Geometric Phase in Quaternionic Quantum Mechanics

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Abstract

Quaternion quantum mechanics is examined at the level of unbroken $SU(2)$ gauge symmetry. A general quaternionic phase expression is derived from formal properties of the quaternion algebra.

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1 Quaternion Quantum Mechanics

Quantum mechanics defined over general algebras have been conjectured since 1934 [1]. In 1936 Birkoff and von Neumann noted that the propositional calculus implies in a representation of pure states of a quantum system by rays on a Hilbert space defined over any associative division algebra [2]. This means that quantum theory would be limited to the real, complex and quaternion algebras. Standard textbooks explain the complex formulation of
quantum mechanics by means of the double slit experiment and the complex phase difference of the wave functions. It is possible to use a real quantum theory, but at the cost of introducing a special operator $J$ satisfying $J^2 = 1$ and $J^T = -J$, so that at the end the complex structure emerges again. The final argument for complex algebra as minimum requirement appears with the spinor structure. In fact, the spinor representations of the rotation group requires the existence of solutions of quadratic algebraic equations related to the invariant operators, which are guaranteed only over a complex algebra\[3\].

The development of quaternion quantum mechanics started with D. Finkelstein in 1959, its relativistic and particle aspects were studied by G. Emch and E. J. Schremp \[4, 5, 6\]. A comprehensive reference list can be found in \[7\].

In an attempt to interpret quaternion quantum mechanics, C. N. Yang suggested that the isospinor symmetry should be contained in the group of automorphisms of the quaternion algebra \[4\]. Indeed, supposing that the spin angular momentum $\vec{M}$ associated with $SO(3)$ and the isospin $\vec{I}$ given by a representation of $SU(2)$, are both present in a single state, their spinor representations are given by the Pauli matrices acting separately on the spinor space $\mathcal{M}$ and the isospinor space $\mathcal{I}$ respectively, generated by two independent complex bases $(1, i)$ and $(1, j)$. The direct sum $\mathcal{M} \oplus \mathcal{I}$ does not close as an algebra, except if third imaginary unit $k = ij$ is introduced, producing a quaternion algebra. The automorphisms of this algebra carries the spin-isospin combined symmetry.

According to this interpretation, quaternion quantum mechanics would be effective at the energy level in which the spin and isospin symmetries remain combined. When this combined symmetry breaks down, the isospin angular momentum may lead to an extra spin degree of freedom \[8, 8, 11, 11, 12\].

The existence and effectiveness of quaternion quantum mechanics at higher energies must be experimentally verified. In one of the experiments proposed by A. Peres, a neutron interferometer with thin plates made of materials with varying proportions of neutrons and protons is used, where the phase difference in one or another case is measured \[13\]. In principle this experiment could be adapted to a variable beam intensity, so that a phase difference between the complex and the quaternion could be detected for different energy levels.

Quaternions keep a one-to-one correspondence with space-time vectors.
Therefore, the quaternion phase can also be set in a one-to-one correspondence with a rotation subgroup of the Lorentz group. In this sense, the geometric quaternion phase is truly geometrical as compared with the geometric complex phase, defined on a projective space [14]. The integration of this quaternionic geometric phase, along a closed loop in space-time, can be associated with the space-time curvature, suggesting a quantum gravitational effect.

Taking the quaternion wave function $\Psi$ as a solution of Schrödinger’s equation defined with an anti-Hermitian quaternionic Hamiltonian operator $H$, then the quaternionic dynamical phase $\omega$ can be described by [15]

$$\oint_c \omega^{-1} d\omega = - \int_C \langle \Psi | H | \Psi \rangle dt$$

where $\langle, \rangle$ denotes the quaternionic Hilbert product. In [15], Adler and Anandan have proposed a solution of this integral as given by

$$\omega(t) = T \exp \left( - \int_0^t \langle \Psi | H | \Psi \rangle dv \right),$$

where $\exp$ is the usual complex exponential function and $T$ denotes a constant quaternion representing a time ordering factor.

On the other hand, the geometric phase $\tilde{\omega}$ is determined by

$$\oint_c \tilde{\omega}^{-1} d\tilde{\omega} = - \int_C \langle \Psi | \frac{d\Psi}{dt} \rangle dt,$$

Again, according to [15] this may be integrated to give the following result

$$\tilde{\omega}(t) = T \exp(- \int_0^t \langle \Psi | \frac{d\Psi}{dv} \rangle dv).$$

The question we address ourselves concerns with the generality of this solution as represented by a Volterra integral combined with a fixed ordering factor $T$. We shall see that the left-hand side of (3) has a solution expressed by the imaginary quaternionic exponential function. We start by examining the meaning and uniqueness of the quaternionic line integral in (3). Denoting a quaternion function of a quaternion variable $X = X_\alpha e^\alpha$ in a quaternion basis $e^\alpha$ by $f(X) = U_\alpha e^\alpha$ where $U_\alpha$ are real components, we may define the
left and right line integrals respectively by

\[ \int_c f(X)dX = e^\alpha e^\beta \int_c U_\alpha dx_\beta, \quad \int_c dX f(X) = e^\beta e^\alpha \int_c U_\alpha dx_\beta. \]

These integrals are not necessarily equal:

\[ \int_c f(X)dX - \int_c dX f(X) = \varepsilon_{ijk} e^k \int_c (U_i dx_j - U_j dx_i). \]

However, for a closed loop \( c \), the above difference vanishes as a consequence of Green’s theorem in the plane \((i, j)\). Therefore, for \( X = \tilde{\omega} \) and \( f(X) = \tilde{\omega}^{-1} \), the phase expression in the left-hand side of (3) is uniquely defined.

To obtain a solution of (3) that is more general than (4) we need to understand the importance of being a division algebra.

## 2 Harmonic Functions

The division algebra condition \( |AB| = |A||B| \) is a basic requirement of the standard mathematical analysis based on limit operations of products. In the complex case, the limit operation is independent of the direction in the Gauss plane, eventually leading to the Cauchy-Riemann equations. However, when we attempt to extend the same concepts to the quaternion algebra, the generalized Cauchy-Riemann conditions become so restrictive that only a few trivial functions survive (see the appendix for a brief review) [16, 17, 18, 19, 20]. A less restrictive condition is given by the harmonic functions [21]

\[ \sum \delta_{ij} \frac{\partial^2 U_\alpha}{\partial X_i \partial X_j} + \frac{\partial^2 U_\alpha}{\partial X_0^2} = \Box^2 U_\alpha = 0, \quad (5) \]

Quaternion harmonicity can be implemented by the introduction of the slash differential operator \( \partial = \sum e^\alpha \partial_\alpha = \sum e^\alpha \partial / \partial X_\alpha \), such that \( \Box^2 = \partial \bar{\partial} \). Clearly this operator may act on the right and on the left of a quaternion function.

\footnote{Greek indices run from 0 to 3 and small Latin indices from 1 to 3. The quaternion multiplication table is \( e^i e^j = -\delta^{ij} + \sum e^{ijk} e^k \), \( e^0 e^0 = e^0 e^0 = e^0 = 1 \). Quaternion conjugate is denoted with overbar: \( \bar{e}^i = -e^i \), \( \bar{e}^0 = e^0 \). The quaternion norm is \( |X|^2 = X \bar{X} \).}
\[ f(X), \text{ giving} \]
\[ \partial /f(X) = \partial U_0 \partial X_0 + \sum \partial U_i \partial X_i e^i + \sum \partial U_0 \partial X_i e^i - \sum \partial U_i \partial X_j \delta_{ij} \]
\[ f(x) \partial \partial = \partial U_0 \partial X_0 + \sum \partial U_i \partial X_i e^i + \sum [\partial U_0 \partial X_i e^i - \sum \partial U_i \partial X_j (\delta_{ij} + \epsilon_{ijk} e^k)] \]

It is clear that \( \partial f(X) \neq f(X) \partial \), unless the condition
\[ \frac{\partial U_i}{\partial X_j} = \frac{\partial U_j}{\partial X_i}, \tag{6} \]
holds. Therefore, three classes of harmonic functions may be defined:

a) The left harmonic functions, characterized by \( \partial f(X) = 0 \)
\[ \frac{\partial U_0}{\partial X_0} = \sum \frac{\partial U_i}{\partial X_i}, \]
\[ \frac{\partial U_k}{\partial X_0} + \frac{\partial U_0}{\partial X_k} = \sum \epsilon_{ijk} \frac{\partial U_i}{\partial X_j}. \]

b) The right harmonic functions, such that \( f(X) \partial = 0 \)
\[ \frac{\partial U_0}{\partial X_0} = \sum \frac{\partial U_i}{\partial X_i}, \]
\[ \frac{\partial U_k}{\partial X_0} + \frac{\partial U_0}{\partial X_k} = -\sum \epsilon_{ijk} \frac{\partial U_i}{\partial X_j}. \]

c) The totally harmonic functions (or simply H-functions), characterized by \( \partial f(X) = 0 \) and \( f(X) \partial = 0 \)
\[ \frac{\partial U_0}{\partial X_0} = \sum \frac{\partial U_i}{\partial X_i}, \]
\[ \frac{\partial U_i}{\partial X_0} = \frac{\partial U_0}{\partial X_i}, \]
\[ \frac{\partial U_i}{\partial X_j} = \frac{\partial U_j}{\partial X_i}. \tag{7} \]
The functions belonging to these three classes satisfy the harmonic condition (6).

A non trivial example of H-function is given by an instanton expressed in terms of quaternions. The connection of an anti self dual $SU(2)$ gauge field is given by the form

$$\Gamma = \sum_{\alpha} A_{\alpha}(X)dx^\alpha,$$

where $A_0 = \sum U_k e^k$ and $A_k = U_0 e^k - \epsilon_{ijk} U_i e^j$ and

$$U_0 = \frac{\frac{1}{2}X_0}{1 + |X|^2}, \quad U_i = \frac{-\frac{1}{2}X_i}{1 + |X|^2},$$

are the components of the quaternion function $f(X) = U_0 e^\alpha$. We can see that $f(X)$ satisfy the conditions (7) in the region of space-time defined by $\sum X_i^2 = -2X_0$.

The above example is a particular case of a wider class of functions with components

$$U_\alpha = g_\alpha(X)/(1 + |X|^2),$$

where $g_\alpha(X)$ are real functions.

However, there are some functions which are clearly analytic, such as a constant quaternion, which does not satisfy (7). Therefore, as it happens in the cases of real and complex functions, an analytic quaternion function should be more generally defined by a convergent positive power series.

### 3 Power Series

The power expansion of a quaternionic function requires the equivalent to Cauchy’s integral theorems. Given a quaternion function $f(X)$ defined on an orientable 3-dimensional hypersurface $S$ with unit normal vector $\eta$, again we may define two hypersurface integrals.

$$\int_S f(X) dS_\eta, \quad \text{and} \quad \int_S dS_\eta f(X),$$

where $dS_\eta = \sum dS_i e^i$ denotes the quaternion hypersurface element with components

$$dS_\alpha = \epsilon_{\alpha\beta\gamma\delta} X_\alpha dX_\beta dX_\gamma.$$
where $\epsilon_{\alpha\beta\gamma\delta}$ is the four-dimensional Levi-Civita symbol. On the other hand, denoting by $dV = dX_0dX_1dX_2dX_3$ the 4-dimensional volume element in a region $\Omega$ bounded by $S$, after integrating in one of the variables, we obtain the following result

$$\int_\Omega \partial /f(X) dV = \int_\Omega e^\alpha \partial_\alpha e^\beta U_\beta dV =$$

$$\int_\Omega [(\partial_0 U_0 - \sum_i \partial_i U_i) + \sum_i (\partial_0 U_i + \partial_i U_0) e^i + \epsilon^{ijk} \partial_i U_j e_k] dV.$$

Noting that

$$\int \partial_\alpha U_\beta dV = \int U_\beta dS_\alpha,$$

it follows that

$$\int_\Omega \partial f(X) dV = \int_\Omega [(U_0 dS_0 - \sum_i \delta^{ij} U_i dS_j)e^0 + \sum_i (U_i dS_0 + U_0 dS_i)e^i - \sum \epsilon^{ijk} U_i dS_j e_k].$$

An straightforward calculation shows that this is exactly the same expression of the surface integral

$$\int_S dS_\eta f(X) = \sum \int_S U_\alpha dS_\beta e^\beta e^\alpha.$$ 

Therefore, we obtain the result

$$\int_\Omega \partial f(X) dV = \int_S dS_\eta f(X). \quad (9)$$

Similarly, for the left surface integral we have

$$\int_\Omega f(X) \partial dV = \int_S f(X) dS_\eta. \quad (10)$$

These integrals are defined for any quaternion functions whose components are integrable and their difference is

$$\sum \epsilon^{ijk} e_k \int_S (U_i dS_j - U_j dS_i) = -\sum \epsilon^{ijk} e_k \int_\Omega (\frac{\partial U_i}{\partial X_j} + \frac{\partial U_j}{\partial X_i}) dV,$$

The right hand side is zero so that only one type of surface integral need to be considered. The following theorem extends the first Cauchy’s Theorem to quaternion functions:
If \( f(X) \) satisfy (7) in the interior of a region \( \Omega \) bounded by a hypersurface \( S \) then

\[
\int_S f(X) dS_\eta = \int_S dS_\eta f(X) = 0. \tag{11}
\]

This property follows immediately from equations (9), (10) and the conditions (7). The second Cauchy’s theorem is also true for H-functions:

If \( f(X) \) satisfy the conditions (7) in a region bounded by a simple closed 3-dimensional hypersurface \( S \), then for a point \( P \) in \( S \), we have

\[
f(P) = \frac{1}{\pi^2} \int_S f(X)(X - P)^{-3} dS_\eta. \tag{12}
\]

The proof is also a trivial generalization of the similar complex theorem: The integrand does not satisfy the conditions (7) in \( \Omega \) as it is not defined at \( P \) and consequently the previous theorem does not apply. However the point \( P \) may be isolated by a sphere with surface \( S_0 \) with center at \( P \) and radius \( \epsilon \) such that it remains inside \( \Omega \). Applying (11) to the region bounded by \( S \) and \( S_0 \) we obtain

\[
\int_S f(X)(X - P)^{-3} dS_\eta + \int_{S_0} f(X)(X - P)^{-3} dS_\eta = 0.
\]

Now, the components \( U_\alpha \) may be assumed to be differentiable and regular so that we may calculate their Taylor expansions around \( P \):

\[
U_\alpha(X) = U_\alpha(P) + \epsilon^\beta \frac{\partial U_\alpha}{\partial x^\beta} \mid_P + \cdots.
\]

Replacing this in the integral over \( S_0 \) and taking the limit \( \epsilon \to 0 \), it follows that

\[
f(P) = \left( \int_S f(X)(X - P)^{-3} dS_\eta \right) \left( \int_{S_0} (X - P)^{-3} dS_\eta \right)^{-1}. \tag{13}
\]

In order to calculate the integral over the sphere \( S_0 \) it is convenient to use four dimensional spherical coordinates \((r, \theta, \phi, \gamma)\), such that \( X_0 = rsin\gamma \), \( X_1 = rcos\gamma sin\theta cos\phi \), \( X_2 = rcos\gamma sin\theta sin\phi \) and \( X_3 = rcos\gamma cos\theta \) where \( \theta \in (0, \pi) \), \( \phi \in (0, 2\pi) \), \( \gamma \in (-\pi/2, \pi/2) \). The volume element in spherical coordinates is \( dv = Jdrd\theta d\phi d\gamma \) where \( J = -r^3 cos^2\gamma sin\theta \) is the Jacobian determinant.

The unit normal to the spherical hypersurface centered at \( P \) and with radius \( \epsilon \) can be written as \( \eta = (X - P)/\epsilon \) so that \((X - P)^{-3} = \hat{\eta}^3/\epsilon^3 \) and

\[
- \int_{S_0} (X - P)^{-3} dS_\eta = \int_{S_0} \hat{\eta}^2 cos^2\gamma sin\theta d\theta d\phi d\gamma = \pi^2.
\]

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After replacing in (13), we obtain the proposed result. Notice that the power
\((-3)\) in (12) is not accidental as it is the right power required to cancel the
Jacobian determinant when \(\epsilon \to 0\).

Now we may prove the following general result:

Let \(f(X)\) be such that it satisfies (7) inside a region \(\Omega\) bounded by a
surface \(S\). Then for all \(X\) inside \(\Omega\) there exists coefficients \(a_n\) such that
\[
f(X) = \sum_{n=0}^{\infty} a_n (X - Q)^n.
\]
(14)

As in the similar complex theorem, consider the largest sphere \(S_0\) inside \(\Omega\),
centered at \(Q\). The integral (12) for a point \(P = X\) inside \(\Omega\) gives
\[
f(X) = \frac{1}{\pi^2} \int_{S} f(X')(X' - Q)^{-3} \left[1 - (X' - Q)^{-1}(X - Q)\right]^{-3} dS'_\eta.
\]

It is a simple matter to see that the particular function \(f(X) = (1 - X)^{-3}\),
with \(|X| < 1\) can be expanded as
\[
(1 - X)^{-3} = \sum_{n=1}^{\infty} \frac{n(n + 1)}{2} X^{n-1} = \sum_{m=0}^{\infty} \frac{(m+1)(m+2)}{2} X^m.
\]
(15)

Assuming that \(|X - Q| < |X' - Q|\) and using (13), the above integrand is
equivalent to
\[
[1 - (X' - Q)^{-1}(X - Q)]^{-3} = \sum_{m=0}^{\infty} \frac{(m+1)(m+2)}{2} (X' - Q)^{-m}(X - Q)^m,
\]
so that
\[
f(X) = \frac{1}{\pi^2} \sum_{m=0}^{\infty} \frac{(m+1)(m+2)}{2} \times \int_{S_0} f(X')(X' - Q)^{-3-m}(X - Q)^m dS'_\eta.
\]

Since \(\eta\) and \((X - Q)\) are proportional, the above expression may be written as
\[
f(X) = \frac{1}{\pi^2} \sum_{m=0}^{\infty} \frac{(m+1)(m+2)}{2} \times \int_{S_0} f(X')(X' - Q)^{-3-m} dS'_\eta (X - Q)^m.
\]
Defining the coefficients

\[ a_m = \frac{1}{\pi^2} \frac{(m+1)(m+2)}{2} \int_{S_0} f(X')(X' - Q)^{-3-m} dS'_y, \tag{16} \]

we obtain expression (14), showing that all functions satisfying (7) can also be expressed as a convergent positive power series. The converse is not generally true.

4 Back to Phase

Now we may define a quaternion exponential function in terms of convergent power series and in particular the pure imaginary quaternionic exponential to represent the quaternionic phase. Let us express the solution of (3) as the quaternionic ordered exponential function defined along a curve by

\[ \tilde{\omega} = \text{qexp} \left( \int_c \tilde{\omega}^{-1}d\tilde{\omega} \right) \]

To find the expression of \( P \exp \), consider the quaternion \( X = X_0 e^0 + \sum X_i e^i \). With the last three components we may associate the 3-vector \( \xi \), and a pure imaginary quaternion \( \xi \) such that \( |\xi|^2 = \sum X_i^2 = \xi \cdot \bar{\xi} \), where the dot means the Euclidean scalar product. The unit vector \( \tilde{\Upsilon} = \xi / \sqrt{\xi \cdot \xi} \), corresponds to the pure imaginary quaternion \( \Upsilon = \xi / |\xi| \), such that \( \Upsilon^2 = -1 \), determined by three angles.

We may now draw the Gauss plane with \( e^0 \) in the real axis and \( \Upsilon \) in a direction orthogonal to \( e^0 \). Then a quaternion \( X \) with modulus \( |X| \), making an angle \( \gamma \) with \( e^0 \) may be expressed as

\[ X = X_0 e^0 + X_i e^i = |X| \left( e^0 \cos \gamma + \Upsilon \sin \gamma \right). \]

Replacing \( \sin \gamma \) and \( \cos \gamma \) by the respective power series expansions, after rearranging the terms, we may define the quaternion exponential \( \text{qexp}(\Upsilon \gamma) \) by the series within the parenthesis, so that

\[ \text{qexp}(\Upsilon \gamma) = \frac{X}{|X|} \]
Therefore, the most general integral of (3) may be expressed as the geometric quaternion phase

\[ \tilde{\omega} = \text{qexp}(\Upsilon \gamma) = e^0 \cos \gamma + \Upsilon \sin \gamma. \]  

(17)

Notice that in contrast to (4) there is no fixed direction \( T \) but rather the unit direction \( \Upsilon \) which varies with the quantum states. Contrarily to the complex phase, \( \tilde{\omega} \) acts automorphically over the quaternion wave functions as

\[ \Psi' = \text{qexp}(\Upsilon \gamma)^{-1} \Psi \text{qexp}(\Upsilon \gamma) = \tilde{\omega}^{-1} \Psi \tilde{\omega}, \]

Consequently, the general quaternion phase is in fact distinct from the complex phase both from the analytic point of view as well as from its the geometric interpretation. In the particular case where the vector \( \Upsilon \) is fixed we obtain a solution equivalent to (4).

It appears that quaternion quantum mechanics should be effective at the level of a combined spin-isospin symmetry. The quaternionic spinor operator transforms under the automorphism of the quaternion algebra, producing a distinct behavior on the phase of the wave functions, as compared with the complex theory.

The neutron interferometry experiment proposed in [13] can be modified to accommodate the high-energy interpretation. Accordingly, we suggest a variable beam experiment over plates made of the same material. A higher energy beam will show a qualitative difference from the lower energy case, evidencing the distinction between the quaternion and complex phases.
Appendix
Basic Quaternionic Analysis

Taking a generic quaternion function \( f(X) = U_\alpha(X)e^\alpha \), and denoting \( \Delta f = [f(X + \Delta X) - f(X)] \), the left and right derivatives of \( f(X) \) are defined respectively by

\[
\begin{align*}
  f'(X) &= \lim_{\Delta X \to 0} \delta f(X)(\Delta X)^{-1}, \\
  'f(X) &= \lim_{\Delta X \to 0} (\Delta X)^{-1} \Delta f(X),
\end{align*}
\]

where the limits are taken with \( |\Delta X| \to 0 \) along the direction of the four-vector \( \Delta X \) which depends on the 3-dimensional vector \( \vec{\Delta X} \). Following the same complex procedure, take the derivatives along a fixed direction \( \Delta X = \Delta X_\beta e^\beta \) (no sum on \( \beta \)), indicated by the index within parenthesis

\[
\begin{align*}
  f'(X)_{(\beta)} &= \frac{\partial U_0}{\partial X_\beta} e^0(e^\beta)^{-1} + \sum_i \frac{\partial U_i}{\partial X_\beta} e^i(e^\beta)^{-1}, \\
  'f(X)_{(\beta)} &= \frac{\partial U_0}{\partial X_\beta} (e^\beta)^{-1} e^0 + \sum_i \frac{\partial U_i}{\partial X_\beta} (e^\beta)^{-1} e^i.
\end{align*}
\]

Straightforward calculation shows that

\[
\begin{align*}
  f'(X)_{(0)} &= 'f(X)_{(0)}, \\
  f'(X)_{(j)} &= 'f(X)_{(j)} - 2 \sum_{i,k} \epsilon^{ijk} \frac{\partial U_i}{\partial X_j} e^k.
\end{align*}
\]

By imposing that these derivatives are selectively equal, four basic classes of complex-like analytic functions can be obtained:
As we have mentioned these conditions are too restrictive for most applications, including quantum mechanics.

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