

# **Canadian Journal of Physics**

**Quaternionic Quantum Particles: New Solutions** 

Journal:	Canadian Journal of Physics
Manuscript ID	cjp-2020-0077
Manuscript Type:	Article
Date Submitted by the Author:	11-Feb-2020
Complete List of Authors:	Giardino, Sergio; UFRGS, Departamento de Matemática Pura e Aplicada
Keyword:	quantum mechanics, quaternions, Schroedinger equation, quantum scattering, mathematical physics
Is the invited manuscript for consideration in a Special Issue? :	Not applicable (regular submission)

SCHOLARONE<sup>™</sup> Manuscripts

# **Quaternionic Quantum Particles: New Solutions**

SERGIO GIARDINO\*

Departamento de Matemática Pura e Aplicada, Universidade Federal do Rio Grande do Sul (UFRGS) Avenida Bento Gonçalves 9500, Caixa Postal 15080, 91501-970 Porto Alegre, RS, Brazil

If  $\Psi$  is a quaternionic wave function, then  $i\Psi \neq \Psi i$ . Thus, there are two versions of the quaternionic Schrödinger equation (QSE). In this article, we present the second possibility for solving the QSE, following on from a previous article. After developing the general methodology, we present the quaternionic free particle solution and the scattering of the quaternionic particle through a scalar barrier.

Contents

PACS numbers:

Concents	
I. INTRODUCTION	1
II. TIME-DEPENDENT EQUATION	2
III. GENERAL TIME-INDEPENDENT EQUATION	а
<b>IV. WAVE FUNCTIONS</b> A. $ \kappa_1  = 0$ B. $\cos W = 0$ and $\kappa_0 \neq 0$ C. $\cos W = 0$ and $\kappa_0 = 0$ D. The $\nabla \Gamma = \nabla \Omega = 0$ case	4 5 5 6 6 6
V. THE FREE QUATERNIONIC PARTICLE	7
VI. THE STEP POTENTIAL	7
VII. CONCLUSION	9
ACKNOWLEDGEMENTS	9
References	9

# I. INTRODUCTION

Quaternions [1–3], represented by  $\mathbb{H}$ , are hyper-complex numbers with three anti-commuting complex units. In general, if  $q \in \mathbb{H}$ , then

$$q = x_0 + x_1 i + x_2 j + x_3 k, \tag{1}$$

where  $x_0$ ,  $x_1$ ,  $x_2$  and  $x_3$  are real and the complex units *i*, *j* and *k* satisfy

ij = -ji = k and ijk = -1. (2)

Using a notation called symplectic, we express (1) as

$$q = z + \zeta j$$
 with  $z, \zeta \in \mathbb{C}$ . (3)

Quantum mechanics is a physical theory based on complex numbers. A generalization that replaces complexes with quaternions has been attempted, and Stephen Adler's textbook [4] surveys this endeavor. In this formulation, quaternionic quantum mechanics (QQM) deploys anti-hermitian operators (AHO), instead of the usual hermitian

<sup>\*</sup>Electronic address: sergio.giardino@ufrgs.br

operators of complex quantum mechanics (CQM). An anti-hermitian operator  $\mathcal{A}$  satisfies  $\mathcal{A}^{\dagger} = -\mathcal{A}$ , where  $\mathcal{A}^{\dagger}$  is the adjoint operator of  $\mathcal{A}$ . QQM has been formulated in terms of AHO, among other reasons, to preserve the conservation of the probability current. In spite of this advantage, the adoption of AHO has several drawbacks. The most visible is the breakdown of Ehrenfest's theorem [4–6]. The lack of simple solutions in anti-hermitian QQM is another drawback. Of course, there are anti-hermitian quaternionic solutions, like [7–27], but they are difficult to grasp and do not have the simplicity that allows them to be compared to either CQM or classical solutions. Experimental tests have been performed as well [28, 29], but no quaternionic effect has been observed at the present time. We further adduce that several interesting quantum applications of quaternions are not  $\mathbb{H}QM$  [30–34].

More recently, novel alternatives have been attempted to build a consistent QQM. One may replace usual QQM wave functions with regular quaternionic functions [35], and maintain anti-hermitian formalism. Another approach emerged after the discovery of quaternionic solutions obtained throughout non-anti-hermitian (NAH) Hamiltonians in the study of the quaternionic Aharonov-Bohm (AB) effect [36]. This discovery has enabled a formal expression of an NAH-QQM, where the probability current and the expectation value were redefined and the Hilbert space is real [37, 38]. Following these results, a solution for the QSE was developed, and the first quaternionic particle solution was obtained [39], the Virial theorem has been proven [40] and scattering phenomena has also been studied [41].

Because of the non commutativity between quaternionic functions and the complex unit *i*, there are two possibilities for the QSE, according to the position of *i*. The first possibility has already been considered in [39], where the mathematical formalis has beed developed, and in this article we entertain the second possibility.

This article is organized as follows: Section II presents a general time-dependent solution for QSE, whereas the time-independent QSE is solved in Section III. In Section IV, the solution method is used in several simple situations and, in Section V, the quaternionic free particle is obtained. Section VI describes the scattering of the quaternionic free particle through a scalar step potential, while section VII rounds off the article with our conclusions and future perspectives.

#### **II. TIME-DEPENDENT EQUATION**

The time-dependent quaternionic Schrödinger is

$$i\hbar\frac{\partial\Psi}{\partial t} = \mathcal{H}\Psi,\tag{4}$$

where  $\Psi$  is a quaternionic wave function and  $\mathcal{H}$  is a quaternionic Hamiltonian. We comment on the position of the complex unit *i* on the *left* side of the time-derivative of  $\Psi$  in (4). In [39] we studied the case where the complex unit *i* lay on the *right* side of  $\Psi$ . We separate the time variable of the wave function as

$$\Psi(\mathbf{x},t) = \Phi(\mathbf{x})\Lambda(t),\tag{5}$$

where  $\Phi(x)$  and  $\Lambda(t)$  are both quaternionic. In a complex wave function, a complex exponential, which is a unitary complex, carries the time dependence. By analogy, the time-dependent function  $\Lambda$  of the quaternionic wave function will be chosen to be a unitary quaternionic function. Accordingly, in symplectic notation (3), we get

$$\Lambda = \cos \Xi e^{iX} + \sin \Xi e^{iY} j, \qquad \text{so that} \qquad \Lambda \Lambda^* = 1. \tag{6}$$

 $\Xi$ , X and Y are time-dependent real functions and  $\Lambda^*$  is the quaternionic conjugate of  $\Lambda$ . In order to eliminate the dependence on time from the wave equation, we multiply the right hand side of (4) by  $\Lambda^*$  and impose

$$\dot{\Lambda}\Lambda^* = \frac{\kappa}{\hbar},\tag{7}$$

where the dot denotes a time derivative and  $\kappa \in \mathbb{H}$  is the separation constant

$$\kappa = \kappa_0 + \kappa_1 j, \quad \text{with} \quad \kappa_0, \, \kappa_1 \in \mathbb{C}.$$
 (8)

Consequently, from (7) we get

$$i\left(\dot{X}\cos^{2}\Xi + \dot{Y}\sin^{2}\Xi\right) + \left[\dot{\Xi} + i\sin\Xi\cos\Xi\left(\dot{Y} - \dot{X}\right)\right]e^{i(X+Y)}j = \frac{\kappa}{\hbar}.$$
(9)

We can obtain several solutions for (9). For  $\dot{\Xi} = 0$ ,  $\dot{X} = \dot{Y} = -i\kappa_0$  and  $\kappa_1 = 0$ , we obtain

$$\Lambda = \exp\left[-\frac{i\mathcal{E}}{\hbar}t\right]\Lambda_0, \quad \text{so that} \quad \dot{\Lambda}\Lambda^* = -\frac{i\mathcal{E}}{\hbar}, \tag{10}$$

where  $\mathcal{E}$  is the energy and  $\Lambda_0$  is a unitary quaternionic constant that can multiply both sides of the complex exponential indifferently. The time solution (10) is very similar to the complex case; conversely, we achieved something more interesting by imposing  $\dot{\Xi} = 0$  and  $X + Y = \tau_0$ , where  $\tau_0$  is a real constant. Thus, we get

$$\Lambda = \left\{ \cos \Xi \exp\left[ -\frac{i\mathcal{E}}{\hbar}t \right] + \sin \Xi \exp\left[ i\left(\frac{\mathcal{E}}{\hbar}t + \tau_0\right) \right] j \right\} \Lambda_0, \quad \text{so that} \quad \dot{\Lambda}\Lambda^* = \frac{i\mathcal{E}}{\hbar} \left( -\cos 2\Xi + \sin 2\Xi e^{i\tau_0}j \right).$$
(11)

We remark that (11) may be written schematically as

$$\Lambda = \Lambda_1 \exp\left[-\frac{i\mathcal{E}}{\hbar}t\right] \Lambda_0 \tag{12}$$

where  $\Lambda_1$  is an arbitrary constant quaternion. Solution (11) is absolutely new, it recovers (10) when sin  $\Xi = 0$ , but the value of the constant quaternion contributes to the eigenvalue. This kind of influence of a constant over the eigenvalue of an eigenfunction is unknown in CQM. We expect that novel quantum solutions, unattainable through CQM may emerge. Nevertheless, there is another simple possibility for time-dependent solutions. If  $\dot{X} = \dot{Y} = 0$ , we achieve

$$\Lambda = \left[ \cos\left(\frac{\mathcal{E}}{\hbar}t\right) e^{-iX} + \sin\left(\frac{\mathcal{E}}{\hbar}t\right) e^{i(X+\tau_0)}j \right] \Lambda_0 \qquad \text{so that} \qquad \dot{\Lambda}\Lambda^* = \frac{\mathcal{E}}{\hbar} e^{i\tau_0}j. \tag{13}$$

In the same fashion as (11), the solution given by (12) is absolutely new, it does not have a complex counterpart and a complex limit is meaningless. If something physical may be described with it, it is probably unknown to CQM.

# **III. GENERAL TIME-INDEPENDENT EQUATION**

Using (4-7), the time-independent Schrödinger equation reads

$$\mathcal{H}\Phi = i\,\Phi\,\kappa.\tag{14}$$

In order to solve (14), we need several assumptions. First of all, we propose the spatial wave function

$$\Phi = \phi \,\lambda,\tag{15}$$

where  $\lambda$  is a time-independent quaternionic function given by

$$\lambda = \rho K$$
, where  $|\lambda| = \rho$ ,  $K = \cos \Theta e^{i\Gamma} + \sin \Theta e^{i\Omega} j$ , and  $KK^* = 1$ ; (16)

and  $\phi$  is a time-independent complex solution of Schrödinger equation with energy *E*, so that

$$\mathcal{H}\phi = E\phi, \tag{17}$$

where the energy *E* is real. Consequently, the Hamiltonian  $\mathcal{H}$  is the hermitian operator

$$\mathcal{H} = -\frac{\hbar^2}{2m}\nabla^2 + V,\tag{18}$$

where V is a real scalar potential. More general hamiltonian operators, with complex potentials and complex energies, are interesting directions for research and they may be examined in a separate article. Using (14-15), (16), we get

$$\nabla^2 \lambda + \frac{2}{\phi} \nabla \phi \cdot \nabla \lambda = \frac{2m}{\hbar^2} (E\lambda - i\lambda\kappa).$$
<sup>(19)</sup>

We also adopt

$$\nabla K = p e^{i\Gamma} + q e^{i\Omega} j$$
 and  $\nabla^2 K = u e^{i\Gamma} + v e^{i\Omega} j$ , (20)

where

$$p = -\sin\Theta\,\nabla\Theta + i\cos\Theta\,\nabla\Gamma, \qquad q = \cos\Theta\,\nabla\Theta + i\sin\Theta\,\nabla\Omega, u = -\cos\Theta\left(\left|\nabla\Gamma\right|^{2} + \left|\nabla\Theta\right|^{2}\right) - \sin\Theta\,\nabla^{2}\Theta + i\left(\cos\Theta\,\nabla^{2}\Gamma - 2\sin\Theta\,\nabla\Gamma\cdot\nabla\Theta\right)$$
(21)  
$$v = -\sin\Theta\left(\left|\nabla\Omega\right|^{2} + \left|\nabla\Theta\right|^{2}\right) + \cos\Theta\,\nabla^{2}\Theta + i\left(\sin\Theta\,\nabla^{2}\Omega + 2\cos\Theta\,\nabla\Omega\cdot\nabla\Theta\right).$$

The complex and quaternionic parts of (19) give

$$\frac{1}{\rho} \left( \nabla + \frac{2}{\phi} \nabla \phi \right) \cdot \nabla \rho + \frac{2}{\rho \phi} \nabla (\rho \phi) \cdot \frac{p}{\cos \Theta} + \frac{u}{\cos \Theta} = \frac{2m}{\hbar^2} \left[ E - i\kappa_0 + i\kappa_1^* \tan \Theta e^{i(\Omega - \Gamma)} \right]$$
(22)

$$\frac{1}{\rho} \left( \boldsymbol{\nabla} + \frac{2}{\phi} \boldsymbol{\nabla} \phi \right) \cdot \boldsymbol{\nabla} \rho + \frac{2}{\rho \phi} \boldsymbol{\nabla} (\rho \phi) \cdot \frac{\boldsymbol{q}}{\sin \Theta} + \frac{v}{\sin \Theta} = \frac{2m}{\hbar^2} \left[ E - i\kappa_0^* - i\kappa_1 \cot \Theta e^{i(\Gamma - \Omega)} \right].$$
(23)

Specific values chosen for  $\kappa$  furnish the three time-dependent solutions (10-12). Four real equations are obtained from the two complex equations (22-23). First of all, we note that

$$i\kappa_0 \in \mathbb{R}$$
 and  $\kappa_1 = |\kappa_1|e^{i\tau_0}$ . (24)

Thence, we define

$$\frac{1}{\rho} \left( \boldsymbol{\nabla} + \frac{2}{\phi} \boldsymbol{\nabla} \phi \right) \cdot \boldsymbol{\nabla} \rho = \mathcal{Z}_0, \qquad \frac{2}{\rho \phi} \boldsymbol{\nabla} (\rho \phi) \cdot \frac{p}{\cos \Theta} = \mathcal{Z}_1 \qquad \text{and} \qquad \frac{2}{\rho \phi} \boldsymbol{\nabla} (\rho \phi) \cdot \frac{q}{\sin \Theta} = \mathcal{Z}_2, \tag{25}$$

where  $Z_0$ ,  $Z_1$  and  $Z_2$  are complex functions. We finally separate (22-23) into real components, so that

$$\Re(\mathcal{Z}_0 + \mathcal{Z}_1) - |\nabla\Gamma|^2 - |\nabla\Theta|^2 - \tan\Theta\nabla^2\Theta = \frac{2m}{\hbar^2} \Big( E - i\kappa_0 + |\kappa_1|\tan\Theta\sinW \Big)$$
(26)

$$\Re(\mathcal{Z}_0 + \mathcal{Z}_2) - |\boldsymbol{\nabla}\Omega|^2 - |\boldsymbol{\nabla}\Theta|^2 + \cot\Theta\nabla^2\Theta = \frac{2m}{\hbar^2} \Big( E + i\kappa_0 + |\kappa_1|\cot\Theta\sinW \Big)$$
(27)

$$\Im(\mathcal{Z}_0 + \mathcal{Z}_1) + \left(\nabla - 2\tan\Theta\nabla\Theta\right) \cdot \nabla\Gamma = \frac{2m}{\hbar^2} |\kappa_1| \tan\Theta\cos W$$
(28)

$$\Im(\mathcal{Z}_0 + \mathcal{Z}_2) + \left(\boldsymbol{\nabla} + 2\cot\Theta\boldsymbol{\nabla}\Theta\right) \cdot \boldsymbol{\nabla}\Omega = -\frac{2m}{\hbar^2} |\kappa_1| \cot\Theta\cos W$$
<sup>(29)</sup>

where

$$W = \Gamma - \Omega + \tau_0, \tag{30}$$

and  $\Re(\mathcal{Z})$  and  $\Im(\mathcal{Z})$  are the real and the imaginary components of a complex  $\mathcal{Z}$ , respectively. Equations (26-29) are the most general time-independent solutions obtained from the three time-dependent cases. In the following section, we examine several simple solutions, and leave more complicated cases for future research.

# IV. WAVE FUNCTIONS

Assuming an arbitrary one-dimensional complex wave function  $\phi$  and also  $\nabla \Theta = \mathbf{0}$ , we impose the constraints

$$\nabla \phi \cdot \nabla \rho = 0, \qquad \nabla \phi \cdot \nabla \Gamma = 0, \qquad \nabla \phi \cdot \nabla \Omega = 0, \qquad \nabla \rho \cdot \nabla \Gamma = 0, \qquad \nabla \rho \cdot \nabla \Omega = 0, \tag{31}$$

remembering that  $\nabla \Gamma \cdot \nabla \Omega \neq 0$ . Thus, (26-29) turn into two equations

$$\frac{1}{\rho}\nabla^2 \rho - |\boldsymbol{\nabla}\Gamma|^2 = \frac{2m}{\hbar^2} \Big( E - i\kappa_0 + |\kappa_1| \tan\Theta\sin W \Big)$$
(32)

$$\frac{1}{\rho}\nabla^2\rho - |\boldsymbol{\nabla}\Omega|^2 = \frac{2m}{\hbar^2} \Big( E + i\kappa_0 + |\kappa_1| \cot\Theta\sin W \Big), \tag{33}$$

$$\nabla^2 \Gamma = \frac{2m}{\hbar^2} |\kappa_1| \tan \Theta \cos W \tag{34}$$

$$\nabla^2 \Omega = -\frac{2m}{\hbar^2} |\kappa_1| \cot \Theta \cos W \tag{35}$$

From (31), we suppose that there is no common variable between either  $\rho$  and  $\Gamma$  or between  $\rho$  and  $\Omega$ ; therefore,  $\nabla^2 \rho / \rho$  has to be constant. After the action of the gradient operator over (32-33), we recover (34-35) with changed signs. This result imposes

$$\nabla^2 \Gamma = \nabla^2 \Omega = 0. \tag{36}$$

Hence, we gain the constraint

$$|\kappa_1|\cos W = 0,\tag{37}$$

and consequently two cases to consider. Let us examine the first one.

**A.**  $|\kappa_1| = 0$ 

We suppose a three-dimensional space, and thus  $\nabla\Gamma$  and  $\nabla\Omega$  are necessarily collinear. The other two directions of the space given by  $\nabla\phi$  and  $\nabla\rho$ . From (32) and (33), we obtain

$$\frac{1}{\rho}\nabla^2\rho = \frac{2mE}{\hbar^2} + \frac{|\nabla\Gamma|^2 + |\nabla\Omega|^2}{2}, \quad \text{and} \quad \frac{2m\mathcal{E}}{\hbar^2} = \frac{|\nabla\Gamma|^2 - |\nabla\Omega|^2}{2}, \quad (38)$$

where

$$\mathcal{E} = i\kappa_0 \tag{39}$$

is the quaternionic energy. Therefore, we reach the following solution

$$\Gamma = \gamma \cdot \mathbf{x} + \Gamma^{(0)}, \qquad \Omega = \boldsymbol{\omega} \cdot \mathbf{x} + \Omega^{(0)}, \qquad \text{and} \qquad \rho = A \, e^{\boldsymbol{\alpha} \cdot \mathbf{x}} + B \, e^{-\boldsymbol{\alpha} \cdot \mathbf{x}}, \tag{40}$$

where  $\Gamma^{(0)}$ ,  $\Omega^{(0)}$ , *A* and *B* are real scalar constants, and  $\alpha$  is a constant real vector. There is no solution for the constant  $\rho$ , and we must have

$$|\boldsymbol{\alpha}|^2 = \frac{2mE}{\hbar^2} + \frac{|\gamma|^2 + |\boldsymbol{\omega}|^2}{2}$$
 and  $|\gamma|^2 - |\boldsymbol{\omega}|^2 \ge 0.$  (41)

The most general wave function is thus

$$\Phi = \phi(\mathbf{x}) \rho(\mathbf{x}) \Big[ \left( \cos \Theta e^{i\Gamma} + \sin \Theta e^{i\Omega} j \right) C_1 + \left( \cos \Theta e^{i\Gamma} + \sin \Theta e^{-i\Omega} j \right) C_2 + \left( \cos \Theta e^{-i\Gamma} + \sin \Theta e^{i\Omega} j \right) C_3 + \left( \cos \Theta e^{-i\Gamma} + \sin \Theta e^{-i\Omega} j \right) C_4 \Big],$$
(42)

where  $C_1$ ,  $C_2$ ,  $C_3$  and  $C_4$  are arbitrary complex constants. (14) is not satisfied for quaternionic integration constants. We can make  $\phi$  constant, so that E = 0, and thus obtain the simplest solution of the case, a truly quaternionic free particle. However, we stress that every one-dimensional complex wave function  $\phi$  generates the same kind of quaternionic solution, where the quaternionic solution may be understood as a geometric phase. A general study concerning quaternionic phases is an interesting direction for research.

## **B.** $\cos W = 0$ and $\kappa_0 \neq 0$

The solutions of this case obey

$$W = \Gamma - \Omega + \tau_0 = \left(n + \frac{1}{2}\right)\pi$$
 so that  $\nabla\Gamma = \nabla\Omega$ , (43)

with  $n \in \mathbb{Z}$ . Using (32-33), (39) and (43), we get

$$\mathcal{E} = -|\kappa_1|\cot 2\Theta \sin W,\tag{44}$$

so that

$$\frac{1}{\rho}\nabla^2 \rho = \frac{2m}{\hbar^2} \Big( E - \mathcal{E}\sec 2\Theta \Big) + |\nabla\Gamma|^2.$$
(45)

Inasmuch as there is no defined sign on the right hand side of (45), two kinds of solutions for  $\rho$  are admitted, either real exponentials or a linear combination of sines and cosines. Even a  $\nabla^2 \rho = 0$  is admitted, and hence there are more possibilities for  $\rho$  in this situation than has been found in the previous  $|\kappa_1| = 0$  case. The general solution is thus

$$\Phi = \phi(\mathbf{x}) \rho(\mathbf{x}) \left( C_1 e^{i\Gamma} + C_2 e^{-i\Gamma} \right) \left( \cos \Theta - i \sin W \sin \Theta e^{i\tau_0} j \right)$$
(46)

with  $C_1$  and  $C_2$  arbitrary complex constants and  $\Gamma$  given by (40). The solution (46) comprises a complex solution and a quaternionic unitary constant that multiplies its right-hand side. The quaternionic energy accomplished through (45) is

$$\mathcal{E} = \cos 2\Theta \left[ E + \frac{\hbar^2}{2m} \left( |\gamma|^2 \pm |\alpha|^2 \right) \right],\tag{47}$$

where the sign of  $|\alpha|^2$  is defined by  $\rho$ . It is totally unexpected that the quaternionic constant influences the energy of the system, and there is no counterpart to this phenomenon in CQM. A physical system described with this solution would be remarkable. We notice that low quaternionic energies, where  $\mathcal{E} < E$ , are admitted, depending on  $\rho$ . This curious and new effect is probably due to the quaternionic character of the eigenvalue  $\kappa$ , which is connected to the energy through (44).

**C.**  $\cos W = 0$  and  $\kappa_0 = 0$ 

This solution is related to the time-dependent solution (13). The solutions of this case follow (43), but (32-33) additionally imposes

$$\Theta = \left(\tilde{n} + \frac{1}{2}\right) \frac{\pi}{2}, \quad \text{where} \quad \tilde{n} \in \mathbb{Z}.$$
(48)

Consequently, the quaternionic wave function is obtained from (46), and the quaternionic energy is

$$\mathcal{E} = |\kappa_1| = -\frac{\cot\Theta}{\sin W} \left[ E + \frac{\hbar^2}{2m} \left( |\gamma|^2 \pm |\alpha|^2 \right) \right].$$
(49)

**D.** The  $\nabla \Gamma = \nabla \Omega = \mathbf{0}$  case

Assuming an arbitrary one-dimensional complex wave function  $\phi$ , we impose the constraints

$$\nabla \phi \cdot \nabla \rho = 0, \qquad \nabla \phi \cdot \nabla \Theta = 0, \qquad \nabla \rho \cdot \nabla \Theta = 0. \tag{50}$$

Thus, (25-28) turns into two equations

$$\frac{1}{\rho}\nabla^2 \rho - |\nabla\Theta|^2 = \frac{2m}{\hbar^2} \Big( E - i\kappa_0 \cos 2\Theta + |\kappa_1| \sin W \sin 2\Theta \Big)$$
(51)

$$\nabla^2 \Theta = \frac{2m}{\hbar^2} \Big( i\kappa_0 \sin 2\Theta + |\kappa_1| \sin W \cos 2\Theta \Big), \tag{52}$$

and the constraint (37) that has already been found for the  $\nabla \Theta = \mathbf{0}$  cases. However, the orthogonality of  $\nabla \rho$  and  $\nabla \Theta$  implies that  $\nabla^2 \rho / \rho$  is a constant. Applying the gradient operator over (51), we recover (52) with a changed sign, and thus  $\nabla^2 \Theta = 0$ , which forces a constant  $\Theta$  because of (52). With exception for an exotic zero energy solution, where  $\kappa = 0$  and  $\nabla \Theta$  is constant. Therefore, we do not have a simple solution for non-constant  $\Theta$ . Maybe this kind of solution exists when (50) includes a non-orthogonal  $\nabla \Theta$ . The research of such solutions is potentially an interesting subject for future work.

6

#### V. THE FREE QUATERNIONIC PARTICLE

Let us take the complex free particle as a reference. Its expression is

$$\phi(\mathbf{x}) = A_1 e^{i\mathbf{k}\cdot\mathbf{x}} + A_2 e^{-i\mathbf{k}\cdot\mathbf{x}}, \quad \text{where} \quad |\mathbf{k}|^2 = \frac{2mE}{\hbar^2},$$
(53)

and *A* and *B* are complex integration constants. In order to understand the physics of the previously calculated solutions, we will entertain the probability current defined in [36?], namely

$$j = \frac{1}{2m} \left\{ \left( \hat{p} \Psi \right) \Psi^* + \left[ \left( \hat{p} \Psi \right) \Psi^* \right]^* \right\} \quad \text{and} \quad \hat{p} \Psi = -i \hbar \nabla \Psi.$$
(54)

Using the general quaternionic time independent wave function (15), we get

$$j = \rho^2 \left[ j_0 + \frac{\hbar}{m} |\phi|^2 \left( \cos^2 \Theta \nabla \Gamma + \sin^2 \Theta \nabla \Omega \right) \right] |C|^2$$
(55)

where *C* is an arbitrary quaternionic constant and  $j_0$  is the probability current due to the complex free particle (53). There is no probability flux along the  $\nabla \Theta$  and  $\nabla \rho$  directions. This fact does not mean that there is no motion along these directions. We remember the complex square well, where a particle oscillates along a confined region without generating a non-zero probability flux. Thus, we interpret that the quaternionic particle freely propagates along directions  $\nabla \Gamma$  and  $\nabla \Omega$  only, while directions  $\nabla \Theta$  and  $\nabla \rho$  allow oscillatory motions only. A simple quaternionic free particle obtained from (42) is

$$\Phi = \rho(\mathbf{x}) \left( \cos \Theta e^{i\gamma \cdot \mathbf{x}} + \sin \Theta e^{i\omega \cdot \mathbf{x}} j \right) C \qquad \Rightarrow \qquad j = \frac{\hbar}{m} \rho^2 |C|^2 \left( \cos^2 \Theta \gamma + \sin^2 \Theta \omega \right), \tag{56}$$

where *C* is a quaternionic constant and  $\nabla \Theta = \mathbf{0}$ . From (38), we get

$$|\alpha|^2 = \frac{|\gamma|^2 + |\omega|^2}{2}, \qquad \frac{2m\mathcal{E}}{\hbar^2} = \frac{|\gamma|^2 - |\omega|^2}{2}.$$
 (57)

An exotic zero-energy wave function is possible for

$$|\alpha| = |\gamma| = |\omega|. \tag{58}$$

The situation is different from the complex case, where null energies imply null momenta. Another particularity is that we cannot recover a complex solution by simply imposing  $\Theta = |\omega| = |\alpha| = 0$ . We remember that  $|\alpha| = 0$  is prohibited by (57), and that a simple quaternionic constant may change the energy of the particle (46-47). Thus, QQM solutions cannot be understood as encompassing a complex solution plus an independent pure quaternionic part. In fact, we have a different theory, which may recover CQM for several situations, but not for all cases.

### VI. THE STEP POTENTIAL

Let us consider the scalar step potential

$$V = \begin{cases} 0 & \text{for } x < 0, & \text{region I} \\ V_0 & \text{for } x \ge 0, & \text{region II}, \end{cases}$$
(59)

where  $V_0$  concerns a real positive constant and the potential *V* divides the three-dimensional space into two parts bordered by the *Oyz* plane. We propose the wave function

$$\Phi_{I} = \rho_{k} \left[ \cos \Theta_{k} e^{i(k+\gamma_{k}^{\perp})\cdot \mathbf{x}} + \sin \Theta_{k} e^{i(-k+\omega_{k}^{\perp})\cdot \mathbf{x}} j \right] + R \rho_{q} \left[ \cos \Theta_{q} e^{i(-q+\gamma_{q}^{\perp})\cdot \mathbf{x}} + \sin \Theta_{q} e^{i(q+\omega_{q}^{\perp})\cdot \mathbf{x}} j \right]$$

$$\Phi_{II} = T \rho_{p} \left[ \cos \Theta_{p} e^{i(p+\gamma_{p}^{\perp})\cdot \mathbf{x}} + \sin \Theta_{p} e^{i(-p+\omega_{p}^{\perp})\cdot \mathbf{x}} j \right]$$
(60)

with *R* and *T* complex constants and *k*, *q*, *p*,  $\gamma_a^{\perp}$  and  $\omega_a^{\perp}$  real vectors for a = k, *q*, *p*. We also adopt real constants for  $\Theta_a$  and real functions for  $\rho_a$ . An arbitrary vector *v* is decomposed as

$$v = v^{\parallel} + v^{\perp}, \tag{61}$$

where the component of v parallel to k is  $v^{\parallel}$ , and the component of v normal to k is  $v^{\perp}$ . We expect that the three terms of the wave function (60) have identical properties, or describe particles of the same type. We choose the time-dependent solution (10), where E = 0. From (38), we obtain several energy relations

$$\frac{2m\mathcal{E}}{\hbar^2} = \frac{|\gamma_k|^2 - |\omega_k|^2}{2} = \frac{|\gamma_q|^2 - |\omega_q|^2}{2}, \qquad \frac{2m(\mathcal{E} - V_0)}{\hbar^2} = \frac{|\gamma_p|^2 - |\omega_p|^2}{2}$$
(62)

and also that

$$|\boldsymbol{\alpha}_{a}|^{2} = |\boldsymbol{a}|^{2} + \frac{|\gamma_{a}|^{2} + |\boldsymbol{\omega}_{a}|^{2}}{2}$$
 where  $\boldsymbol{a} = k, q, p.$  (63)

At the point of incidence  $x_0 = (0, y_0, z_0)$ , which we set to  $x_0 = (0, 0, 0)$  without loss of generality, we consider the continuity of the wave function,

$$\Phi_{I}(\mathbf{x}_{0}) = \Phi_{II}(\mathbf{x}_{0}) \qquad \Rightarrow \qquad \begin{cases} \rho_{k}(0)\cos\Theta_{k}^{(0)} + R\rho_{q}(0)\cos\Theta_{q}^{(0)} = T\rho_{p}(0)\cos\Theta_{p}^{(0)} \\ \rho_{k}(0)\sin\Theta_{k}^{(0)} + R\rho_{q}(0)\sin\Theta_{q}^{(0)} = T\rho_{p}(0)\sin\Theta_{p}^{(0)} \end{cases}$$
(64)

$$\nabla \Phi_{I}^{\parallel}(\mathbf{x}_{0}) = \nabla \Phi_{II}^{\parallel}(\mathbf{x}_{0}) \qquad \Rightarrow \qquad \begin{cases} \mathbf{k}\rho_{k}(0)\cos\Theta_{k}^{(0)} - \mathbf{q}R\rho_{q}(0)\cos\Theta_{q}^{(0)} = \mathbf{p}T\rho_{p}(0)\cos\Theta_{p}^{(0)} \\ -\mathbf{k}\rho_{k}(0)\sin\Theta_{k}^{(0)} + \mathbf{q}R\rho_{q}(0)\sin\Theta_{q}^{(0)} = -\mathbf{p}T\rho_{p}(0)\sin\Theta_{p}^{(0)}. \end{cases}$$
(65)

and thus

$$|T|^{2} = \frac{|\mathbf{k} + \mathbf{q}|^{2}}{|\mathbf{p} + \mathbf{q}|^{2}} \left(\frac{\rho_{k}(0)}{\rho_{p}(0)}\right)^{2} \quad \text{and} \quad |R|^{2} = \frac{|\mathbf{k} - \mathbf{p}|^{2}}{|\mathbf{p} + \mathbf{q}|^{2}} \left(\frac{\rho_{k}(0)}{\rho_{q}(0)}\right)^{2}.$$
(66)

The normal directions place further boundary conditions

$$\boldsymbol{\nabla} \Phi_{I}^{\perp}(\mathbf{0}) = \boldsymbol{\nabla} \Phi_{II}^{\perp}(\mathbf{0}) \qquad \Rightarrow \qquad \begin{cases} \boldsymbol{\nabla} \rho_{k}(0) \ K_{k} + \boldsymbol{\nabla} \rho_{q}(0) \ R \ K_{q} = \boldsymbol{\nabla} \rho_{p}(0) \ T \ K_{p} \\ \boldsymbol{\gamma}_{k}^{\perp} \ \rho_{k}(0) \ \cos \Theta_{k}^{(0)} + R \boldsymbol{\gamma}_{q}^{\perp} \ \rho_{q}(0) \ \cos \Theta_{q}^{(0)} = T \boldsymbol{\gamma}_{p}^{\perp} \ \rho_{p}(0) \ \cos \Theta_{p}^{(0)} \\ \boldsymbol{\omega}_{k}^{\perp} \ \rho_{k}(0) \ \sin \Theta_{k}^{(0)} + R \boldsymbol{\omega}_{q}^{\perp} \ \rho_{q}(0) \ \sin \Theta_{q}^{(0)} = T \boldsymbol{\omega}_{p}^{\perp} \ \rho_{p}(0) \ \sin \Theta_{p}^{(0)}, \end{cases}$$
(67)

where

$$K_a = \cos \Theta_a^{(0)} + \sin \Theta_a^{(0)} j, \qquad \nabla \rho_a(0) = \alpha_a (A_a - B_a) \qquad \text{and} \qquad a = k, q, p.$$
(68)

We propose a solution using the constraint

$$\sin^2 \Theta_k^{(0)} = \sin^2 \Theta_q^{(0)} = \sin^2 \Theta_p^{(0)}.$$
(69)

If |k| = |q|, we benefit from the identity

$$|\mathbf{k}| - |\mathbf{q}| R \frac{\rho_q(0)}{\rho_k(0)} = |\mathbf{p}| T \frac{\rho_p(0)}{\rho_k(0)},$$
(70)

which is valid for the scattering of quantum particles in CQM. Thus, (67), (69) and (70) give rise to

$$\frac{|\boldsymbol{\gamma}_q|}{|\boldsymbol{\gamma}_k|} = \frac{|\boldsymbol{\omega}_q|}{|\boldsymbol{\omega}_k|} = \frac{|\boldsymbol{\nabla}\rho_q(0)|}{|\boldsymbol{\nabla}\rho_k(0)|} = 1 \qquad \qquad \frac{|\boldsymbol{\gamma}_p|}{|\boldsymbol{\gamma}_k|} = \frac{|\boldsymbol{\omega}_p|}{|\boldsymbol{\omega}_k|} = \frac{|\boldsymbol{\nabla}\rho_p(0)|}{|\boldsymbol{\nabla}\rho_k(0)|} = \frac{|\boldsymbol{p}|}{|\boldsymbol{k}|}.$$
(71)

From (62-63) and (71) we finally obtain

$$\frac{|\boldsymbol{\alpha}_p|^2}{|\boldsymbol{\alpha}_k|^2} = \frac{|\boldsymbol{p}|^2}{|\boldsymbol{k}|^2} \qquad \qquad \frac{|\boldsymbol{p}|^2}{|\boldsymbol{k}|^2} = 1 - \frac{V_0}{\mathcal{E}}.$$
(72)

Consequently, every parameter of the reflected and transmitted particles may be written in terms of the incident particle parameters. The results are similar to the CQM case, but the transmission and reflection coefficients have multiplying factors that are characteristic of quaternionic particles. These factors are related to the oscillation along the  $\nabla \rho$  direction; as discussed in section V, the quaternionic particle propagates along  $\nabla \Gamma$  and  $\nabla \Omega$ , whereas along  $\nabla \rho$  and  $\nabla \Theta$  it only oscillates.

8

#### VII. CONCLUSION

In this article, we have used a general method for solving the QSE (4) that has been developed in [39] to the solution of the QSE with a right multiplying complex unit *i*. We have proven that there are time-dependent solutions for Schrödinger equation (4), which are fundamentally different from the time-function of CQM. We have also developed a general method for solving the time-independent solution, and we have obtained free particle solutions without a CQM counterpart. These solutions present oscillations that are normal to the propagation direction. This result is unknown in CQM, and now we need to find more physical examples where this kind of situation is found. Another interesting new feature is the influence of quaternionic constants on the energies of solutions. This is another quaternionic feature unknown in CQM, and other physical systems where this kink of behavior is found are also of interest for further research.

In summary, we expect that these two articles will foster new developments in QQM. First of all, because the presented solutions are simple, and do not assume the anti-hermitian constraint that has been supposed for the QQM. Secondly, we have a method for finding new solutions, and then every result of CQM is at risk of being studied using the quaternionic formalism deployed here. We expect that more physical solutions may be found in the future, which may inspire either mathematical or physics investigations, including experimental ones.

#### ACKNOWLEDGEMENTS

Sergio Giardino is grateful for the hospitality at the Institute of Science and Technology of Unifesp in São José dos Campos.

- [1] J. Vaz; R. da Rocha. "An Introduction to Clifford Algebras and Spinors". Oxford University Press (2016).
- [2] G. M. Dixon. "Division Algebras: octonions, quaternions, complex numbers and the qlgebraic design of physics". Springer (1994).
- [3] J. P. Ward. "Quaternions and Cayley Numbers". Springer Dordrecht (1997).
- [4] S. L. Adler. "Quaternionic Quantum Mechanics and Quantum Fields". Oxford University Press (1995).
- [5] S. L. Adler. "Quaternionic quantum field theory". Commun. Math. Phys., 104:611, 1986.
- [6] S. L. Adler. "Quaternionic quantum field theory". In: C. Teitelboim (Ed.), Quantum Mechanics of Fundamental Systems 1, Springer (1988).
- [7] A. J. Davies; B. H. J. McKellar. "Nonrelativistic quaternionic quantum mechanics in one dimension". Phys. Rev., A40:4209–4214, (1989).
- [8] A. J. Davies; B. H. J. McKellar. "Observability of quaternionic quantum mechanics". Phys. Rev., A46:3671-3675, (1989).
- [9] S. De Leo; G. Ducati. "Quaternionic differential operators". J. Math. Phys, 42:2236-2265, (2001).
- [10] S. De Leo; G. Ducati; C. Nishi. " Quaternionic potentials in non-relativistic quantum mechanics". J. Phys, A35:5411– 5426, (2002).
- [11] S. De Leo; G. Ducati. "Quaternionic bound states". J. Phys, A35:3443-3454, (2005).
- [12] S. De Leo; G. Ducati; T. Madureira. "Analytic plane wave solutions for the quaternionic potential step". J. Math. Phys, 47:082106-15, (2006).
- [13] S. De Leo; G. Ducati. "Quaternionic wave packets". J. Math. Phys, 48:052111–10, (2007).
- [14] A. J. Davies. "Quaternionic Dirac equation". Phys.Rev., D41:2628-2630, (1990).
  [15] S. De Leo; S. Giardino. "Dirac solutions for quaternionic potentials". J. Math. Phys., 55:022301-10, (2014) arXiv:1311.6673[math-ph].
- [16] S. De Leo; G. Ducati; S. Giardino. "Quaternioninc Dirac Scattering". J. Phys. Math., 6:1000130, (2015) arXiv:1505.01807[math-ph].
- [17] S. Giardino. "Quaternionic particle in a relativistic box". Found. Phys., 46(4):473-483, (2016)arXiv:1504.00643[quant-ph].
- [18] H. Sobhani; H. Hassanabadi. "Scattering in quantum mechanics under quaternionic Dirac delta potential". Can. J. Phys., 94:262–266, (2016).
- [19] L. M. Procopio; L. A. Rozema; B Dakic; P. Walther. "Comment on Peres experiment using photons: No test for hypercomplex (quaternionic) quantum theories". *Phys. Rev.*, A96(3):036101, (2017).
- [20] H. Sobhani; H; Hassanabadi; W. S. Chung. "Observations of the RamsauerTownsend effect in quaternionic quantum mechanics". Eur. Phys. J., C77(6):425, (2017).
- [21] H. Hassanabadi; H. Sobhani; A. Banerjee. "Relativistic scattering of fermions in quaternionic quantum mechanics". Eur. Phys. J., C77(9):581, (2017).
- [22] H. Hassanabadi, H. Sobhani; W. S. Chung. "Scattering Study of Fermions Due to Double Dirac Delta Potential in Quaternionic Relativistic Quantum Mechanics". Adv. High Energy Phys., 2018:8124073, 2018.

- [23] H. Sobhani; H; Hassanabadi. "New face of RamsauerTownsend effect by using a Quaternionic double Dirac potential". Indian J. Phys., 91(1):1–5, (2017).
- [24] S. De Leo; C A. A. de Souza; G. Ducati. "Quaternionic perturbation theory". Eur. Phys. J. Plus, 134(3):113, (2019).
- [25] M. Cahay; G. B. Purdy; D. Morris. "On the quaternion representation of the Pauli spinor of an electron". Phys. Scripta, 94(8):085205, (2019).
- [26] P. A. Bolokhov. "Quaternionic wave function". Int. J. Mod. Phys., A34(02):1950001, (2019).
- [27] B. C. Chanyal; Sandhya Karnatak. "A comparative study of quaternionic rotational Dirac equation and its interpretation". accept by Int. J. Geom. Meth. Mod. Phys. (2019).
- [28] L. M. Procopio; L. A. Rozema; Z. J. Wong; D. R. Hamel; K. O'Brien; X. Zhang; B. Dakic; P. Walther. "Single-photon test of hyper-complex quantum theories using a metamaterial". Nature Communications 8, Article number: 15044 (2017).
- [29] S. P. Brumby; G. C. Joshi. "Experimental status of quaternionic quantum mechanics". Chaos Solitons Fractals, 7:747–752, (1996) quant-ph/9610009.
- [30] A. I. Arbab. "The Quaternionic Quantum Mechanics". Appl. Phys. Res., 3:160-170, (2011).
- [31] D. C. Brody; E.-V. Graefe. "Six-dimensional space-time from quaternionic quantum mechanics". Phys. Rev., D84:125016, (2011).
- [32] J. Morais. "On the quaternion representation of the Pauli spinor of an electron". Ann. Phys., 349:171-188, (2014).
- "Quaternionic quantization principle in general relativity and supergravity". [33] M. Kober. Int. J. Mod. Phys., A31(04n05):1650004, (2016).
- [34] S. B. Tabeu; F. Fotsa-Ngaffo; A. Kenfack-Jiotsa. "Non-Hermitian Hamiltonian of two-level systems in complex quaternionic space: An introduction in electronics". EPL, 125(2):24002, (2019).
- [35] B. Muraleetharan; K. Thirulogasanthar; I. Sabadini. "A Representation of Weyl-Heisenberg Lie Algebra in the Quaternionic Setting ". Ann. Phys. 385 180-213 (2017).
- [36] S. Giardino. "Quaternionic Aharonov-Bohm effect". Adv. Appl. Cliff. Alg. 27 24452456 (2017).
- [37] S. Giardino. "Non-anti-hermitian Quaternionic Quantum Mechanics". Adv. Appl. Clifford Algebras, 28(1):19, (2018).
- [38] S. Giardino. "Quaternionic quantum mechanics in real Hilbert space". arXiv:1803.11523[math-ph] (2018).
- [39] S. Giardino. Quaternionic quantum particles. Adv. Appl. Clifford Algebras, 29(4):83, (2019).
  [40] S. Giardino. "Virial theorem and generalized momentum in quaternic quantum mechanics". Eur. Phys. J. Plus, 135(1):114, (2020).
- [41] M. Hasan; B. P. Mandal. "New scattering features of quaternionic pointinteraction in non-Hermitian quantum mechanics". arXiv:1901.02357 (2019).