Complex four-vectors and the Dirac equation

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Abstract

The Dirac relativistic wave equation is normally expressed using four by four complex matrices. However, the equation can also be expressed without loss of generality within the simpler algebra of complex four-vectors, which is equivalent to the Pauli algebra of two by two complex matrices.

The conventional formulation uses four-component spinors which are expressed relative to an arbitrarily chosen axis (normally the z axis of the frame of reference). The direction of this axis, and even its existence, are normally hidden in the choice of basis matrices. The simpler formulation uses only quantities which are expressed in complex four-vector notation, which is symmetrical in its treatment of three-dimensional space, and the chosen axis appears explicitly in the equation.

The same axis also appears unexpectedly in the interaction with an electromagnetic four-potential, suggesting that the conventional formulation of the equation might be misleading in this case. In particular, a gauge transformation involves a rotation of the wave function about the chosen axis rather than a scalar phase transformation.

1 Complex four-vector terminology and notation

Complex four-vectors extend conventional real four-vectors to include complex components. The resulting objects can then be algebraically multiplied and divided in ways which result in useful physical equations. Complex four-vectors can be represented using the Pauli algebra of 2 by 2 complex matrices, where the unit vectors correspond to the Pauli spin matrices. This representation is closely related to *spin vectors* in spinor theory [Pen86] except that a scale factor of $1/\sqrt{2}$ used to make spin vectors compatible with two-component spinors does not apply in complex four-vector notation.

This algebra is also equivalent to the Clifford algebra $C\ell_3$. In multivector [Hes84, Lou97] terminology (often used with Clifford algebra) the imaginary scalar (timelike) part of a complex four-vector could be called the *pseudoscalar* part and the imaginary three-vector (spacelike) part would be called the *bivector* part.

The term "complex four-vector" describes the structure of the numerical object, like "complex number", but is not intended to be limited to quantities which transform as vectors under a Lorentz transformation. Some quantities such as displacements transform as four-vectors, but others are invariant or transform in a similar way to spinors. Quantities such as the electromagnetic field strength or the complex four-vector equivalent of the angular momentum transform in yet another way which can be called a *field spinor* or *algebraic spinor* [Hil87].

All simpler numerical quantities such as scalars and three-vectors can be treated as complex four-vector quantities where some of the parts are zero. This includes *quaternions*, which have a pure real scalar part and a pure imaginary three-vector part.

The alternative term "p-number" used for this type of numerical object by Hestenes [Hes66] avoids the misleading use of the word "vector" but gives no clue to the novice as to what it might be. These objects are also equivalent to Clifford's "biquaternions" but that term is also unsuitable because it refers to complexified quaternions, and a quaternion is already considered to have an imaginary vector part in this terminology. Some authors appear to have reused the term "octonions" for this purpose, but this term is already in use for a different group, also known as "Cayley numbers", which has seven imaginary components and is in no way related to four-vectors.

1.1 Notation

The notation used here is intended to maximize consistency with notation conventionally used for simpler cases such as classical vectors and complex numbers. As complex four-vectors can be represented using the Pauli matrices, some of the terminology is based on the matrix representation.

i — is the square root of minus one.

$\mathbf{i}$, $\mathbf{j}$, $\mathbf{k}$ — are the unit vectors in the x, y and z directions, which (like the Pauli spin matrices) have the following algebraic properties:

$$\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = 1$$

$$\mathbf{i}\,\mathbf{j} = -\,\mathbf{j}\,\mathbf{i} = i\,\mathbf{k},\ \ \mathbf{j}\,\mathbf{k} = -\,\mathbf{k}\,\mathbf{j} = i\,\mathbf{i},\ \ \mathbf{k}\,\mathbf{i} = -\,\mathbf{i}\,\mathbf{k} = i\,\mathbf{j}$$

These can also be written as $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$.

a — normally denotes a complex four-vector $a_0 + a_1\,\mathbf{i} + a_2\,\mathbf{j} + a_3\,\mathbf{k}$.

ab — represents algebraic multiplication between four-vectors a and b.

$a.b$ — normally represents multiplication by or between scalars.

$\mathbf{a}$ — in boldface type represents a conventional three-vector.

$\mathbf{a}.\mathbf{b}$ denotes the scalar product of two three-vectors.

$\mathbf{a} \times \mathbf{b}$ denotes the vector "cross" product of two three-vectors.

1.2 Algebraic product

Using the abbreviated notation $\mathbf{a}_{123}$ for the three-vector part, the algebraic product ab can be expanded as follows:

$$\begin{aligned} ab &= a_0.b_0 + \mathbf{a}_{123}.\mathbf{b}_{123} \\ &+ a_0.\mathbf{b}_{123} + \mathbf{a}_{123}.b_0 \\ &+ i\,\mathbf{a}_{123} \times \mathbf{b}_{123} \end{aligned}$$

Multiplication is not generally commutative, but $ab = ba$ when either a or b is scalar, and when the vector parts are parallel, i.e. when $\mathbf{a}_{123} = k.\mathbf{b}_{123}$ for some complex scalar constant k, as it is only the vector cross-product terms which are not commutative.

1.3 Complex conjugate

The complex conjugate of a four-vector is obtained by taking the complex conjugate of each component,

$$a^* = a_0^* + a_1^*\,\mathbf{i} + a_2^*\,\mathbf{j} + a_3^*\,\mathbf{k}.$$

In the Pauli algebra matrix representation, this operation is the complex conjugate transpose (also known as the Hermitian conjugate), and in multivector algebra, the corresponding operation is called reversion.

The complex conjugate of a product reverses the order of the terms,

$$(ab)^* = b^*\,a^*.$$

1.4 Vector conjugate

The vector conjugate of a four-vector switches the sign of the three-vector part.

$$\overline{a} = a_0 - a_1\,\mathbf{i} - a_2\,\mathbf{j} - a_3\,\mathbf{k}.$$

In the matrix representation, this is the *adjugate* matrix, and in multivector algebra, this is called the Clifford conjugate.

The vector conjugate of a product reverses the order of the terms,

$$\overline{(ab)} = \overline{b}\,\overline{a}.$$

1.5 Determinant and magnitude

The determinant or magnitude square of a four-vector is equal to the determinant of the corresponding matrix in the Pauli algebra representation.

$$\begin{aligned} \det(a) \text{ or } |a|^2 &= a\overline{a} \text{ or } \overline{a}a \\ &= {a_0}^2 - {a_1}^2 - {a_2}^2 - {a_3}^2 \end{aligned}$$

Note that this is generally a complex scalar, not necessarily pure real.

1.6 Multiplicative inverse

Any four-vector with a non-zero determinant has a multiplicative inverse.

$$a^{-1} = \frac{\overline{a}}{\det(a)}$$

The inverse of a product reverses the order of the terms:

$$(ab)^{-1} = b^{-1}a^{-1}$$

1.7 Division

Dividing by a four-vector is equivalent to multiplying by its inverse.

$$a/b = ab^{-1} = a\overline{b}/\det(b)$$

1.8 The partial derivative operator

The three-vector partial derivative operator ∇ is extended to include a time-like part, combining the operators div, grad, curl and $\partial/\partial t$ into a single four-vector operator $\Box$.

$$\Box = 1/c\ \partial/\partial t + \mathbf{i}\,\partial/\partial x + \mathbf{j}\,\partial/\partial y + \mathbf{k}\,\partial/\partial z$$

Following the general rules on conjugates, the complex conjugate $\Box^*$ and the vector conjugate $\overline{\Box}$ operate on the term on the left, and the vector complex conjugate $\overline{\Box}^*$ operates on the term on the right again. As displacements in space are real, complex conjugation has no other effect than switching the operator from the right to the left.

The combinations $\overline{\Box}^*\Box$ or $\Box\overline{\Box}^*$ form the D'Alembertian operator $|\Box|^2$ which in conventional components expands to

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2}.$$

For theoretical purposes, it is convenient to assume that space, time and energy are measured in consistent units, which eliminates the need for any explicit factors of c or $\hbar$.

2 Lorentz transformations

When a four-vector quantity such as displacement or velocity is transformed from one inertial frame of reference to another, relative angles and invariant quantities must be preserved, and real quantities must remain independent of imaginary quantities. The general form of four-vector transformation which preserves local angles and preserves real and imaginary parts separately is

$$p' = W\,p\,W^*,$$

where W may be any complex four-vector. The transformations produced are the proper Lorentz tranformations, which cover all combinations of rotations in space, velocity (boost) transformations and scale changes.

Complex four-vector objects can have several other possible transformation laws.

An *inverse four-vector* is the vector conjugate of an ordinary four-vector, so its transformation law is the vector conjugate of the vector transformation,

$$q' = \overline{W}^*\,q\,\overline{W}.$$

The four-gradient operator $\Box$ transforms as an inverse vector.

A *spinor* is defined as a quantity S such that $S\,S^*$ is a four-vector, so its transformation law is

$$S' = W\,S.$$

This definition of spinor is not restricted to quantities which can be represented in the conventional two-component spinor notation (which applies when the scalar part is zero and the three-vector part consists of perpendicular real and imaginary vectors of equal magnitude) but also includes all other complex four-vector quantities which transform in the same way.

Finally, certain physical quantities are formed from the algebraic product of a vector and an inverse vector. These quantities have a *field spinor* or *algebraic spinor* transformation law

$$F' = W\,F\,W^{-1},$$

with a matching law for the complex conjugate which occurs when the inverse vector precedes the vector. The scalar (timelike) part of this type of quantity is unchanged by this transformation law, so it is invariant. The four-vector equivalent of the angular momentum, $x\,\overline{p}$, transforms as a field spinor. The electromagnetic field $\mathbf{E} + i\mathbf{B}$ is equal to the four-gradient of the four-potential, $\Box A$, so it transforms as a complex conjugate field spinor.

3 The Dirac equation

3.1 The first-order Klein-Gordon equation

The purpose behind the invention of the Dirac relativistic equation of the electron was to find a first-order equation similar to the Schrödinger equations which at the same time agreed with the second-order Klein-Gordon relativistic wave equation. In four-vector notation, the Klein-Gordon equation is

$$|\Box|^2\,\Psi = -m^2\Psi$$

A simple first-order equation in complex four-vector notation which leads directly to this equation is

$$\Box\,\Psi = im\,\overline{\Psi}^*\,\overline{k}^* \qquad (1)$$

where k is a constant such that $k\overline{k}^* = -1$.

The Klein-Gordon equation can then be obtained directly from equation (1) as follows:

$$\begin{aligned}
|\Box|^2\,\Psi &= \overline{\Box}^*\,\Box\,\Psi \\
&= \overline{\Box}^*(im\,\overline{\Psi}^*\,\overline{k}^*) \quad \text{using equation (1)} \\
&= im\,\overline{(\Box\,\Psi)}^*\overline{k}^* \quad \text{since } m \text{ and } k \text{ are constant} \\
&= im\,\overline{(im\,\overline{\Psi}^*\,\overline{k}^*)}^*\,\overline{k}^* \quad \text{using equation (1) again} \\
&= im\,(-im\,\Psi k)\overline{k}^* \quad \text{applying the conjugations} \\
&= m^2\,\Psi\,k\overline{k}^* \\
&= -m^2\,\Psi
\end{aligned}$$

The value of k obviously cannot be pure scalar. The most basic form of quantity k which satisfies $k\overline{k}^* = -1$ is a unit magnitude three-vector.

As it is possible to postmultiply Ψ by an arbitrary non-null complex four-vector constant with a corresponding change in k, it is necessary to make an arbitrary choice as to whether Ψ transforms as a simple spinor or a field spinor, and correspondingly whether k is an invariant constant or transforms as a field spinor, and the choice of direction of k in a given frame is similarly arbitrary, as it only affects Ψ by a constant factor.

In order to maintain a simple correspondence with the Dirac bispinor representation, it is simplest to adopt the convention here that Ψ transforms like a spinor and that k is an invariant three-vector constant, equal to the unit vector $\mathbf{k}$ in the z direction, which means that $\overline{k}^* = -\mathbf{k}$. (The easiest way to understand the concept of an invariant vector is that it is a vector expressed in a frame of reference associated with the wave function itself, so it does not depend on the observer frame).

3.2 Plane wave solutions

In order for equation (1) to match the usual form of eigenvalue equation needed for quantum mechanics, it must be expressed in a form where all operators on Ψ are linear and do not involve conjugates.

Provided that Ψ is not null, it can be split up into four factors of the form $UWab$ corresponding to a unit magnitude real vector, a quaternion, a scalar amplitude and a scalar phase. Equation (1) can then be expanded in terms of these factors:

$$\begin{aligned}
\Box(UWab) &= -im\,\overline{(UWab)}^{*}\,\mathbf{k} \\
&= -im\,\overline{U}^{*}Wab^{*}\,\mathbf{k} \;\; \text{applying the conjugations} \\
&= -im\,\overline{(UU^{*})}(UWab)\,(b^{*})^{2}\,\mathbf{k} \\
&= -im\,\overline{u}(UWab)\,(b^{*})^{2}\,\mathbf{k} \;\; \text{where } u = UU^{*}
\end{aligned}$$

For this to be in the correct form, u must be a constant proper four-velocity, so $m\overline{u}$ is the reversed momentum $\overline{p}$. The phase b must also be a constant and $(b^*)^2$ must be real for consistency between the sides of the equation, which means that $(b^*)^2$ must be ± 1 (distinguishing between electron and positron solutions).

Moving some constants across then gives the Dirac equation in complex four-vector form (for the free space case, where no external potential is present):

$$iu\Box\Psi\,\mathbf{k} = \pm m\Psi$$

The above constraints mean that in the expansion of Ψ, only the quaternion factor W and the amplitude a can vary, and for a free space wave even the amplitude is a constant. The basic solution in this case is that Ψ is a plane quaternion wave of the form $UWa\exp(-ix.\overline{p}\,\mathbf{k})$ where U determines the velocity, W is now a constant quaternion giving the orientation of the spin axis relative to the z axis, a is the amplitude factor and the exponential expression is a quaternion wave in the direction of the z axis. If applied as a transformation, this quaternion wave rotates local vectors around the spin axis $W\,\mathbf{k}\,W^*$ at twice the angular frequency associated with the energy of the wave function.

In the matrix form, the spin axis quaternion W is closely related to the two-component spinor representation relative to the z axis:

$$W = \begin{bmatrix} \alpha & -\beta^* \\ \beta & \alpha^* \end{bmatrix}$$

3.3 The effect of an external potential

In the presence of an external four-potential A, equation (1) acquires an extra term, giving the complete Dirac equation in complex four-vector notation:

$$\Box\Psi + ie\overline{A}\Psi\,\mathbf{k} = im\,\overline{\Psi}^{*}\,\overline{\mathbf{k}}^{*} \qquad (2)$$

Note the factor of $\mathbf{k}$ in the four-potential term. In the Dirac algebra formulation of this equation, the effect of the four-potential appears at first glance to be equivalent to adding the four-potential components to the four-derivative components, which in complex four-vector notation would be equivalent to replacing $\Box$ by $(\Box + ie\,\overline{A})$. However, in the Dirac notation the value $\mathbf{k}$ is the implicit axis of quantization, which is hidden by the choice of basis matrices.

3.4 Gauge transformations

Maxwell's equations are gauge-invariant, which means that the physical electromagnetic field derived from the four-potential is unaffected by a gauge transformation:

$$\overline{A} \rightarrow \overline{A'} = \overline{A} - \frac{1}{e}\Box\alpha \tag{3}$$

where α is any differentiable scalar function of space and time. However, if a transformed four-potential is inserted in the Dirac equation without any other change, the additional term means that the equation can no longer hold for the same wave function Ψ. In order for the Dirac equation itself to be unaffected by this transformation, a corresponding transformation has to be applied to the wave function Ψ. In the complex four-vector notation, this transformation is given by:

$$\Psi' = \Psi \exp(i\alpha\,\mathbf{k})$$

This again differs from the Dirac algebra formulation by the explicit appearance of $\mathbf{k}$. Note that the exponential term commutes with $\mathbf{k}$. Vector and complex conjugation each switch the sign of the exponential term, so the double conjugate leaves the exponential term unchanged:

$$\overline{\Psi'}^* = \overline{\Psi}^* \exp(i\alpha\,\mathbf{k})$$

The four-derivative of the exponential term is very simple (since i and $\mathbf{k}$ are constant):

$$\begin{aligned}\Box \exp(i\alpha\,\mathbf{k}) &= \Box(i\alpha\,\mathbf{k})\exp(i\alpha\,\mathbf{k}) \\ &= i(\Box\alpha)\exp(i\alpha\,\mathbf{k})\,\mathbf{k}\end{aligned}$$

The four-derivative of Ψ' includes a corresponding term:

$$\begin{aligned}\Box\Psi' &= (\Box\Psi)\exp(i\alpha\,\mathbf{k}) + i(\Box\alpha)\Psi\exp(i\alpha\,\mathbf{k})\,\mathbf{k} \\ &= (\Box\Psi)\exp(i\alpha\,\mathbf{k}) + i(\Box\alpha)\Psi'\,\mathbf{k}\end{aligned}$$

Note that α, being scalar, commutes with Ψ, and this allows us to place it in the conventional position to be acted on by the $\Box$ operator.

Now, when we replace Ψ with Ψ' and A with A' in equation (2), the extra terms generated by each transformation cancel out. The transformed equation is identical in form to the original, and the transformation has merely postmultiplied both sides of the original equation by $\exp(i\alpha\,\mathbf{k})$.

$$\Box\Psi' + ie\overline{A'}\Psi'\,\mathbf{k} = im\,\overline{\Psi'}^*\,\overline{\mathbf{k}}^*$$

This shows that the Dirac equation is unaffected by a gauge transformation of the four-potential provided that the appropriate transformation is simultaneously applied to the wave function Ψ.

3.5 Comparison with bispinors

Although Ψ can be represented as a complex four-vector or as a two by two complex matrix, the components of Ψ in the Dirac bispinor representation match neither four-vector components nor the matrix components. If we represent the bispinor form as

$$\begin{bmatrix} \Psi_A \\ \Psi_B \\ \Psi_C \\ \Psi_D \end{bmatrix}$$

and use the form of the Dirac matrices given in "Principles of Quantum Mechanics" [Dir58], then by writing out the component equations we can establish that the matrix form is

$$\begin{bmatrix} \Psi_{00} & \Psi_{01} \\ \Psi_{10} & \Psi_{11} \end{bmatrix} = \begin{bmatrix} \Psi_A + \Psi_C & \Psi_B^* - \Psi_D^* \\ \Psi_B + \Psi_D & -\Psi_A^* + \Psi_C^* \end{bmatrix}$$

From this matrix, we can obtain the four-vector components in the usual way:

$$\begin{aligned}
\Psi_0 &= (\Psi_A + \Psi_C - \Psi_A^* + \Psi_C^*)/2 \\
&= \mathrm{Re}(\Psi_C) + i\,\mathrm{Im}(\Psi_A) \\
\Psi_1 &= (\Psi_B + \Psi_D + \Psi_B^* - \Psi_D^*)/2 \\
&= \mathrm{Re}(\Psi_B) + i\,\mathrm{Im}(\Psi_D) \\
\Psi_2 &= (\Psi_B + \Psi_D - \Psi_B^* + \Psi_D^*)/2i \\
&= \mathrm{Im}(\Psi_B) - i\,\mathrm{Re}(\Psi_D) \\
\Psi_3 &= (\Psi_A + \Psi_C + \Psi_A^* - \Psi_C^*)/2 \\
&= \mathrm{Re}(\Psi_A) + i\,\mathrm{Im}(\Psi_C)
\end{aligned}$$

3.6 Operators

As shown in the previous section, there is a simple systematic relationship between the Dirac matrix representation and the complex four-vector representation of the Dirac equation.

Dirac matrices and bispinor notation effectively provide an ingenious but somewhat obscure way of simulating postmultiplication by a structured constant (the axis of quantization) while retaining a notation like that for the non-relativistic Schrödinger equation where operators simply premultiply the wave function.

In contrast, the complex four-vector representation expresses the wave function in a form which is more closely related to conventional space-time, but the corresponding quantum mechanical operators need to include a postmultiplicative constant, which means that they cannot be written simply as a sequence of premultiplicative operators, but rather need to be written with a dummy argument to make clear the multiplication sequence.

Where the non-relativistic Schrödinger operator carries directly over to the relativistic case, the Dirac form of the equation multiplies each component by a Dirac matrix, but the complex four-vector form of the operator simply postmultiplies the result by the constant **k**.

For example, in the Schrödinger representation, the linear momentum operator in the x direction can be written simply as

$$\hat{p}_x = -i\frac{\partial}{\partial x}$$

but the corresponding operator in the complex four-vector representation of the Dirac equation is

$$\hat{p}_x(\Psi) = -i\frac{\partial}{\partial x}\Psi\,\mathbf{k}$$

where Ψ is the dummy argument to indicate the multiplication order. The dummy argument may appear more than once in the expansion if only some of the terms involve postmultiplicative factors.

This means that the complex four-vector representation does make it just a little more complicated to write out operator expressions and especially the products of multiple operators, but by avoiding the use of Dirac matrices it also means that such expressions are usually simpler to interpret and evaluate.

3.7 The probability current

If Ψ varies as a spinor, then $j = \Psi\Psi^*$ is a real four-vector which is equal to Dirac's probability current density vector. Whether it is evaluated using the Dirac matrices or by algebraically multiplying the complex four-vector form, the resulting expression in terms of the Dirac components is identical.

$$\begin{aligned}
j_0 &= (\Psi_A\Psi_A^* + \Psi_B\Psi_B^* + \Psi_C\Psi_C^* + \Psi_D\Psi_D^*) \\
j_1 &= (\Psi_A\Psi_D^* + \Psi_D\Psi_A^* + \Psi_C\Psi_B^* + \Psi_B\Psi_C^*) \\
j_2 &= (\Psi_B\Psi_C^* - \Psi_C\Psi_B^* + \Psi_D\Psi_A^* - \Psi_A\Psi_D^*)/i \\
j_3 &= (\Psi_A\Psi_C^* + \Psi_C\Psi_A^* - \Psi_B\Psi_D^* - \Psi_D\Psi_B^*)
\end{aligned}$$

There is no obvious evidence of symmetry in terms of the Dirac components, but in the four-vector representation the product $\Psi\Psi^*$ is automatically symmetrical between the different components and has no explicit dependence on the choice of axes.

3.8 Physical spin axis representation

Equation (1) requires the choice of an arbitrary direction for k, and our above choice of **k** for this purpose appears to introduce an unexpected asymmetry between the axes. However, the same equation can be written in terms of the physical spin axis $\mathbf{e}_s$ which can be obtained by transforming the unit vector **k** from the rest frame of Ψ (where the speed is zero and average orientation is scalar) to the frame of the observer. This axis transforms like an angular momentum value; the transformed value still has a zero scalar part, but acquires an imaginary vector component if the speed is non-zero, in exactly the same way that an electric field gives rise to a magnetic component when viewed from a moving frame of reference. By writing out the transformation factors, we find that $\Psi\,\mathbf{k}$ is equal to $\mathbf{e}_s\,\Psi$, with the order of the terms reversed, so the equation becomes:

$$\Box\,\Psi = im\,\overline{\mathbf{e}_s}^*\,\overline{\Psi}^* \tag{4}$$

This representation is less useful for finding solutions to the equation because $\mathbf{e}_s$ is not a constant in this case, but it demonstrates that the equation can be written without any need for an arbitrary choice of axis in the notation.

In this form, any explicit solution for Ψ still involves an arbitrary choice of axis as long as Ψ is assumed to transform like a conventional spinor. However, if Ψ is instead assumed to transform like an algebraic spinor, the equation can then be interpreted as referring entirely to physical fields whose properties do not depend on the choice of notation. (Note that most of the previous equations involving Ψ assume the spinor transformation law and would need some modification if Ψ were to be redefined as an algebraic spinor).

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