{\dagger*}$. The former transformation is natural for a 6-vector, as

$$(q^* \mathbf{F} q^{\dagger*})^\dagger = q^* \mathbf{F}^\dagger q^{\dagger*} = -q^* \mathbf{F} q^{\dagger*}.$$

The latter transformation may be justified on general principle: if the column vector of the $x'_\alpha = \lambda_\alpha x_\alpha$ is transformed by the matrix Δ , then the column vector of the $\partial/\partial x'_\alpha = \lambda_\alpha \partial/\partial x_\alpha$ is transformed by the inverse of Δ^\dagger . Now, if Δ leaves $x_0^2 - x_1^2 - x_2^2 - x_3^2$ invariant, the inverse of Δ^\dagger is Δ ; hence,

$$\frac{d}{dx} = \sum_\alpha \lambda_\alpha^* \frac{\partial}{\partial x_\alpha}$$

transforms like x .

In summary, the following hermitian quaternions are transformed by $q(\)q^{\dagger*}$:

$$x = t + i\mathbf{r} \quad (\text{position in space-time}),$$

$$\frac{d}{dx} = \frac{\partial}{\partial t} - i\nabla \quad (\text{partial derivation}),$$

$$p = m + im\mathbf{v} \quad (\text{energy-momentum}),$$

$$J = \rho + i\mathbf{j} \quad (\text{charge-current density}),$$

$$\Phi = \varphi + i\mathbf{A} \quad (4\text{-potential}).$$

On the other hand, the 6-vector

$$\mathbf{F} = \mathbf{B} + i\mathbf{E} \quad (\text{electromagnetic field})$$

is transformed by $q(\cdot)q^\dagger$. The quaternion form of Maxwell's equations is

$$\frac{d}{dx} \mathbf{F} + J = 0.$$

Operating on this equation by $(d/dx)^\dagger$ and noting that $(d/dx)^\dagger (d\mathbf{F}/dx)$ is a 6-vector, we infer that the scalar part of $(d/dx)^\dagger J$ is zero. This is the equation of continuity. We should also add the observation that $(d/dx)^\dagger \Phi + \mathbf{F}$ is a scalar, which is sometimes put equal to zero.

Maxwell's equations describe the electromagnetic field created by a continuous distribution of charge in motion, as expressed by the charge-current biquaternion J . Conversely, a given electromagnetic field also acts on a moving charge, this time viewed as a discrete charge q_0 moving with velocity \mathbf{v} , by exerting a force $q_0(\mathbf{E} + \mathbf{v} \times \mathbf{B})$. According to Newton, this should be the rate of change of momentum, but special relativity requires that the rate be measured by d/ds , not by d/dt . Moreover, according to the dictates of special relativity, this should be augmented by a term $q_0(\mathbf{v} \times \mathbf{E} + \mathbf{B})$, expressing the rate of change of energy. Thus, we obtain the relativistic form of the *equation of motion* of an electron, with $q_0 = -e$,

$$\frac{dp}{ds} = e \frac{dx}{ds} \mathbf{F} + ig,$$

where g is some hermitian biquaternion.

There remains a contradiction: we described the charge as continuously distributed in Maxwell's equation, but as discrete in the equation of motion. This contradiction will only be resolved when we pass to the quantum-mechanical treatment of the electron.

Application to Quantum Mechanics

Quantum mechanics prescribes that the momentum $p = m_0 dx/ds$ be replaced by the differential operator $-(h/2\pi i)(d/dx)$, where h is Planck's constant. Choosing units so that $h/2\pi = 1$, we thus expect the equation $pp^\dagger = m_0^2$ to be replaced by the relativistic wave equation

$$\left(\frac{d}{dx}\right) \left(\frac{d}{dx}\right)^\dagger \varphi = -m_0^2 \varphi,$$

where $\varphi = \varphi_0 + i\varphi_1$ is a function of position in space-time. This is usually referred to as the *Klein–Gordon equation*; but, as a recent biography of Schrödinger points out (Moore [1989]), Schrödinger himself had considered this form of the wave equation before introducing the time-evolving form which is named after him.

Dirac obtained his celebrated first-order equation by extracting the square root of this second-order differential operator, thus rediscovering the main idea behind Clifford algebras. It does not seem to be widely realized that such *ad hoc* methods are not needed and that Dirac's first-order equation is in fact *equivalent* to the Klein–Gordon equation, provided we do not insist that φ remain a scalar. In fact, we shall assume that φ is a biquaternion and write

$$\frac{d\varphi}{dx} = m_0 \chi,$$

where $\chi = \chi_0 + i\chi_1$ is another biquaternion. Then

$$m_0 \left(\frac{d\chi}{dx}\right)^\dagger = \left(\frac{d}{dx}\right)^\dagger \left(\frac{d}{dx}\right) \varphi = -m_0^2 \varphi,$$

so the Klein–Gordon equation is equivalent to the following pair of biquaternion equations:

$$\frac{d\varphi}{dx} = m_0 \chi, \quad \left(\frac{d\chi}{dx}\right)^\dagger = -m_0 \varphi.$$

How can these be combined into a single first-order equation?

Assume, for the moment, that there is an entity j such that $j^2 = -1$, $ji = -ij$, and $ji_\alpha = i_\alpha j$ for $\alpha = 0, 1, 2$, or 3 . Then we have

$$\begin{aligned} \left(\frac{d}{dx}\right) (\varphi + j\chi) &= \left(\frac{d}{dx}\right) \varphi + \left(\frac{d}{dx}\right) j\chi \\ &= m_0 \chi + j \left(\frac{d}{dx}\right)^\dagger \chi \\ &= m_0 (\chi - j\varphi) \\ &= -jm_0 (\varphi + j\chi). \end{aligned}$$

There is certainly no 4-by-4 matrix which anticommutes with the complex number i . But let us pass to real 4-by-4 matrices and identify i_α with the matrix $L(i_\alpha)$ representing it. We shall take $j_\alpha = R(i_\alpha)$, the contravariant representation; then

$$j_1^2 = j_2^2 = j_3^2 = j_3 j_2 j_1 = -1, \quad j_\alpha i_\beta = i_\beta j_\alpha$$

for $\alpha, \beta = 1, 2$, or 3 . Now replace the complex number i by the real matrix j_1 and identify j with j_2 . Putting

$$\Psi = \varphi + j_2 \chi = \varphi_0 + j_1 \varphi_1 + j_2 \chi_0 + j_3 \chi_1,$$

we may write the above first-order equation as

$$\frac{d}{dx} \Psi + j_2 m_0 \Psi = 0,$$

where now

$$\frac{d}{dx} = \frac{\partial}{\partial t} - j_1 \nabla,$$

and we have essentially recaptured Dirac's equation for the free electron.

A word of warning: having replaced i by j_1 , we must now write $x = t + j_1 r$, and so on, and even the biquaternion $q = u + iv$ in the Lorentz transformation has now become the matrix $u + j_1 v$.

To make sure that our first-order equation is preserved under the Lorentz transformation which sends x to qxq^{\dagger} , hence d/dx to $q(d/dx)q^{\dagger}$, it suffices to let Ψ be transformed into $q^*\Psi$. (There are other possibilities, namely, sending Ψ to $q^*\Psi q^{\dagger}$ or $q^*\Psi q^{\dagger}$, but we shall not consider these.) We note that the Lorentz transformation $q(\)q^{\dagger}$ is unchanged when q is replaced by $-q$, but that it corresponds to two distinct ways of transforming Ψ : into $q^*\Psi$ and $-q^*\Psi$, respectively. The transformations of Ψ do not constitute a representation of the Lorentz group, but what has been called a *projective representation*. This is the mathematical reason for saying that the electron has spin $\frac{1}{2}$.

It can be shown that the 16 matrices $1, i_\alpha, j_\beta$, and $i_\alpha i_\beta$ ($\alpha, \beta = 1, 2$, or 3) span the space of all 4-by-4 real matrices. The reason is that \mathbb{H} is a central simple algebra of degree 4 over \mathbb{R} , hence $\mathbb{H} \otimes \mathbb{H}^{\text{op}}$ is isomorphic to $M_4(\mathbb{R})$ (see Jacobson [1980], Theorem 4.6). Thus, Ψ is just an arbitrary 4-by-4 real matrix. However, the transformation rule $\Psi \mapsto q^*\Psi$ permits us to multiply Ψ in the Dirac equation by the column vector $(1, 0, 0, 0)^{\dagger}$, so we may assume, without loss in generality, that Ψ is the real column vector $(\psi_0, \psi_1, \psi_2, \psi_3)^{\dagger}$; we may write $\Psi = [\psi]$, where $\psi = \psi_0 + i_1\psi_1 + i_2\psi_2 + i_3\psi_3$ is a real quaternion. There is nothing to prevent us from introducing a complex column vector here; on the other hand, there seems to be no necessity for doing so either, at least as long as we confine attention to the *free* electron, not influenced by an electromagnetic field.

Dirac's equation for the free electron may be written more explicitly in matrix form as follows:

$$\left(\frac{\partial}{\partial t} - R(i_1) \sum_{\alpha=1}^3 L(i_\alpha) \frac{\partial}{\partial x_\alpha} \right) [\psi] = -m_0 R(i_2) [\psi].$$

Now $L(i_\alpha)[\psi] = [i_\alpha\psi]$ and $R(i_\alpha)[\psi] = [\psi i_\alpha]$, so this is really an equation in real quaternions:

$$\frac{\partial \psi}{\partial t} - \nabla \psi i_1 + m_0 \psi i_2 = 0.$$

When written in this way, the equation is less apparently Lorentz-invariant.

When taking $j_1 = R(i_1)$ and $j_2 = R(i_2)$, we made an arbitrary choice. We might just as well have taken $j_1 = R(i_2)$ and $j_2 = R(i_3)$ or, more generally, $j_\alpha = R(r i_\alpha r^{\dagger})$ ($\alpha = 1, 2$, or 3), where r is a real quaternion such that $rr^{\dagger} = 1$, that is, where $r(\)r^{\dagger}$ is a rotation in 3-space. What would happen to Dirac's equation had we chosen a different coordinate frame in 3-space? In its quaternionic form, it would then become

$$\frac{\partial \psi}{\partial t} - \nabla \psi r i_1 r^{\dagger} + m_0 \psi r i_2 r^{\dagger} = 0.$$

Multiplying by r on the right, we would then obtain

$$\frac{\partial \psi r}{\partial t} - \nabla \psi r i_1 + m_0 \psi r i_2 = 0,$$

which is the same as the original equation with ψ replaced by ψr .

I recall telling Dirac in 1949 that I could derive his equation with the help of quaternions. After thinking quietly for several minutes, as was his habit before speaking, he said, "Unless you can do it with *real* quaternions, I am not interested." As I had biquaternions in mind, it was perhaps this remark which finally persuaded me to abandon theoretical physics for pure mathematics. Looking at the problem again almost half a century later, in connection with a project to write an undergraduate textbook on the history and philosophy of mathematics (together with Bill Anglin), I realize that I should have replied: "Yes; but can you do it using a *real* wave vector?" It is only quite recently that I became aware of Dirac's 1945 article, which shows how to express Lorentz transformations with the help of *real* quaternions in a roundabout way. I don't know whether this idea was ever followed up.

The Electron in an Electromagnetic Field

What happens to an electron when an electromagnetic field is present? Classical physics requires that the kinetic energy m should be augmented by the potential energy $-e\varphi$, where $-e$ is the charge of the electron and φ is the potential. According to special relativity, the energy-momentum 4-vector p should then be augmented by $-e\Phi$, where $\Phi = \varphi + j_1 \mathbf{A}$ is the 4-potential. Finally, quantum mechanics requires that p be replaced by $i(d/dx)$; hence, $p - e\Phi$ by $i(d/dx) - e\Phi$. Multiplying this by $-i$, we see that Dirac's equation becomes

$$\left(\frac{d}{dx} + i e \Phi \right) \Psi + j_2 m_0 \Psi = 0,$$

where $\Psi = [\psi]$, ψ being a quaternion.

One is tempted to replace the complex number i by the real matrix j_1 as before, in which case Dirac's equation would become

$$\frac{\partial \psi}{\partial t} - e \mathbf{A} \psi - (\nabla \psi - e \varphi \psi) i_1 + m_0 \psi i_2 = 0.$$

As long as ψ is nonzero, we could multiply this equation by ψ^{-1} and solve for \mathbf{A} . I do not know whether this makes any sense, so I shall allow i to remain a complex number, thus forcing Ψ to be a complex vector, hence ψ a biquaternion.

Now Φ was only determined inasmuch as $(d/dx)^{\dagger} \Phi + \mathbf{F}$ is a scalar. As pointed out by Hermann Weyl [1950], this property is not affected by a so-called *gauge transformation*: replacing Φ by $\Phi + d\alpha/dx$, where α is a real scalar.

The same result could have been achieved replacing Ψ in Dirac's equation by

$$\Psi \exp(i\epsilon\alpha) = \Psi(\cos(\epsilon\alpha) + i \sin(\epsilon\alpha)),$$

for

$$\frac{d}{dx}(\Psi \exp(i\epsilon\alpha)) = \left(\frac{d\Psi}{dx} + ie \frac{d\alpha}{dx} \right) \exp(i\epsilon\alpha).$$

[The argument depends on the fact that Ψ commutes with $\exp(i\epsilon\alpha)$; it would not have worked had we replaced i by j_1 .]

Dirac's equation expresses the action of the electromagnetic field, as determined by Φ , on the electron. It replaces the equation of motion discussed earlier. On the other hand, the contribution of the electron to the electromagnetic field was expressed by Maxwell's equations. In terms of Φ these can be written

$$\frac{d}{dx} \left(\frac{d}{dx} \right)^\dagger \Phi = J,$$

where J is the charge-current density. Only now we can calculate J with the help of the wavefunction Ψ . The following considerations are adapted from Sudbury [1986], after translation into our language.

Recall the matrix form of Dirac's equation for an electron in an electromagnetic field:

$$\left(\frac{d}{dx} + ie\Phi \right) \Psi = -j_2 m_0 \Psi, \quad (1)$$

where $\Psi = [\psi]$ is a complex column vector, ψ now being a biquaternion. Since the old symbols $*$ and \dagger have changed their meanings in the course of our discussion, we shall now write Ψ^T for the transpose of Ψ and $\Psi^C = [\psi^C]$ for the complex conjugate of Ψ . It will be convenient to invoke the *hermitian conjugate* $\Psi^H = \Psi^{CT} = [\psi^C]^T$. Now

$$\frac{d}{dx} = \frac{\partial}{\partial t} - j_1 \nabla, \quad \Phi = \varphi + j_1 \mathbf{A}$$

are real symmetric matrices, but j_2 is antisymmetric. Multiplying (1) by Ψ^H , we obtain

$$\Psi^H \left(\frac{d}{dx} + ie\Phi \right) \Psi = -\Psi^H j_2 m_0 \Psi, \quad (2)$$

and the hermitian conjugate of this is

$$\Psi^H \left(\overleftarrow{\frac{d}{dx}} - ie\Phi \right) \Psi = +\Psi^H j_2 m_0 \Psi, \quad (3)$$

where the arrow indicates that differentiation operates leftwards. Adding (2) and (3), we obtain

$$\Psi^H \overleftrightarrow{\frac{d}{dx}} \Psi = 0,$$

that is,

$$\frac{\partial}{\partial t}(\Psi^H \Psi) - \sum_{\alpha=0}^3 \frac{\partial}{\partial x_\alpha} (\Psi^H j_1 i_\alpha \Psi) = 0.$$

This equation resembles the equation of continuity

$$\sum_{\alpha=0}^3 \frac{\partial}{\partial x_\alpha} J_\alpha = 0,$$

which suggests that we define

$$J_\alpha = e\Psi^H i_\alpha \lambda_\alpha^* \Psi$$

and consider $J = \sum_{\alpha=0}^3 J_\alpha \lambda_\alpha i_\alpha$ as a candidate for the charge-current density. Here λ_α is defined as before, except that i has now been replaced by j_1 , thus $\lambda_\alpha = j_1 i_\alpha$ when $\alpha > 0$ but $\lambda_0 = 1$. It remains to check that J is transformed by a Lorentz transformation into $qJq^{*\dagger}$. Indeed, J transforms into

$$\sum_{\beta} e\Psi^H q^\dagger i_\beta \lambda_\beta^* q^* \Psi \lambda_\beta i_\beta,$$

and, by Lemma 1, this is

$$\sum_{\alpha,\beta} e\Psi^H i_\alpha \lambda_\alpha^* \Psi \Lambda_{\alpha\beta} \lambda_\beta i_\beta = \sum_{\alpha,\beta} J_\alpha \Lambda_{\alpha\beta} \lambda_\beta i_\beta = qJq^{*\dagger},$$

as was to be shown.

The wave vector Ψ appearing in the Dirac equation (1) depends on the following three data:

- A point in Minkowski space represented by $x = t + j_1 \mathbf{r}$. The Lorentz transformation $x \mapsto qxq^{*\dagger}$ corresponds to a transformation $\Psi \mapsto q^* \Psi$.
- A choice of the 4-potential Φ , compatible with the electromagnetic field, which itself depends on x . The gauge transformation $\Phi \mapsto \Phi + d\alpha/dx$ is equivalent to the transformation $\Psi \mapsto \Psi \exp(ei\alpha)$.
- The choice of j_1 and j_2 , which determines $j_3 = j_2 j_1$. We had assumed that $j_\alpha = R(i_\alpha)$ but allowed i_α to be replaced by $ri_\alpha r^T$, r being a quaternion with $rr^T = 1$. However, since Ψ is now allowed to be a complex vector, we may as well allow i_α to be replaced by $ri_\alpha r^H$, where r is a biquaternion with $rr^H = 1$. This induces a transformation $\psi \mapsto \psi r$, or $\Psi \mapsto R(r)\Psi$.

The group acting on Ψ according to (a) is the group $SU(2)$ of unitary transformations of determinant 1. The group acting on Ψ according to (b) is the group $U(1)$ of the complex numbers with absolute value 1. The group acting on Ψ according to (c) is a projective representation of $SU(3)$.

The physical theories underlying the foregoing discussion have been known for a long time; they are all discussed in the classic text by Hermann Weyl [1950], a

translation of the German edition of 1930. Even some further steps are indicated there, in particular the so-called *second quantization* (accompanied by some hocus pocus to remove unwanted infinities). Following this procedure, one is told to replace the functions Φ and Ψ by operators; but, according to Sudbury [1986], the form of the Dirac equation remains the same. These ideas culminate in quantum-electro-dynamics (QED), which has succeeded in making highly accurate predictions. More recent developments exploit the gauge theories initiated by Weyl. Thus, the strong force acting on a fermion is explained with the help of the group $SU(3)$ and the electro-weak force with the help of the group $SU(2) \times U(1)$. There does not seem to be any significance to the observation that these same groups arise in the above discussion.

What then is the final verdict on the usefulness of quaternions for physics? I am told that they are catching on as a tool for computation, but in the more general framework of Clifford algebras. Indeed, Dirac's original derivation of his equation implicitly used a Clifford algebra argument. One may cling to a feeling that there is something special about quaternions: their 4-dimensionality and the fact that they form a division algebra. These special properties of quaternions might be expected to put restraints on the nature of our universe.

Unfortunately, the 4-dimensionality of Hamiltonian quaternions does not account for the difference between space and time in Minkowski space, and division plays no role in our story. These aspects of quaternions are called upon, however, when one expresses the algebra of 4-by-4 real matrices as a tensor product of \mathbb{H} and \mathbb{H}^{op} , which fact we have exploited here. Be that as it may, I firmly believe that quaternions can supply a shortcut for pure mathematicians who wish to familiarize themselves with certain aspects of theoretical physics.

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