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Quaternionic differential operators

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Motivated by a quaternionic formulation of quantum mechanics, we discuss quaternionic and complex linear differential equations. We touch only a few aspects of the mathematical theory, namely the resolution of the second order differential equations with constant coefficients. We overcome the problems coming out from the loss of the fundamental theorem of the algebra for quaternions and propose a practical method to solve quaternionic and complex linear second order differential equations with constant coefficients. The resolution of the complex linear Schrödinger equation, in the presence of quaternionic potentials, represents an interesting application of the mathematical material discussed in this paper. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1360195]

I. INTRODUCTION

There is substantial literature analyzing the possibility to discuss quantum systems by adopting quaternionic wave functions.[1–14] This research field has been attacked by a number of people leading to substantial progress. In the last years, many articles,[15–31] review papers[32–34] and books[35–37] provided a detailed investigation of group theory, eigenvalue problem, scattering theory, relativistic wave equations, Lagrangian formalism and variational calculus within a quaternionic formulation of quantum mechanics and field theory. In this context, by observing that the formulation of physical problems in mathematical terms often requires the study of partial differential equations, we develop the necessary theory to solve quaternionic and complex linear differential equations. The main difficulty in carrying out the solution of quaternionic differential equations is obviously represented by the noncommutative nature of the quaternionic field. The standard methods of resolution break down and, consequently, we need to modify the classical approach. It is not our purpose to develop a complete quaternionic theory of differential equations. This exceeds the scope of this paper. The main objective is to include what seemed to be most important for an introduction to this subject. In particular, we restrict ourselves to second order differential equations and give a practical method to solve such equations when quaternionic constant coefficients appear.

Some of the results given in this paper can be obtained by translation into a complex formalism.[15,16,31] Nevertheless, many subtleties of quaternionic calculus are often lost by using the translation trick. See, for example, the difference between quaternionic and complex geometry in quantum mechanics,[32,34] generalization of variational calculus,[9,10] the choice of a one-dimensional quaternionic Lorentz group for special relativity,[21] the new definitions of transpose and determinant for quaternionic matrices.[29] A wholly quaternionic derivation of the general solution of second order differential equations requires a detailed discussion of the fundamental theorem of algebra for quaternions, a revision of the resolution methods and a quaternionic generalization of the complex results.

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The study of quaternionic linear second order differential equations with constant coefficients is based on the explicit resolution of the characteristic quadratic equation.[38–41] We shall show that the loss of fundamental theorem of the algebra for quaternions does not represent a problem in solving quaternionic linear second order differential equations with constant coefficients. From there, we introduce more advanced concepts, like diagonalization and Jordan form for quaternionic and complex linear matrix operators, which are developed in detail in the recent literature[22–31] and we apply them to solve quaternionic and complex linear second order differential equations with constant coefficients.

As an application of the mathematical material presented in this paper, we discuss the complex linear Schrödinger equation in the presence of quaternionic potentials and solve such an equation for stationary states and constant potentials. We also calculate the relation between the reflection and transmition coefficients for the step and square potential and give the quaternionic solution for bound states.

This work was intended as an attempt at motivating the study of quaternionic and complex linear differential equations in view of their future applications within a quaternionic formulation of quantum mechanics. In particular, our future objective is to understand the role that such equations could play in developing nonrelativistic quaternionic quantum dynamics[4] and the meaning that quaternionic potentials[15,16] could play in discussing CP violation in the kaon system.[36]

In order to give a clear exposition and to facilitate access to the individual topics, the sections are rendered as self-contained as possible. In Sec. II, we review some of the standard concepts used in quaternionic quantum mechanics, i.e., state vector, probability interpretation, scalar product and left/right quaternionic operators.[29,35,42–45] Section III contains a brief discussion of the momentum operator. In Sec. IV, we summarize without proofs the relevant material on quaternionic eigenvalue equations from Ref. 31. Section V is devoted to the study of the one-dimensional Schrödinger equation in quaternionic quantum mechanics. Sections VI and VII provide a detailed exposition of quaternionic and complex linear differential equations. In Sec. VIII, we apply the results of previous sections to the one-dimensional Schrödinger equation with quaternionic constant potentials. Our conclusions are drawn in the final section.

II. STATES AND OPERATORS IN QUATERNIONIC QUANTUM MECHANICS

In this section, we give a brief survey of the basic mathematical tools used in quaternionic quantum mechanics.[32–37] The quantum state of a particle is defined, at a given instant, by a quaternionic wave function interpreted as a probability amplitude given by

$$\Psi(\mathbf{r})=[f_0+\mathbf{h}\cdot\mathbf{f}](\mathbf{r}), \tag{1}$$

where $\mathbf{h}=(i,j,k)$, $\mathbf{f}=(f_1,f_2,f_3)$ and $f_m:\mathbb{R}^3\to\mathbb{R}$, $m=0,1,2,3$. The probabilistic interpretation of this wave function requires that it belong to the Hilbert vector space of square-integrable functions. We shall denote by $\mathcal{F}$ the set of wave functions composed of sufficiently regular functions of this vector space. The same function $\Psi(\mathbf{r})$ can be represented by several distinct sets of components, each one corresponding to the choice of a particular basis. With each pair of elements of $\mathcal{F}$, $\Psi(\mathbf{r})$, and $\Phi(\mathbf{r})$, we associate the quaternionic scalar product,

$$(\Psi,\Phi)=\int d^3r\,\overline{\Psi}(\mathbf{r})\Phi(\mathbf{r}), \tag{2}$$

where

$$\overline{\Psi}(\mathbf{r})=[f_0-\mathbf{h}\cdot\mathbf{f}](\mathbf{r}) \tag{3}$$

represents the quaternionic conjugate of $\boldsymbol{\Psi}(\mathbf{r})$.

A quaternionic linear operator, $\mathcal{O}_{\mathbb{H}}$, associates with every wave function $\Psi(\mathbf{r})\in\mathcal{F}$ another wave function $\mathcal{O}_{\mathbb{H}}\Psi(\mathbf{r})\in\mathcal{F}$, the correspondence being linear from the right on $\mathbb{H}$,

$$\mathcal{O}_{\mathbb{H}}[\Psi_1(\mathbf{r})q_1+\Psi_2(\mathbf{r})q_2]=[\mathcal{O}_{\mathbb{H}}\Psi_1(\mathbf{r})]q_1+[\mathcal{O}_{\mathbb{H}}\Psi_2(\mathbf{r})]q_2,$$

$q_{1,2}\in\mathbb{H}$. Due to the noncommutative nature of the quaternionic field we need to introduce complex and real linear quaternionic operators, respectively, denoted by $\mathcal{O}_{\mathbb{C}}$ and $\mathcal{O}_{\mathbb{R}}$, the correspondence being linear from the right on $\mathbb{C}$ and $\mathbb{R}$

$$\mathcal{O}_{\mathbb{C}}[\Psi_1(\mathbf{r})z_1+\Psi_2(\mathbf{r})z_2]=[\mathcal{O}_{\mathbb{C}}\Psi_1(\mathbf{r})]z_1+[\mathcal{O}_{\mathbb{C}}\Psi_2(\mathbf{r})]z_2,$$

$$\mathcal{O}_{\mathbb{R}}[\Psi_1(\mathbf{r})\lambda_1+\Psi_2(\mathbf{r})\lambda_2]=[\mathcal{O}_{\mathbb{H}}\Psi_1(\mathbf{r})]\lambda_1+[\mathcal{O}_{\mathbb{H}}\Psi_2(\mathbf{r})]\lambda_2,$$

$z_{1,2}\in\mathbb{C}$ and $\lambda_{1,2}\in\mathbb{R}$.

As a concrete illustration of these operators let us consider the case of a finite, say n-dimensional, quaternionic Hilbert space. The wave function $\Psi(\mathbf{r})$ will then be a column vector,

$$\Psi=\begin{pmatrix}\Psi_1\\ \Psi_2\\ \vdots\\ \Psi_n\end{pmatrix},\quad \Psi_{1,2,\ldots,n}\in\mathcal{F}.$$

Quaternionic, complex and real linear operators will be represented by $n\times n$ quaternionic matrices $M_n[\mathcal{A}\otimes\mathcal{O}]$, where $\mathcal{O}$ represents the space of real operators acting on the components of Ψ and $\boldsymbol{\mathcal{A}}=(\mathcal{A}_{\mathbb{H}},\mathcal{A}_{\mathbb{C}},\mathcal{A}_{\mathbb{R}})$ denote the real algebras,

$$\mathcal{A}_{\mathcal{H}}\ :\ \{\mathbf{1},\ \mathbf{L},\ \mathbf{R},\ \mathbf{L}*\mathbf{R}\}_{16},$$

$$\mathcal{A}_{\mathbb{C}}\ :\ \{\mathbf{1},\ \mathbf{L},\ R_i,\ \mathbf{L}R_i\}_{8},$$

$$\mathcal{A}_{\mathbb{R}}\ :\ \{\mathbf{1},\ \mathbf{L}\}_{4},$$

generated by the left and right operators,

$$\mathbf{L}:=(L_i,L_j,L_k),\quad \mathbf{R}:=(R_i,R_j,R_k),\tag{4}$$

and by the mixed operators,

$$\mathbf{L}*\mathbf{R}:=\{L_pR_q\},\quad p,q=i,j,k.\tag{5}$$

The action of these operators on the quaternionic wave function Ψ is given by

$$\mathbf{L}\Psi\equiv\mathbf{h}\Psi,\quad \mathbf{R}\Psi\equiv\Psi\mathbf{h}.$$

The operators $\mathbf{L}$ and $\mathbf{R}$ satisfy the left/right quaternionic algebra,

$$L_i^2=L_j^2=L_k^2=L_iL_jL_k=R_i^2=R_j^2=R_k^2=R_kR_jR_i=-\mathbf{1},$$

and the following commutation relations:

$$[L_p,R_q]=0.$$

III. SPACE TRANSLATIONS AND QUATERNIONIC MOMENTUM OPERATOR

Space translation operators in quaternionic quantum mechanics are defined in the coordinate representation by the real linear anti-Hermitian operator,[36]

$$\boldsymbol{\partial}\equiv(\partial_x,\partial_y,\partial_z).\tag{6}$$

To construct an observable momentum operator we must look for a Hermitian operator that has all the properties of the momentum expected by analogy with the momentum operator in complex quantum mechanics. The choice of the quaternionic linear operator,

$$\boldsymbol{\mathcal{P}}_L = -L_i \hbar \boldsymbol{\partial}, \tag{7}$$

as a Hermitian momentum operator, would appear completely satisfactory, until we consider the translation invariance for quaternionic Hamiltonians, $\mathcal{H}_q$. In fact, due to the presence of the left acting imaginary unit i, the momentum operator (7) does not commute with the j/k-part of $\mathcal{H}_q$. Thus, although this definition of the momentum operator gives a Hermitian operator, we must return to the anti-Hermitian operator $\boldsymbol{\partial}$ to get a translation generator, $[\boldsymbol{\partial}, \mathcal{H}_q] = 0$. A second possibility to be considered is represented by the complex linear momentum operator, introduced by Rotelli in Ref. 44,

$$\boldsymbol{\mathcal{P}}_R = -R_i \hbar \boldsymbol{\partial}. \tag{8}$$

The commutator of $\boldsymbol{\mathcal{P}}_R$ with a quaternionic linear operator $\mathcal{O}_{\mathbb{H}}$ gives

$$[\boldsymbol{\mathcal{P}}_R, \mathcal{O}]\Psi = \hbar[\mathcal{O}, \boldsymbol{\partial}]\Psi i.$$

Taking $\mathcal{O}_{\mathbb{H}}$ to be a translation invariant quaternionic Hamiltonian $\mathcal{H}_q$, we have

$$[\boldsymbol{\mathcal{P}}_R, \mathcal{H}_q] = 0.$$

However, this second definition of the momentum operator has the following problem: the complex linear momentum operator $\boldsymbol{\mathcal{P}}_R$ does not represent a quaternionic Hermitian operator. In fact, by computing the difference

$$(\Psi, \boldsymbol{\mathcal{P}}_R \Phi) - \overline{(\Phi, \boldsymbol{\mathcal{P}}_R \Psi)},$$

which should vanish for a Hermitian operator $\boldsymbol{\mathcal{P}}_R$, we find

$$(\Psi, \boldsymbol{\mathcal{P}}_R \Phi) - (\boldsymbol{\mathcal{P}}_R \Psi, \Phi) = \hbar[i, (\Psi, \boldsymbol{\partial}\Phi)], \tag{9}$$

which is in general nonvanishing. There is one important case in which the right-hand side of Eq. (9) does vanish. The operator $\boldsymbol{\mathcal{P}}_R$ gives a satisfactory definition of the Hermitian momentum operator when restricted to a *complex geometry*,[45] that is a *complex projection* of the quaternionic scalar product, $(\Psi, \boldsymbol{\mathcal{P}}_R \Phi)_{\mathbb{C}}$. Note that the assumption of a complex projection of the quaternionic scalar product does not imply complex wave functions. The state of quaternionic quantum mechanics with complex geometry will be again described by vectors of a quaternionic Hilbert space. In quaternionic quantum mechanics with complex geometry observables can be represented by the quaternionic Hermitian operator, H, obtained taking the *spectral decomposition*[31] of the corresponding anti-Hermitian operator, A, or simply by the complex linear operator, $-AR_i$, obtained by multiplying A by the operator representing the right action of the imaginary unit i. These two possibilities represent equivalent choices in describing quaternionic observables within a quaternionic formulation of quantum mechanics based on complex geometry. In this scenario, the complex linear operator $\boldsymbol{\mathcal{P}}_R$ has all the expected properties of the momentum operator. It satisfies the standard commutation relations with the coordinates. It is a translation generator. Finally, it represents a *quaternionic observable*. A review of quaternionic and complexified quaternionic quantum mechanics by adopting a complex geometry is found in Ref. 34.

IV. OBSERVABLES IN QUATERNIONIC QUANTUM MECHANICS

In a recent paper,[31] we find a detailed discussion of eigenvalue equations within a quaternionic formulation of quantum mechanics with quaternionic and complex geometry. Quaternionic eigenvalue equations for quaternionic and complex linear operators require eigenvalues from the right. In particular, without loss of generality, we can reduce the eigenvalue problem for quaternionic and complex linear anti-Hermitian operators $A \in M_n[\mathcal{A}_{\mathbb{H}} \otimes \mathcal{O}]$ to

$$A\Psi_m = \Psi_m \lambda_m i, \quad m = 1,2,\ldots,n, \tag{10}$$

where λ_m are real eigenvalues.

There is an important difference between the structure of Hermitian operators in complex and quaternionic quantum mechanics. In complex quantum mechanics we can always trivially relate an anti-Hermitian operator, A, to a Hermitian operator, H, by removing a factor i, i.e., $A = iH$. In general, due to the noncommutative nature of the quaternionic field, this does not apply to quaternionic quantum mechanics.

Let $\{\Psi_m\}$ be a set of normalized eigenvectors of A with complex imaginary eigenvalues $\{i\lambda_m\}$. The anti-Hermitian operator A is then represented by

$$A = \sum_{r=1}^{n} \Psi_r \lambda_r i \Psi_r^\dagger, \tag{11}$$

where $\Psi^\dagger := \overline{\Psi^t}$. It is easy to verify that

$$A\Psi_m = \sum_{r=1}^{n} \Psi_r \lambda_r i \Psi_r^\dagger \Psi_m = \sum_{r=1}^{n} \Psi_r \lambda_r i \delta_{rm} = \Psi_m \lambda_m i.$$

In quaternionic quantum mechanics with quaternionic geometry,[36] the observable corresponding to the anti-Hermitian operator A is represented by the following Hermitian quaternionic linear operator:

$$H = \sum_{r=1}^{n} \Psi_r \lambda_r \Psi_r^\dagger. \tag{12}$$

The action of these operators on the eigenvectors Ψ_m gives

$$H\Psi_m = \Psi_m \lambda_m.$$

The eigenvalues of the operator H are real and eigenvectors corresponding to different eigenvalues are orthogonal.

How to relate the Hermitian operator H to the anti-Hermitian operator A? A simple calculation shows that the operators $L_i H$ and HL_i does not satisfy the same eigenvalue equation of A. In fact,

$$L_i H \Psi_m = \left[L_i \left(\sum_{r=1}^{n} \Psi_r \lambda_r \Psi_r^\dagger \right) \right] \Psi_m = i \sum_{r=1}^{n} \Psi_r \lambda_r \Psi_r^\dagger \Psi_m = i \Psi_m \lambda_m$$

and

$$HL_i \Psi_m = \left[\left(\sum_{r=1}^{n} \Psi_r \lambda_r \Psi_r^\dagger \right) L_i \right] \Psi_m = \sum_{r=1}^{n} \Psi_r \lambda_r \Psi_r^\dagger i \Psi_m.$$

These problems can be avoided by using the right operator R_i instead of the left operator L_i. In fact, the operator HR_i satisfies the same eigenvalue equation of A,

$$HR_i \Psi_m = \left[\left(\sum_{r=1}^{n} \Psi_r \lambda_r \Psi_r^\dagger \right) R_i \right] \Psi_m = \sum_{r=1}^{n} \Psi_r \lambda_r \Psi_r^\dagger \Psi_m i = \Psi_m \lambda_m i.$$

The eigenvalues of the operator $-AR_i$ are real and eigenvectors corresponding to different eigenvalues are orthogonal. The right hermiticity of this operator is recovered within a quaternionic formulation of quantum mechanics based on complex geometry.[34]

When the space state is finite-dimensional, it is always possible to form a basis with the eigenvectors of the operators H and $-AR_i$. When the space state is infinite-dimensional, this is no longer necessarily the case. So, it is useful to introduce a new concept, that of an observable. By definition, the Hermitian operators H or $-AR_i$ are observables if the orthonormal system of vectors forms a basis in the state space.

In quaternionic quantum mechanics with quaternionic geometry, the Hermitian operator corresponding to the anti-Hermitian operator A of Eq. (11) is thus given by the operator H of Eq. (12). By adopting a complex geometry, observables can also be represented by complex linear Hermitian operators obtained by multiplying the corresponding anti-Hermitian operator A by $-R_i$. We remark that for complex eigenvectors, the operators L_iH, HL_i, HR_i and A reduce to the same complex operator,

$$iH = i\sum_{r=1}^{n} \lambda_r \Psi_r \Psi_r^\dagger .$$

We conclude this section by giving an explicit example of quaternionic Hermitian operators in a finite two-dimensional space state. Let

$$A = \begin{pmatrix} -i & 3j \\ 3j & i \end{pmatrix} \tag{13}$$

be an anti-Hermitian operator. An easy computation shows that the eigenvalues and the eigenvectors of this operator are given by

$$\{2i, 4i\} \quad \text{and} \quad \left\{ \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ j \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} k \\ 1 \end{pmatrix} \right\}.$$

It is immediate to verify that iA and Ai are characterized by complex eigenvalues and so cannot represent quaternionic observables. In quaternionic quantum mechanics with quaternionic geometry, the quaternionic observable corresponding to the anti-Hermitian operator of Eq. (13) is given by the Hermitian operator,

$$H = \Psi_1 2 \Psi_1^\dagger + \Psi_2 4 \Psi_2^\dagger = \begin{pmatrix} 3 & k \\ -k & 3 \end{pmatrix}. \tag{14}$$

Within a quaternionic quantum mechanics with complex geometry, a second equivalent definition of the quaternionic observable corresponding to the anti-Hermitian operator of Eq. (13) is given by the complex linear Hermitian operator,

$$\tilde{H} = \begin{pmatrix} -i & 3j \\ 3j & i \end{pmatrix} R_i . \tag{15}$$

V. THE QUATERNIONIC SCHRÖDINGER EQUATION

For simplicity, we shall assume a one-dimensional description. In the standard formulation of quantum mechanics, the wave function of a particle whose potential energy is $V(x,t)$ must satisfy the Schrödinger equation,

$$i\hbar\, \partial_t \Phi(x,t) = \mathcal{H}\, \Phi(x,t) = \left(-\frac{\hbar^2}{2m} \partial_{xx} + V(x,t) \right) \Phi(x,t). \tag{16}$$

Let us modify the previous equation by introducing the quaternionic potential,

$$[V+\mathbf{h}\cdot\mathbf{V}](x,t).$$

The i-part of this quaternionic potential violates the norm conservation. In fact,

$$\partial_t\int_{-\infty}^{+\infty}\mathrm{d}x\,\bar{\Phi}\,\Phi=\int_{-\infty}^{+\infty}\mathrm{d}x\left[\frac{\hbar}{2m}\bar{\Phi}\,i\,\partial_{xx}\Phi-\frac{\hbar}{2m}(\partial_{xx}\bar{\Phi})i\,\Phi-\frac{1}{\hbar}\bar{\Phi}\{i,\mathbf{h}\}\cdot\mathbf{V}\Phi\right]$$
$$=\frac{2}{\hbar}\int_{-\infty}^{+\infty}\mathrm{d}x\,\bar{\Phi}\,V_1\Phi.$$

The j/k-part of $\mathbf{h}\cdot\mathbf{V}$ is responsible for T-violation.[4] To show that, we briefly discuss the time reversal invariance in quaternionic quantum mechanics. The quaternionic Schrödinger equation in the presence of a quaternionic potential which preserves norm conservation, is given by[4,15,16,36]

$$i\,\hbar\,\partial_t\Phi(x,t)=[\mathcal{H}-j\,W]\Phi(x,t), \tag{17}$$

where $W\in\mathbb{C}$. Evidently, quaternionic conjugation,

$$-\hbar\,\partial_t\bar{\Phi}(x,t)i=\mathcal{H}\,\bar{\Phi}(x,t)+\bar{\Phi}(x,t)j\,W,$$

does not yield a time-reversed version of the original Schrödinger equation

$$-i\,\hbar\,\partial_t\Phi_{\mathrm{T}}(x,-t)=[\mathcal{H}-j\,W]\Phi_{\mathrm{T}}(x,-t). \tag{18}$$

To understand why the T-violation is proportional to the j/k-part of the quaternionic potential, let us consider a real potential W. Then, the Schrödinger equation has a T-invariance. By multiplying Eq. (17) by j from the left, we have

$$-i\,\hbar\,\partial_t\,j\,\Phi(x,t)=[\mathcal{H}-j\,W]j\,\Phi(x,t),\qquad W\in\mathbb{R},$$

which has the same form of Eq. (18). Thus,

$$\Phi_{\mathrm{T}}(x,-t)=j\,\Phi(x,t).$$

A similar discussion applies for imaginary complex potential $W\in i\,\mathbb{R}$. In this case, we find

$$\Phi_{\mathrm{T}}(x,-t)=k\,\Phi(x,t).$$

However, when both V_2 and V_3 are nonzero, i.e., $W\in\mathbb{C}$, this construction does not work, and the quaternionic physics is T-violating. The system of neutral kaons is the natural candidate to study the presence of *effective* quaternionic potentials, $V+\mathbf{h}\cdot\mathbf{V}$. In studying such a system, we need of V_1 and $V_{2,3}$ in order to include the decay rates of $K_{\mathrm{S}}/K_{\mathrm{L}}$ and CP-violation effects.

A. Quaternionic stationary states

For stationary states,

$$V(x,t)=V(x)\quad\text{and}\quad W(x,t)=W(x),$$

we look for solutions of the Schrödinger equation of the form

$$\Phi(x,t)=\Psi(x)\zeta(t). \tag{19}$$

Substituting (19) in the quaternionic Schrödinger equation, we obtain

$$i\,\hbar\,\Psi(x)\dot{\zeta}(t)=[\mathcal{H}-j\,W(x)]\Psi(x)\zeta(t). \tag{20}$$

Multiplying by $-\overline{\Psi}(x)i$ from the left and by $\overline{\zeta}(t)$ from the right, we find

$$\hbar\,\dot{\zeta}(t)\overline{\zeta}(t)/|\zeta(t)|^2=\overline{\Psi}(x)[-i\,\mathcal{H}+k\,W(x)]\Psi(x)/|\Psi(x)|^2. \tag{21}$$

In this equation we have a function of t on the left-hand side and a function of x on the right-hand side. The previous equality is only possible if

$$\hbar\,\dot{\zeta}(t)\overline{\zeta}(t)/\,|\zeta(t)|^2=\overline{\Psi}(x)[-i\,\mathcal{H}+k\,W(x)]\Psi(x)/|\Psi(x)|^2=q, \tag{22}$$

where q is a quaternionic constant. The energy operator $-i\,\mathcal{H}+k\,W(x)$ represents an anti-Hermitian operator. Consequently, its eigenvalues are purely imaginary quaternions, $q=\mathbf{h}\cdot\mathbf{E}$. By applying the unitary transformation u,

$$\overline{u}\,\mathbf{h}\cdot\mathbf{E}\,u=-\,i\,E,\quad E=\sqrt{E_1^2+E_2^2+E_3^2},$$

Eq. (22) becomes

$$\hbar\,\overline{u}\,\dot{\zeta}(t)\overline{\zeta}(t)u/|\zeta(t)|^2=\overline{u}\,\overline{\Psi}(x)[-i\,H+k\,W(x)]\Psi(x)u/|\Psi(x)|^2=-i\,E. \tag{23}$$

The solution $\Phi(x,t)$ of the Schrödinger equation is not modified by this similarity transformation. In fact,

$$\Phi(x,t)\to\Psi(x)u\,\overline{u}\,\zeta(t)=\Psi(x)\zeta(t).$$

By observing that $|\Phi(x,t)|^2=|\Psi(x)|^2|\zeta(t)|^2$, the norm conservation implies $|\zeta(t)|^2$ constant. Without loss of generality, we can choose $|\zeta(t)|^2=1$. Consequently, by equating the first and the third term in Eq. (23) and solving the corresponding equation, we find

$$\zeta(t)=\exp[-iEt/\hbar]\zeta(0), \tag{24}$$

with $\zeta(0)$ unitary quaternion. Note that the position of $\zeta(0)$ in Eq. (24) is very important. In fact, it can be shown that $\zeta(0)\exp[-iEt/\hbar]$ is not solution of Eq. (23). Finally, to complete the solution of the quaternionic Schrödinger equation, we must determine $\Psi(x)$ by solving the following second order (right complex linear) differential equation,

$$\left[i\,\frac{\hbar^2}{2m}\,\partial_{xx}-i\,V(x)+k\,W(x)\right]\Psi(x)=-\Psi(x)i\,E. \tag{25}$$

B. Real potential

For $W(x)=0$, Eq. (25) becomes

$$\left[\frac{\hbar^2}{2m}\,\partial_{xx}-V(x)\right]\{[\Psi(x)]_{\mathbb{C}}-j[j\Psi(x)]_{\mathbb{C}}\}=i\,\{[\Psi(x)]_{\mathbb{C}}-j[j\Psi(x)]_{\mathbb{C}}\}i\,E. \tag{26}$$

Consequently,

$$\left[\frac{\hbar^2}{2m}\,\partial_{xx}-V(x)\right][\Psi(x)]_{\mathbb{C}}=-[\Psi(x)]_{\mathbb{C}}E,$$

and

$$\left[\frac{\hbar^2}{2m}\,\partial_{xx}-V(x)\right][j\Psi(x)]_{\mathbb{C}}=[j\Psi(x)]_{\mathbb{C}}E.$$

By solving these complex equations, we find

$$\Psi(x)=\exp\left[\sqrt{\frac{2m}{\hbar^2}(V-E)}\,x\right]k_1+\exp\left[-\sqrt{\frac{2m}{\hbar^2}(V-E)}\,x\right]k_2+j\times\left\{\exp\left[\sqrt{\frac{2m}{\hbar^2}(V+E)}\,x\right]k_3+\exp\left[-\sqrt{\frac{2m}{\hbar^2}(V+E)}\,x\right]k_4\right\},$$

where k_n, $n=1,\ldots,4$, are complex coefficients determined by the initial conditions.

C. Free particles

For free particles, $V(x)=W(x)=0$, the previous solution reduces to

$$\Psi(x)=\exp\left[i\frac{p}{\hbar}x\right]k_1+\exp\left[-i\frac{p}{\hbar}x\right]k_2+j\left\{\exp\left[\frac{p}{\hbar}x\right]k_3+\exp\left[-\frac{p}{\hbar}x\right]k_4\right\},$$

where $p=\sqrt{2mE}$. For scattering problems with a wave function incident from the left on quaternionic potentials, we have

$$\Psi(x)=\exp\left[i\frac{p}{\hbar}x\right]+r\exp\left[-i\frac{p}{\hbar}x\right]+j\,\tilde{r}\exp\left[\frac{p}{\hbar}x\right], \tag{27}$$

where $|r|^2$ is the standard coefficient of reflection and $|\tilde{r}\exp[(p/\hbar)x]|^2$ represents an additional evanescent probability of reflection. In our study of quaternionic potentials, we shall deal with the rectangular potential barrier of width a. In this case, the particle is free for $x<0$, where the solution is given by (27), and $x>a$, where the solution is

$$\Psi(x)=t\exp\left[i\frac{p}{\hbar}x\right]+j\,\tilde{t}\exp\left[-\frac{p}{\hbar}x\right]. \tag{28}$$

Note that, in Eqs. (27) and (28), we have, respectively, omitted the complex exponential solution $\exp[-(p/\hbar)x]$ and $\exp[(p/\hbar)x]$ which are in conflict with the boundary condition that $\Psi(x)$ remain finite as $x\to-\infty$ and $x\to\infty$. In Eq. (28), we have also omitted the complex exponential solution $\exp[-i(p/\hbar)x]$ because we are considering a wave incident from the left.

VI. QUATERNIONIC LINEAR DIFFERENTIAL EQUATION

Consider the second order quaternionic linear differential operator,

$$\mathcal{D}_{\mathbb{H}}=\partial_{xx}+(a_0+\mathbf{L}\cdot\mathbf{a})\partial_x+b_0+\mathbf{L}\cdot\mathbf{b}\in\mathcal{A}_{\mathbb{H}}\otimes\mathcal{O}.$$

We are interested in finding the solution of the quaternionic linear differential equation,

$$\mathcal{D}_{\mathbb{H}}\,\varphi(x)=0. \tag{29}$$

In analogy to the complex case, we look for solutions of exponential form

$$\varphi(x)=\exp[qx],$$

where $q\in\mathbb{H}$ and $x\in\mathbb{R}$. To satisfy Eq. (29), the constant q has to be a solution of the quaternionic quadratic equation,[38–41]

$$q^2+(a_0+\mathbf{h}\cdot\mathbf{a})q+b_0+\mathbf{h}\cdot\mathbf{b}=0. \tag{30}$$

A. Quaternionic quadratic equation

To simplify our discussion, it is convenient to modify Eq. (30) by removing the real constant a_0. To do this, we introduce a new quaternionic constant p defined by $p=q+a_0/2$. The quadratic equation (30) then becomes

$$p^2+\mathbf{h}\cdot\mathbf{a}\,p+c_0+\mathbf{h}\cdot\mathbf{c}=0, \tag{31}$$

where $c_0=b_0-a_0^2/4$ and $\mathbf{c}=\mathbf{b}-(a_0/2)\mathbf{a}$. We shall give the solution of Eq. (31) in terms of real constant c_0 and of the real vectors $\mathbf{a}$ and $\mathbf{c}$. Let us analyze the following cases:

- $\mathbf{a}\neq 0$, $\mathbf{c}\neq 0$:
  - **(i)** $\mathbf{a}\times\mathbf{c}=0$,
  - **(ii)** $\mathbf{a}\cdot\mathbf{c}=0$,
  - **(iii)** $\mathbf{a}\times\mathbf{c}\neq 0\neq\mathbf{a}\cdot\mathbf{c}$;
- $\mathbf{a}=0$, $\mathbf{c}\neq 0$;
- $\mathbf{a}\neq 0$, $\mathbf{c}=0$;
- $\mathbf{a}=\mathbf{c}=0$.

• **(i)** $\mathbf{a}\times\mathbf{c}=0$. In this case $\mathbf{a}$ and $\mathbf{c}$ are parallel vectors, so Eq. (31) can be easily reduced to a complex equation. In fact, by introducing the imaginary unit $\mathcal{I}=\mathbf{h}\cdot\mathbf{a}/|\mathbf{a}|$ and observing that $\mathbf{h}\cdot\mathbf{c}=\mathcal{I}\,\alpha$, with $\alpha\in\mathbb{R}$, we find

$$p^2+\mathcal{I}|\mathbf{a}|p+c_0+\mathcal{I}\,\alpha=0,$$

whose *complex* solutions are immediately found.

• **(ii)** $\mathbf{a}\cdot\mathbf{c}=0$. By observing that $\mathbf{a}$, $\mathbf{c}$ and $\mathbf{a}\times\mathbf{c}$ are orthogonal vectors, we can rearrange the imaginary part of p, $\mathbf{h}\cdot\mathbf{p}$, in terms of the new basis $(\mathbf{a},\mathbf{c},\mathbf{a}\times\mathbf{c})$, i.e.,

$$p=p_0+\mathbf{h}\cdot(x\,\mathbf{a}+y\,\mathbf{c}+z\,\mathbf{a}\times\mathbf{c}). \tag{32}$$

Substituting (32) in Eq. (31), we obtain the following system of equations for the real variables p_0, x, y and z:

$$\begin{array}{ll}
\mathbb{R}: & p_0^2-(x^2+x)|\mathbf{a}|^2-y^2\,|\mathbf{c}|^2-z^2|\mathbf{a}|^2|\mathbf{c}|^2+c_0=0,\\
\mathbf{h}\cdot\mathbf{a}: & p_0(1+2\,x)=0,\\
\mathbf{h}\cdot\mathbf{c}: & 1+2\,p_0 y-z|\mathbf{a}|^2=0,\\
\mathbf{h}\cdot\mathbf{a}\times\mathbf{c}: & y+2\,p_0\,z=0.
\end{array}$$

The second equation, $p_0(1+2\,x)=0$, implies $p_0=0$ and/or $x=-\frac{1}{2}$. For $p_0=0$, it can be shown that the solution of Eq. (31), in terms of p_0, x, y and z, is given by

$$p_0=0,\quad x=-\frac{1}{2}\pm\sqrt{\Delta},\quad y=0,\quad z=\frac{1}{|\mathbf{a}|^2}, \tag{33}$$

where

$$\Delta=\frac{1}{4}+\frac{1}{|\mathbf{a}|^2}\left(c_0-\frac{|\mathbf{c}|^2}{|\mathbf{a}|^2}\right)\geqslant 0.$$

For $x=-\frac{1}{2}$, we find

$$y=-\frac{2\,p_0}{4\,p_0^2+|\mathbf{a}|^2},\quad z=\frac{1}{4\,p_0^2+|\mathbf{a}|^2}, \tag{34}$$

and

$$p_0^2 = \tfrac{1}{4}[\pm 2\sqrt{c_0^2 + |\mathbf{c}|^2} - 2\,c_0 - |\mathbf{a}|^2].$$

It is easily verified that

$$\Delta \leqslant 0 \Rightarrow \sqrt{c_0^2 + |\mathbf{c}|^2} - c_0 \geqslant \frac{|\mathbf{a}|^2}{2};$$

thus

$$p_0 = \pm\,\tfrac{1}{2}\sqrt{2(\sqrt{c_0^2 + |\mathbf{c}|^2} - c_0) - |\mathbf{a}|^2}. \tag{35}$$

Summarizing, for $\Delta \neq 0$, we have two quaternionic solutions, $p_1 \neq p_2$,

$$\begin{aligned}
\Delta > 0 \ : \quad & p_0 = 0, \\
& x = -\tfrac{1}{2} \pm \sqrt{\Delta}, \\
& y = 0, \\
& z = \frac{1}{|\mathbf{a}|^2};
\end{aligned} \tag{36}$$

$$\begin{aligned}
\Delta < 0 \ : \quad & p_0 = \pm\,\tfrac{1}{2}\sqrt{2(\sqrt{c_0^2 + |\mathbf{c}|^2} - c_0) - |\mathbf{a}|^2}, \\
& x = -\tfrac{1}{2}, \\
& y = -\frac{2\,p_0}{4\,p_0^2 + |\mathbf{a}|^2}, \\
& z = \frac{1}{4\,p_0^2 + |\mathbf{a}|^2}.
\end{aligned} \tag{37}$$

For $\Delta = 0$, these solutions tend to the same solution $p_1 = p_2$ given by

$$\Delta = 0 \ : \quad p_0 = 0, \quad x = -\frac{1}{2}, \quad y = 0, \quad z = \frac{1}{|\mathbf{a}|^2}. \tag{38}$$

• **(iii)** $\mathbf{a} \times \mathbf{c} \neq 0 \neq \mathbf{a} \cdot \mathbf{c}$. In discussing this case, we introduce the vector $\mathbf{d} = \mathbf{c} - d_0\,\mathbf{a}$, $d_0 = \mathbf{a} \cdot \mathbf{c}/|\mathbf{a}|^2$ and the imaginary part of p in terms of the orthogonal vectors $\mathbf{a}$, $\mathbf{d}$ and $\mathbf{a} \times \mathbf{d}$,

$$p = p_0 + \mathbf{h} \cdot (x\,\mathbf{a} + y\,\mathbf{d} + z\,\mathbf{a} \times \mathbf{d}). \tag{39}$$

By using this decomposition, from Eq. (31) we obtain the following system of real equations:

$\mathbb{R}$:	$p_0^2 - (x^2 + x)\lvert\mathbf{a}\rvert^2 - y^2\,\lvert\mathbf{d}\rvert^2 - z^2\,\lvert\mathbf{a}\rvert^2\lvert\mathbf{d}\rvert^2 + c_0 = 0$,
$\mathbf{h} \cdot \mathbf{a}$:	$p_0(1 + 2\,x) + d_0 = 0$,
$\mathbf{h} \cdot \mathbf{d}$;	$1 + 2\,p_0\,y - z\,\lvert\mathbf{a}\rvert^2 = 0$,
$\mathbf{h} \cdot \mathbf{a} \times \mathbf{d}$:	$y + 2\,p_0 z = 0$.

The second equation of this system, $p_0(1 + 2\,x) + d_0 = 0$, implies $p_0 \neq 0$ since $d_0 \neq 0$. Therefore, we have

$$x = -\frac{p_0 + d_0}{2p_0}, \quad y = -\frac{2p_0}{4p_0^2 + |\mathbf{a}|^2}, \quad z = \frac{1}{4p_0^2 + |\mathbf{a}|^2}, \tag{40}$$

and

$$16w^3 + 8[|\mathbf{a}|^2 + 2c_0]w^2 + 4\left[|\mathbf{a}|^2(c_0 - d_0^2) + \frac{|\mathbf{a}|^4}{4} - |\mathbf{d}|^2\right]w - d_0^2|\mathbf{a}|^4 = 0, \tag{41}$$

where $w = p_0^2$. By using the Descartes rule of signs it can be proved that Eq. (41) has only one real positive solution,[38] $w = \alpha^2$, $\alpha \in \mathbb{R}$. This implies $p_0 = \pm\alpha$. Thus, we also find two quaternionic solutions.

• $\mathbf{a} = 0$ and $\mathbf{c} \neq 0$. By introducing the imaginary *complex* unit $\mathcal{I} = \mathbf{h} \cdot \mathbf{c}/|\mathbf{c}|$, we can reduce Eq. (31) to the following *complex* equation:

$$p^2 + c_0 + \mathcal{I}|\mathbf{c}| = 0.$$

• $\mathbf{a} \neq 0$ and $\mathbf{c} = 0$. This case is similar to the previous one. We introduce the imaginary *complex* unit $\mathcal{I} = \mathbf{h} \cdot \mathbf{a}/|\mathbf{a}|$ and reduce Eq. (31) to the *complex* equation,

$$p^2 + \mathcal{I}|\mathbf{a}|p + c_0 = 0.$$

• $\mathbf{a} = \mathbf{c} = 0$. Equation (31) becomes

$$p^2 + c_0 = 0.$$

For $c_0 = -\alpha^2$, $\alpha \in \mathbb{R}$, we find two real solutions. For $c_0 = \alpha^2$, we obtain an *infinite* number of quaternionic solutions, i.e., $p = \mathbf{h} \cdot \mathbf{p}$, where $|\mathbf{p}| = |\alpha|$.

Let us resume our discussion on a quaternionic linear quadratic equation. For $\mathbf{a} = 0$ and/or $\mathbf{c} = 0$ and for $\mathbf{a} \times \mathbf{c} = 0$ we can reduce quaternionic linear quadratic equations to *complex* equations. For non null vectors satisfying $\mathbf{a} \cdot \mathbf{c} = 0$ or $\mathbf{a} \times \mathbf{c} \neq 0 \neq \mathbf{a} \cdot \mathbf{c}$, we have *effective* quaternionic equations. In these cases, we always find two quaternionic solutions (36), (37) and (40)–(41). For $\mathbf{a} \cdot \mathbf{c} = 0$ and $\Delta = 0$, these solutions tend to the same solution (38). Finally, the fundamental theorem of algebra is lost for a *restricted* class of quaternionic quadratic linear equations, namely

$$q^2 + \alpha^2 = 0, \quad \alpha \in \mathbb{R}.$$

B. Second order quaternionic differential equations with constant coefficients

Due to the quaternionic linearity from the right of Eq. (29), we look for general solutions which are of the form

$$\varphi(x) = \varphi_1(x)c_1 + \varphi_2(x)c_2,$$

where $\varphi_1(x)$ and $\varphi_2(x)$ represent two linear independent solutions of Eq. (29) and c_1 and c_2 are quaternionic constants fixed by the initial conditions. In analogy to the complex case, we can distinguish between quaternionic linear dependent and independent solutions by constructing a Wronskian functional. To do this, we need to define a quaternionic determinant. Due to the noncommutative nature of quaternions, the standard definition of the determinant must be revised. The study of quaternionic, complex and real functionals, extending the complex determinant to quaternionic matrices, has been extensively developed in quaternionic linear algebra.[46–49] In a recent paper,[50] we find an interesting discussion on the impossibility to obtain a quaternionic functional with the main properties of the complex determinant. For quaternionic matrices, M, a *real positive* functional, $|\det M| = \sqrt{\det[MM^\dagger]}$, which reduces to the absolute value of the standard determinant for complex matrices, was introduced by Study[51] and its properties axiomatized by Dieudonné.[52] The details can be found in the excellent survey paper of Aslaksen.[53] This functional allows us to construct a real positive Wronskian,[31]

$$\begin{aligned}\mathcal{W}(x)&=\left|\det\begin{pmatrix}\varphi_1(x) & \varphi_2(x)\\ \dot{\varphi}_1(x) & \dot{\varphi}_2(x)\end{pmatrix}\right|\\&=|\varphi_1(x)||\dot{\varphi}_2(x)-\dot{\varphi}_1(x)\varphi_1^{-1}(x)\varphi_2(x)|\\&=|\varphi_2(x)||\dot{\varphi}_1(x)-\dot{\varphi}_2(x)\varphi_2^{-1}(x)\varphi_1(x)|\\&=|\dot{\varphi}_1(x)||\varphi_2(x)-\varphi_1(x)\dot{\varphi}_1^{-1}(x)\dot{\varphi}_2(x)|\\&=|\dot{\varphi}_2(x)||\varphi_1(x)-\varphi_2(x)\dot{\varphi}_2^{-1}(x)\dot{\varphi}_1(x)|.\end{aligned}$$

Solutions of Eq. (29),

$$\varphi_{1,2}(x)=\exp[q_{1,2}\,x]=\exp\left[\left(p_{1,2}-\frac{a_0}{2}\right)x\right],$$

are given in terms of the solutions of the quadratic equation (31), $p_{1,2}$, and of the real variable x. In this case, the Wronskian becomes

$$\mathcal{W}(x)=|p_1-p_2||\exp[q_1x]||\exp[q_2x]|.$$

This functional allows us to distinguish between quaternionic linear dependent ($\mathcal{W}=0$) and independent ($\mathcal{W}\neq 0$) solutions. A generalization for quaternionic second order differential equations with nonconstant coefficients should be investigated.

For $p_1\neq p_2$, the solution of Eq. (29) is then given by

$$\varphi(x)=\exp\left[-\frac{a_0}{2}x\right]\{\exp[p_1\,x]c_1+\exp[p_2\,x]c_2\}. \tag{42}$$

As observed at the end of the previous subsection, the fundamental theorem of algebra is lost for a *restricted* class of quaternionic quadratic equation, i.e., $p^2+\alpha^2=0$ where $\alpha\in\mathbb{R}$. For these equations we find an infinite number of solutions, $p=\mathbf{h}\cdot\boldsymbol{\alpha}$ with $|\boldsymbol{\alpha}|^2=\alpha^2$. Nevertheless, the general solution of the second order differential equation,

$$\ddot{\varphi}(x)+\alpha^2\,\varphi(x)=0, \tag{43}$$

is also expressed in terms of *two* linearly independent exponential solutions,

$$\varphi(x)=\exp[i\,\alpha\,x]c_1+\exp[-i\,\alpha\,x]c_2. \tag{44}$$

Note that any other exponential solution, $\exp[\mathbf{h}\cdot\boldsymbol{\alpha}x]$, can be written as a linear combination of $\exp[i\,\alpha x]$ and $\exp[-i\,\alpha x]$,

$$\exp[\mathbf{h}\cdot\boldsymbol{\alpha}x]=\frac{1}{2\alpha}\{\exp[i\,\alpha\,x](\alpha-i\,\mathbf{h}\cdot\boldsymbol{\alpha})+\exp[-i\,\alpha\,x](\alpha+i\,\mathbf{h}\cdot\boldsymbol{\alpha})\}.$$

As a consequence, the loss of the fundamental theorem of algebra for quaternions does *not* represent an obstacle in solving second order quaternionic linear differential equations with constant coefficients. To complete our discussion, we have to examine the case $p_1=p_2$. From Eq. (38) we find

$$p_1=p_2=-\frac{\mathbf{h}\times\mathbf{a}}{2}+\frac{1}{|\mathbf{a}|^2}\mathbf{h}\cdot\mathbf{a}\times\left(\mathbf{b}-\frac{a_0}{2}\mathbf{a}\right),$$

Thus, a first solution of the differential equation (29) is

$$\xi(x)=\exp\left\{\left[\mathbf{h}\cdot\left(\frac{\mathbf{a}\times\mathbf{b}}{|\mathbf{a}|^2}-\frac{\mathbf{a}}{2}\right)-\frac{a_0}{2}\right]x\right\}.$$

For $\mathbf{a}\times\mathbf{b}=0$, we can immediately obtain a second linearly independent solution by multiplying $\exp[-(a/2)x]$ by x, $\eta(x)=x\,\xi(x)$. For $\mathbf{a}\times\mathbf{b}\neq 0$, the second linearly independent solution takes a more complicated form, i.e.,

$$\eta(x)=\left(x+\frac{\mathbf{h}\cdot\mathbf{a}}{|\mathbf{a}|^2}\right)\xi(x). \tag{45}$$

It can easily be shown that $\eta(x)$ is a solution of the differential equation (29),

$$\begin{aligned}
&\ddot{\eta}(x)+a\,\dot{\eta}(x)+b\,\eta(x)\\
&\quad=\left[x(q^2+a\,q+b)+2\,q+a+\frac{\mathbf{h}\cdot\mathbf{a}}{|\mathbf{a}|^2}(q^2+a\,q)+b\,\frac{\mathbf{h}\cdot\mathbf{a}}{|\mathbf{a}|^2}\right]\xi(x)\\
&\quad=\left(2\,q+a+\left[b,\frac{\mathbf{h}\cdot\mathbf{a}}{|\mathbf{a}|^2}\right]\right)\xi(x)\\
&\quad=\left(2\,\mathbf{h}\cdot\frac{\mathbf{a}\times\mathbf{b}}{|\mathbf{a}|^2}+\left[\mathbf{h}\cdot\mathbf{b},\frac{\mathbf{h}\cdot\mathbf{a}}{|\mathbf{a}|^2}\right]\right)\xi(x)=0.
\end{aligned}$$

Thus, for $p_1=p_2=p=\mathbf{h}\cdot((\mathbf{a}\times\mathbf{b})/|\mathbf{a}|^2-\mathbf{a}/2$, the general solution of the differential equation (29) is given by

$$\varphi(x)=\exp\left[-\frac{a_0}{2}x\right]\left\{\exp[p\,x]c_1+\left(x+\frac{\mathbf{h}\cdot\mathbf{a}}{|\mathbf{a}|^2}\right)\exp[p\,x]c_2\right\}. \tag{46}$$

C. Diagonalization and Jordan form

To find the general solution of linear differential equations, we can also use quaternionic formulations of eigenvalue equations, matrix diagonalization and Jordan form. The quaternionic linear differential equation (29) can be written in matrix form as follows:

$$\dot{\Phi}(x)=M\,\Phi(x), \tag{47}$$

where

$$M=\begin{pmatrix}0 & 1\\ -b & -a\end{pmatrix}\quad\text{and}\quad \Phi(x)=\begin{bmatrix}\varphi(x)\\ \dot{\varphi}(x)\end{bmatrix}.$$

By observing that x is real, the formal solution of the matrix equation (47) is given by

$$\Phi(x)=\exp[M\,x]\Phi(0), \tag{48}$$

where $\Phi(0)$ represents a constant quaternionic column vector determined by the initial conditions $\varphi(0)$, $\dot{\varphi}(0)$ and $\exp[M\,x]=\Sigma_{n=0}^{\infty}[(Mx)^n/n!]$. In the sequel, we shall use right eigenvalue equations for quaternionic linear matrix operators equations,

$$M\,\Phi=\Phi\,q. \tag{49}$$

Without loss of generality, we can work with *complex* eigenvalue equations. By setting $\Psi=\Phi u$, from the previous equation, we have

$$M\,\Psi=M\,\Phi u=\Phi\,q\,u=\Phi u\,\bar{u}qu=\Psi\,z, \tag{50}$$

where $z\in\mathbb{C}$ and u is a unitary quaternion. In a recent paper,[31] we find a complete discussion of the eigenvalue equation for quaternionic matrix operators. In such a paper was shown that the complex counterpart of the matrix M has an eigenvalue spectrum characterized by eigenvalues which appear in conjugate pairs $\{z_1,\bar{z}_1,z_2,\bar{z}_2\}$. Let Ψ_1 and Ψ_2 be the quaternionic eigenvectors corresponding to the complex eigenvalues z_1 and z_2,

$$M\,\Psi_1=\Psi_1\,z_1 \quad \text{and} \quad M\,\Psi_2=\Psi_2\,z_2.$$

It can be shown that for $|z_1|\neq|z_2|$, the eigenvectors Ψ_1 and Ψ_2 are linearly independent on $\mathbb{H}$ and consequently there exists a 2×2 quaternionic matrix $S=[\Psi_1\,\Psi_2]$ which diagonalizes M,

$$\exp[M\,x]=S\,\exp\left[\begin{pmatrix} z_1 & 0\\ 0 & z_2\end{pmatrix}x\right]S^{-1}=S\begin{pmatrix}\exp[z_1x] & 0\\ 0 & \exp[z_2x]\end{pmatrix}S^{-1}.$$

In this case, the general solution of the quaternionic differential equation can be written in terms of the elements of the matrices S and S^{-1} and of the complex eigenvalues z_1 and z_2,

$$\begin{bmatrix}\varphi(x)\\ \dot{\varphi}(x)\end{bmatrix}=\begin{pmatrix}S_{11}\exp[z_1x] & S_{12}\exp[z_2x]\\ S_{21}\exp[z_1x] & S_{22}\exp[z_2x]\end{pmatrix}\begin{bmatrix}S_{11}^{-1}\,\varphi(0)+S_{12}^{-1}\,\dot{\varphi}(0)\\ S_{21}^{-1}\,\varphi(0)+S_{22}^{-1}\,\dot{\varphi}(0)\end{bmatrix}.$$

Hence,

$$\begin{aligned}\varphi(x)&=S_{11}\exp[z_1\,x][S_{11}^{-1}\,\varphi(0)+S_{12}^{-1}\,\dot{\varphi}(0)]\\ &\quad+S_{12}\exp[z_2\,x][S_{21}^{-1}\,\varphi(0)+S_{22}^{-1}\,\dot{\varphi}(0)]\\ &=\exp[S_{11}\,z_1(S_{11})^{-1}\,x]S_{11}[S_{11}^{-1}\,\varphi(0)+S_{12}^{-1}\,\dot{\varphi}(0)]\\ &\quad+\exp[S_{12}\,z_2(S_{12})^{-1}\,x]S_{12}[S_{21}^{-1}\,\varphi(0)+S_{22}^{-1}\,\dot{\varphi}(0)]\\ &=\exp[S_{21}(S_{11})^{-1}\,x]S_{11}[S_{11}^{-1}\,\varphi(0)+S_{12}^{-1}\,\dot{\varphi}(0)]\\ &\quad+\exp[S_{22}(S_{12})^{-1}\,x]S_{12}[S_{21}^{-1}\,\varphi(0)+S_{22}^{-1}\,\dot{\varphi}(0)].\end{aligned} \tag{51}$$

We remark that a different choice of the eigenvalue spectrum does *not* modify the solution (51). In fact, by taking the following quaternionic eigenvalue spectrum:

$$\{q_1,q_2\}=\{\bar{u}_1z_1u_1,\bar{u}_2z_2u_2\},\quad |q_1|\neq|q_2|, \tag{52}$$

and observing that the corresponding linearly independent eigenvectors are given by

$$\{\,\Phi_1=\Psi_1u_1,\Phi_2=\Psi_2u_2\}, \tag{53}$$

we obtain

$$
\begin{aligned}
M &= [\Phi_1\, \Phi_2]\,\mathrm{diag}\{q_1, q_2\}[\Phi_1\, \Phi_2]^{-1} \\
&= [\Psi_1 u_1\, \Psi_2 u_2]\,\mathrm{diag}\{\overline{u_1} z_1 u_1, \overline{u_2} z_2 u_2\}[\Psi_1 u_1\, \Psi_2 u_2]^{-1} \\
&= [\Psi_1\, \Psi_2]\,\mathrm{diag}\{z_1, z_2\}[\Psi_1\, \Psi_2]^{-1}.
\end{aligned}
$$

Let us now discuss the case $|z_1| = |z_2|$. If the eigenvectors $\{\Psi_a, \Psi_b\}$, corresponding to the eigenvalue spectrum $\{z, z\}$, are linearly independent on $\mathbb{H}$, we can obviously repeat the previous discussion and diagonalize the matrix operator M by the 2×2 quaternionic matrix $U = [\Psi_1\, \Psi_2]$. Then, we find

$$
\begin{aligned}
\varphi(x) &= \exp[U_{11} z (U_{11})^{-1} x] U_{11}[U_{11}^{-1}\, \varphi(0) + U_{12}^{-1}\, \dot{\varphi}(0)] \\
&\quad + \exp[U_{12} z (U_{12})^{-1} x] U_{12}[U_{21}^{-1}\, \varphi(0) + U_{22}^{-1}\, \dot{\varphi}(0)] \\
&= \exp[U_{21} (U_{11})^{-1} x] U_{11}[{}_{11}^{-1}\, \varphi(0) + U_{12}^{-1}\, \dot{\varphi}(0)] \\
&\quad + \exp[U_{22} (U_{12})^{-1} x] U_{12}[U_{21}^{-1}\, \varphi(0) + U_{22}^{-1}\, \dot{\varphi}(0)].
\end{aligned} \tag{54}
$$

For linearly dependent eigenvectors, we cannot construct a matrix which diagonalizes the matrix operator M. Nevertheless, we can transform the matrix operator M to Jordan form,

$$
M = J \begin{pmatrix} z & 1 \\ 0 & z \end{pmatrix} J^{-1}. \tag{55}
$$

It follows that the solution of our quaternionic differential equation can be written as

$$
\Phi(x) = J \exp\left[\begin{pmatrix} z & 1 \\ 0 & z \end{pmatrix} x \right] J^{-1}\, \Phi(0) = \begin{pmatrix} J_{11} & x\, J_{11} + J_{12} \\ J_{21} & x\, J_{21} + J_{22} \end{pmatrix} \exp[zx] \begin{bmatrix} J_{11}^{-1}\, \varphi(0) + J_{12}^{-1}\, \dot{\varphi}(0) \\ J_{21}^{-1}\, \varphi(0) + J_{22}^{-1}\, \dot{\varphi}(0) \end{bmatrix}.
$$

Thus,

$$
\begin{aligned}
\varphi(x) &= J_{11} \exp[z\, x][J_{11}^{-1}\, \varphi(0) + J_{12}^{-1}\, \dot{\varphi}(0)] \\
&\quad + (x\, J_{11} + J_{12}) \exp[z\, x][J_{21}^{-1}\, \varphi(0) + J_{22}^{-1}\, \dot{\varphi}(0)] \\
&= \exp[J_{11} z (J_{11})^{-1} x] J_{11}[J_{11}^{-1}\, \varphi(0) + J_{12}^{-1}\, \dot{\varphi}(0)] \\
&\quad + [x + J_{12}(J_{11})^{-1}] \exp[J_{11} z (J_{11})^{-1} x] \\
&\quad \times J_{11}[J_{21}^{-1}\, \varphi(0) + J_{22}^{-1}\, \dot{\varphi}(0)] \\
&= \exp[J_{21} (J_{11})^{-1} x] J_{11}[J_{11}^{-1}\, \varphi(0) + J_{12}^{-1}\, \dot{\varphi}(0)] \\
&\quad + [x + J_{12}(J_{11})^{-1}] \exp[J_{21} (J_{11})^{-1} x] \\
&\quad \times J_{11}[J_{21}^{-1}\, \varphi(0) + J_{22}^{-1}\, \dot{\varphi}(0)].
\end{aligned} \tag{56}
$$

The last equality in the previous equation follows from the use of Eq. (55) and the definition of M.

Finally, the general solution of the quaternionic differential equation (29) can be given by solving the corresponding eigenvalue problem. We conclude this section by observing that the quaternionic exponential solution, $\exp[q\, x]$, can also be written in terms of complex exponential solutions, $u \exp[z\, x] u^{-1}$, where $q = u\, z\, u^{-1}$. The elements of the similarity transformations S, U or J and the complex eigenvalue spectrum of M determine the quaternion u and the complex number z. This form for exponential solutions will be very useful in solving complex linear differential equations with constant coefficients. In fact, due to the presence of the right acting operator R_i, we cannot use quaternionic exponential solutions for complex linear differential equations.

VII. COMPLEX LINEAR QUATERNIONIC DIFFERENTIAL EQUATIONS

Consider now the second order complex linear quaternionic differential operator,

$$\begin{aligned}\mathcal{D}_{\mathbb{C}}=&[a_{02}+\mathbf{L}\cdot\mathbf{a}_2+(b_{02}+\mathbf{L}\cdot\mathbf{b}_2)R_i]\partial_{xx}\\&+[a_{01}+\mathbf{L}\cdot\mathbf{a}_1+(b_{01}+\mathbf{L}\cdot\mathbf{b}_1)R_i]\partial_x\\&+a_{00}+\mathbf{L}\cdot\mathbf{a}_0+(b_{00}+\mathbf{L}\cdot\mathbf{b}_0)R_i\\&\in\mathcal{A}_{\mathbb{C}}\otimes\mathcal{O},\end{aligned}$$

and look for solutions of the complex linear quaternionic differential equation,

$$\mathcal{D}_{\mathbb{C}}\,\varphi(x)=0. \tag{57}$$

Due to the presence of R_i in (57), the general solution of the complex linear quaternionic differential equation cannot be given in terms of quaternionic exponentials. In matrix form, Eq. (57) reads as

$$\dot{\Phi}(x)=M_{\mathbb{C}}\,\Phi(x), \tag{58}$$

where

$$M_{\mathbb{C}}=\begin{pmatrix}0 & 1\\ -b_{\mathbb{C}} & -a_{\mathbb{C}}\end{pmatrix}\quad\text{and}\quad\Phi(x)=\begin{bmatrix}\varphi(x)\\ \dot{\varphi}(x)\end{bmatrix}.$$

The complex counterpart of complex linear quaternionic matrix operator $M_{\mathbb{C}}$ has an eigenvalue spectrum characterized by four complex eigenvalues $\{z_1,z_2,z_3,z_4\}$. It can be shown that $M_{\mathbb{C}}$ is diagonalizable if and only if its complex counterpart is diagonalizable. For diagonalizable matrix operator $M_{\mathbb{C}}$, we can find a complex linear quaternionic linear similarity transformation $S_{\mathbb{C}}$ which reduces the matrix operator $M_{\mathbb{C}}$ to diagonal form,[31]

$$M_{\mathbb{C}}=S_{\mathbb{C}}\begin{pmatrix}\dfrac{z_1+\overline{z_2}}{2}+\dfrac{z_1-\overline{z_2}}{2i}R_i & 0\\ 0 & \dfrac{z_3+\overline{z_4}}{2}+\dfrac{z_3-\overline{z_4}}{2i}R_i\end{pmatrix}S_{\mathbb{C}}^{-1}.$$

It is immediate to verify that

$$\left\{\begin{pmatrix}1\\0\end{pmatrix},\ \begin{pmatrix}j\\0\end{pmatrix},\ \begin{pmatrix}0\\1\end{pmatrix},\ \begin{pmatrix}0\\j\end{pmatrix}\right\}$$

are eigenvectors of the diagonal matrix operator,

$$\begin{pmatrix}\dfrac{z_1+\overline{z_2}}{2}+\dfrac{z_1-\overline{z_2}}{2i}R_i & 0\\ 0 & \dfrac{z_3+\overline{z_4}}{2}+\dfrac{z_3-\overline{z_4}}{2i}R_i\end{pmatrix},$$

with right complex eigenvalues z_1, z_2, z_3 and z_4. The general solution of the differential equation (57) can be given in terms of these complex eigenvalues,

$$\begin{aligned}\varphi(x)=&S_{\mathbb{C}\,11}\exp\left[\left(\frac{z_1+\overline{z_2}}{2}+\frac{z_1-\overline{z_2}}{2i}R_i\right)x\right][S^{-1}_{\mathbb{C}\,11}\,\varphi(0)+S^{-1}_{\mathbb{C}\,12}\,\dot{\varphi}(0)]\\&+S_{\mathbb{C}\,12}\exp\left[\left(\frac{z_3+\overline{z_4}}{2}+\frac{z_3-\overline{z_4}}{2i}R_i\right)x\right][S^{-1}_{\mathbb{C}\,21}\,\varphi(0)+S^{-1}_{\mathbb{C}\,22}\,\dot{\varphi}(0)]\\=&u_1\exp[z_1x]k_1+u_2\exp[z_2x]k_2\\&+u_3\exp[z_3x]k_3+u_4\exp[z_4x]k_4,\end{aligned}\tag{59}$$

where k_n are complex coefficients determined by the initial conditions. This solution holds for diagonalizable matrix operator $M_{\mathbb{C}}$. For nondiagonalizable matrix operators we need to find the similarity transformation $J_{\mathbb{C}}$ which reduces $M_{\mathbb{C}}$ to the Jordan form. For instance, it can be shown that for equal eigenvalues, $z_1=z_2$, the general solution of the differential equation (57) is

$$\varphi(x)=u\exp[zx]k_1+(ux+\tilde{u})\exp[zx]k_2+u_3\exp[z_3x]k_3+u_4\exp[z_4x]k_4. \tag{60}$$

A. Schrödinger equation

Let us now examine the complex linear Schrödinger equation in the presence of a constant quaternionic potential,

$$\left[\frac{\hbar^2}{2m}\partial_{xx}-V+jW\right]\Psi(x)=i\,\Psi(x)\,i\,E. \tag{61}$$

In this case, the complex linear matrix operator,

$$M_{\mathbb{C}}=\begin{pmatrix}0 & 1\\ -b_{\mathbb{C}} & 0\end{pmatrix},\quad b_{\mathbb{C}}=V-jW+iER_i,$$

represents a diagonalizable operator. Consequently, the general solution of the Schrödinger equation is given by

$$\varphi(x)=u_1\exp[z_1x]k_1+u_2\exp[z_2x]k_2+u_3\exp[z_3x]k_3+u_4\exp[z_4x]k_4. \tag{62}$$

The quaternions u_n and the complex eigenvalues z_n are obtained by solving the eigenvalue equation for the complex linear operator $M_{\mathbb{C}}$. We can also obtain the general solution of Eq. (61) by substituting $u\exp[\sqrt{2m/\hbar^2}\,zx]$ in the Schrödinger equation. We find the following quaternionic equation:

$$uz^2-(V-jW)u-iEui=0,$$

where $u=z_u+j\tilde{z}_u$. This equation can be written as two complex equations:

$$[z^2-(V-E)]z_u-\overline{W}\tilde{z}_u=[z^2-(V+E)]\tilde{z}_u+Wz_u=0.$$

An easy calculation shows that z satisfies the complex equation,

$$z^4-2Vz^2+V^2+|W|^2-E^2=0, \tag{63}$$

whose roots are

$$z_{1,2}=\pm\sqrt{V-\sqrt{E^2-|W|^2}}=\pm z_-\quad\text{and}\quad z_{3,4}=\pm\sqrt{V+\sqrt{E^2-|W|^2}}=\pm z_+. \tag{64}$$

By setting $(u_{1,2})_{\mathbb{C}}=(-ju_{3,4})_{\mathbb{C}}=1$, we find

$$u_- = \left(1 + j\,\frac{W}{E+\sqrt{E^2-|W|^2}}\right) \quad \text{and} \quad u_+ = \left(\frac{\bar{W}}{E+\sqrt{E^2-|W|^2}} + j\right). \tag{65}$$

The solution of the complex linear quaternionic Schrödinger equation is then given by

$$\begin{aligned}\Psi(x) = u_- \left\{\exp\left[\sqrt{\frac{2m}{\hbar^2}}\, z_-\, x\right] k_1 + \exp\left[-\sqrt{\frac{2m}{\hbar^2}}\, z_-\, x\right] k_2\right\} \\ + u_+ \left\{\exp\left[\sqrt{\frac{2m}{\hbar^2}}\, z_+\, x\right] k_3 + \exp\left[-\sqrt{\frac{2m}{\hbar^2}}\, z_+\, x\right] k_4\right\}.\end{aligned} \tag{66}$$

Equation (63) can also be obtained by multiplying the complex linear Schrödinger equation (61) from the left by the operator,

$$\frac{\hbar^2}{2m}\,\partial_{xx} - V - j\,W.$$

This gives

$$\begin{aligned}\left[\left(\frac{\hbar^2}{2m}\right)^2 \partial_{xxxx} - 2\,\frac{\hbar^2}{2m}\,V\,\partial_{xx} + V^2 + |W|^2\right]\Psi(x) &= i\left[\frac{\hbar^2}{2m}\,\partial_{xx} - V + j\,W\right]\Psi(x)\,i\,E \\ &= E^2\,\Psi(x).\end{aligned}$$

By substituting the exponential solution $u\exp[\sqrt{2m/\hbar^2}\,z\,x]$ in the previous equation, we immediately re-obtain Eq. (63).

VIII. QUATERNIONIC CONSTANT POTENTIALS

Of all Schrödinger equations the one for a constant potential is mathematically the simplest. The reason for resuming the study of the Schrödinger equation with such a potential is that the qualitative features of a physical potential can often be approximated reasonably well by a potential which is pieced together from a number of constant portions.

A. The potential step

Let us consider the quaternionic potential step,

$$V(x) - j\,W(x) = \begin{cases} 0, & x<0, \\ V - j\,W, & x>0, \end{cases}$$

where V and W represent constant potentials. For scattering problems with a wave function incident from the left on the quaternionic potential step, the complex linear quaternionic Schrödinger equation has the solution

$$\Psi(x) = \begin{cases} x<0: \quad \exp\left[i\,\frac{p}{\hbar}\,x\right] + r\exp\left[-i\,\frac{p}{\hbar}\,x\right] + j\,\tilde{r}\exp\left[\frac{p}{\hbar}\,x\right]; & \\ x>0: \quad u_-\,t\exp\left[\sqrt{\frac{2m}{\hbar^2}}\,z_-\,x\right] + u_+\,\tilde{t}\exp\left[-\sqrt{\frac{2m}{\hbar^2}}\,z_+\,x\right] & [E>\sqrt{V^2+|W|^2}], \\ u_-\,t\exp\left[-\sqrt{\frac{2m}{\hbar^2}}\,z_-\,x\right] + u_+\,\tilde{t}\exp\left[-\sqrt{\frac{2m}{\hbar^2}}\,z_+\,x\right] & [E<\sqrt{V^2+|W|^2}], \end{cases} \tag{67}$$

where r, $\tilde{r}$, t and $\tilde{t}$ are complex coefficients to be determined by matching the wave function $\Psi(x)$ and its slope at the discontinuity of the potential $x=0$.

For $E>\sqrt{V^2+|W|^2}$, the complex exponential solutions of the quaternionic Schrödinger equation are characterized by

$$z_-=i\sqrt{\sqrt{E^2-|W|^2}-V}\in i\,\mathbb{R} \quad \text{and} \quad z_+=\sqrt{\sqrt{E^2-|W|^2}+V}\in\mathbb{R}.$$

The complex linearly independent solutions,

$$u_-\exp\left[-\sqrt{\frac{2m}{\hbar^2}}z_-x\right] \quad \text{and} \quad u_+\exp\left[\sqrt{\frac{2m}{\hbar^2}}z_+x\right],$$

have been omitted, $k_2=k_3=0$ in (66), because we are considering a wave incident from the left and because the second complex exponential solution, $\exp[\sqrt{2m/\hbar^2}\,z_+x]$, is in conflict with the boundary condition that $\Psi(x)$ remain finite as $x\to\infty$. The standard result of complex quantum mechanics are immediately recovered by considering $W=0$ and taking the complex part of the quaternionic solution.

For $E<\sqrt{V^2+|W|^2}$, the complex exponential solutions of the quaternionic Schrödinger equation are characterized by

$$z_-=\sqrt{V-\sqrt{E^2-|W|^2}}, \quad z_+=\sqrt{V+\sqrt{E^2-|W|^2}} \quad \in\mathbb{R} \quad [E>|W|],$$

$$z_\pm=(V^2+|W|^2-E^2)^{1/4}\exp\left[\pm i\frac{\theta}{2}\right], \quad \tan\theta=\frac{\sqrt{|W|^2-E^2}}{V} \quad \in\mathbb{C} \quad [E<|W|].$$

The complex linearly independent solutions,

$$u_-\exp\left[\sqrt{\frac{2m}{\hbar^2}}z_-x\right] \quad \text{and} \quad u_+\exp\left[\sqrt{\frac{2m}{\hbar^2}}z_+x\right],$$

have been omitted, $k_1=k_3=0$ in (66), because they are in conflict with the boundary condition that $\Psi(x)$ remain finite as $x\to\infty$.

A relation between the complex coefficients of reflection and transmission can immediately be obtained by the continuity equation,

$$\partial_t\rho(x,t)+\partial_xJ(x,t)=0, \tag{68}$$

where

$$\rho(x,t)=\bar{\Phi}(x,t)\Phi(x,t),$$

and

$$J(x,t)=\frac{\hbar}{2m}\{[\partial_x\bar{\Phi}(x,t)]i\,\Phi(x,t)-\bar{\Phi}(x,t)i\,\partial_x\Phi(x,t)\}.$$

Note that, due to the noncommutative nature of the quaternionic wave functions, the position of the imaginary unit i in the probability current density $J(x,t)$ is important to recover a continuity equation in quaternionic quantum mechanics. For stationary states, $\Phi(x,t)=\Psi(x)\exp[-i(E/\hbar)t]\zeta(0)$, it can easily be shown that the probability current density,

$$J(x,t)=\frac{\hbar}{2m}\bar{\zeta}(0)\exp\left[i\frac{E}{\hbar}t\right]\{[\partial_x\bar{\Psi}(x)]i\,\Psi(x)-\bar{\Psi}(x)i\,\partial_x\Psi(x)\}\exp\left[-i\frac{E}{\hbar}t\right]\zeta(0),$$

must be independent of x, $J(x,t)=f(t)$. Hence,

$$\frac{\hbar}{2m}\{[\partial_x\overline{\Psi}(x)]i\,\Psi(x)-\overline{\Psi}(x)i\,\partial_x\Psi(x)\}=\exp\left[-i\frac{E}{\hbar}t\right]\zeta(0)f(t)\overline{\zeta}(0)\exp\left[i\frac{E}{\hbar}t\right]=\alpha,$$

where α is a real constant. This implies that the quantity

$$\mathcal{J}=\frac{p}{2m}\{[\partial_x\overline{\Psi}(x)]i\,\Psi(x)-\overline{\Psi}(x)i\,\partial_x\Psi(x)\},$$

has the same value at all points x. In the free potential region, $x<0$, we find

$$\mathcal{J}_-=\frac{p}{m}(1-|r|^2).$$

In the potential region, $x>0$, we obtain

$$\mathcal{J}_+=\begin{cases}\sqrt{\dfrac{2}{m}(\sqrt{E^2-|W|^2}-V)}\left[1-\left(\dfrac{|W|}{E+\sqrt{E^2-|W|^2}}\right)^2\right]|t|^2 \quad [E>\sqrt{V^2+|W|^2}],\\ 0 \quad [E<\sqrt{V^2+|W|^2}].\end{cases}$$

Finally, for stationary states, the continuity equation leads to

$$\begin{gathered}|r|^2+\frac{\sqrt{E^2-|W|^2}-V}{E}\left[1-\left(\frac{|W|}{E+\sqrt{E^2-|W|^2}}\right)^2\right]|t|^2=1 \quad [E>\sqrt{V^2+|W|^2}],\\ |r|^2=1 \quad [E<\sqrt{V^2+|W|^2}].\end{gathered}\tag{69}$$

Thus, by using the concept of a probability current, we can define the following coefficients of transmission and reflection:

$$R=|r|^2,\quad T=\frac{\sqrt{E^2-|W|^2}-V}{E}\left[1-\left(\frac{|W|}{E+\sqrt{E^2-|W|^2}}\right)^2\right]|t|^2 \quad [E>\sqrt{V^2+|W|^2}],$$

$$R=|r|^2,\quad T=0 \quad [E<\sqrt{V^2+|W|^2}].$$

These coefficients give the probability for the particle, arriving from $x=-\infty$, to pass the potential step at $x=0$ or to turn back. The coefficients R and T depend only on the ratios E/V and $|W|/V$. The predictions of complex quantum mechanics are recovered by setting $W=0$.

B. The rectangular potential barrier

In our study of quaternionic potentials, we now reach the rectangular potential barrier,

$$V(x)-j\,W(x)=\begin{cases}0, & x<0,\\ V-j\,W, & 0<x<a,\\ 0, & x>a.\end{cases}$$

For scattering problems with a wave function incident from the left on the quaternionic potential barrier, the complex linear quaternionic Schrödinger equation has the solution

$$\Psi(x)=\begin{cases} x<0: \ \exp\left[i\frac{p}{\hbar}x\right]+r\exp\left[-i\frac{p}{\hbar}x\right]+j\,\tilde{r}\exp\left[\frac{p}{\hbar}x\right]; \\ 0<x<a: \quad u_-\left\{\exp\left[\sqrt{\frac{2m}{\hbar^2}}z_-x\right]k_1+\exp\left[-\sqrt{\frac{2m}{\hbar^2}}z_-x\right]k_2\right\} \\ \qquad\qquad +u_+\left\{\exp\left[\sqrt{\frac{2m}{\hbar^2}}z_+x\right]k_3+\exp\left[-\sqrt{\frac{2m}{\hbar^2}}z_+x\right]k_4\right\}; \\ x>a: \quad t\exp\left[i\frac{p}{\hbar}x\right]+j\,\tilde{t}\exp\left[-\frac{p}{\hbar}x\right]. \end{cases} \tag{70}$$

The complex coefficients r, $\tilde{r}$, t and $\tilde{t}$ are determined by matching the wave function $\Psi(x)$ and its slope at the discontinuity of the potential $x=0$ and will depend on $|W|$.

By using the continuity equation, we immediately find the following relation between the transmission, $T=|t|^2$, and reflection, $R=|r|^2$, coefficients

$$R+T=1. \tag{71}$$

C. The rectangular potential well

Finally, we briefly discuss the quaternionic rectangular potential well,

$$V(x)-j\,W(x)=\begin{cases} 0, & x<0, \\ -V+j\,W, & 0<x<a, \\ 0, & x>a. \end{cases}$$

In the potential region, the solution of the complex linear quaternionic Schrödinger equation is then given by

$$\Psi(x)=u_-\left\{\exp\left[\sqrt{\frac{2m}{\hbar^2}}z_-x\right]k_1+\exp\left[-\sqrt{\frac{2m}{\hbar^2}}z_-x\right]k_2\right\} \\ +u_+\left\{\exp\left[\sqrt{\frac{2m}{\hbar^2}}z_+x\right]k_3+\exp\left[-\sqrt{\frac{2m}{\hbar^2}}z_+x\right]k_4\right\}, \tag{72}$$

where

$$u_-=\left(1-j\frac{W}{E+\sqrt{E^2-|W|^2}}\right), \quad u_+=\left(j-\frac{\bar{W}}{E+\sqrt{E^2-|W|^2}}\right),$$

and

$$z_-=i\sqrt{\sqrt{E^2-|W|^2}+V}, \quad z_+=\sqrt{\sqrt{E^2-|W|^2}-V}.$$

Depending on whether the energy is positive or negative, we distinguish two separate cases. If $E>0$, the particle is unconfined and is scattered by the potential; if $E<0$, it is confined and in a bound state. We limit ourselves to discussing the case $E<0$. For $|W|<|E|<\sqrt{V^2+|W|^2}$, solution (72) becomes

$$u_-\left\{\exp\left[i\sqrt{\frac{2m}{\hbar^2}}\sqrt{\sqrt{E^2-|W|^2}+V}\,x\right]k_1+\exp\left[-i\sqrt{\frac{2m}{\hbar^2}}\sqrt{\sqrt{E^2-|W|^2}+V}\,x\right]k_2\right\}$$
$$+u_+\left\{\exp\left[i\sqrt{\frac{2m}{\hbar^2}}\sqrt{V-\sqrt{E^2-|W|^2}}\,x\right]k_3+\exp\left[-i\sqrt{\frac{2m}{\hbar^2}}\sqrt{V-\sqrt{E^2-|W|^2}}\,x\right]k_4\right\}. \tag{73}$$

For $|E|<|W|$, the solution is given by

$$u_-\left\{\exp\left[\sqrt{\frac{2m}{\hbar^2}\rho}\exp\left[i\frac{\theta+\pi}{2}x\right]\right]k_1+\exp\left[-\sqrt{\frac{2m}{\hbar^2}\rho}\exp\left[i\frac{\theta-\pi}{2}x\right]\right]k_2\right\}$$
$$+u_+\left\{\exp\left[\sqrt{\frac{2m}{\hbar^2}\rho}\exp\left[i\frac{\pi-\theta}{2}\right]x\right]k_3+\exp\left[-\sqrt{\frac{2m}{\hbar^2}\rho}\exp\left[-i\frac{\theta+\pi}{2}x\right]\right]k_4\right\}, \tag{74}$$

where $\rho=\sqrt{V^2+|W|^2-E^2}$ and $\tan\theta=\sqrt{|W|^2-E^2}/V$. In the region of zero potential, by using the boundary conditions at large distances, we find

$$\Psi(x)=\begin{cases} x<0: & \exp\left[\sqrt{\frac{2m}{\hbar^2}|E|}\,x\right]c_1+j\exp\left[-i\sqrt{\frac{2m}{\hbar^2}|E|}\,x\right]c_4;\\ x>a: & \exp\left[-\sqrt{\frac{2m}{\hbar^2}|E|}\,x\right]d_2+j\exp\left[i\sqrt{\frac{2m}{\hbar^2}|E|}\,x\right]d_3.\end{cases} \tag{75}$$

The matching conditions at the discontinuities of the potential yield the energy eigenvalues.

IX. CONCLUSIONS

In this paper, we have discussed the resolution of quaternionic, $\mathcal{D}_{\mathbb{H}}\,\varphi(x)=0$, and complex, $\mathcal{D}_{\mathbb{C}}\,\varphi(x)=0$, linear differential equations with constant coefficients within a quaternionic formulation of quantum mechanics. We emphasize that the only *quaternionic quadratic* equation involved in the study of second order linear differential equations with constant coefficients is given by Eq. (30) following from $\mathcal{D}_{\mathbb{H}}\,\varphi(x)=0$. Due to the right action of the factor i in complex linear differential equations, we cannot factorize a quaternionic exponential and consequently we are not able to obtain a *quaternionic quadratic* equation from $\mathcal{D}_{\mathbb{C}}\,\varphi(x)=0$. Complex linear differential equations can be solved by searching for quaternionic solutions of the form $q\exp[z\,x]$, where $q\in\mathbb{H}$ and $z\in\mathbb{C}$. The complex exponential factorization gives a *complex quartic* equation. A similar discussion can be extended to real linear differential equations, $\mathcal{D}_{\mathbb{R}}\,\varphi(x)=0$. In this case, the presence of left/right operators **L** and **R** in $\mathcal{D}_{\mathbb{R}}$ requires quaternionic solutions of the form $q\exp[\lambda\,x]$, where $q\in\mathbb{H}$ and $\lambda\in\mathbb{R}$. A detailed discussion of real linear differential equations deserves a further investigation.

The use of quaternionic mathematical structures in solving the complex linear Schrödinger equation could represent an important direction for the search of new physics. The open question of whether quaternions could play a significant role in quantum mechanics is strictly related to the whole understanding of resolutions of quaternionic differential equations and eigenvalue problems. The investigation presented in this work is only a first step towards a whole theory of quaternionic differential, integral and functional equations. Obviously, due to the great variety of problems in using a noncommutative field, it is very difficult to define the precise limit of the subject.

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APPENDIX A: QUATERNIONIC LINEAR QUADRATIC EQUATIONS

In this appendix, we give some examples of quaternionic linear quadratic equations; see cases (i)–(iii) and find their solutions.

• **(i):** $p^2+\sqrt{2}(i+j)p-1-2\sqrt{2}(i+j)=0$.

In solving such an equation we observe that $\mathbf{a}=(\sqrt{2},\sqrt{2},0)$ and $\mathbf{c}=-(2\sqrt{2},2\sqrt{2},0)$ are parallel vectors, $\mathbf{c}=-2\,\mathbf{a}$. Consequently, by introducing the *complex* imaginary unit $\mathcal{I}=(i+j)/\sqrt{2}$, we can reduce the quadratic quaternionic equation to the following *complex* equation:

$$p^2+2\,\mathcal{I}p-1-4\,\mathcal{I}=0,$$

whose solutions are $p_{1,2}=-\mathcal{I}\pm 2\sqrt{\mathcal{I}}$. It follows that the quaternionic solutions are

$$p_{1,2}=\pm\sqrt{2}-(1\mp\sqrt{2})\frac{i+j}{\sqrt{2}}.$$

• **(ii):** $p^2+i\,p+\frac{1}{2}k=0, \quad \Delta=0$.

We note that $\mathbf{a}=(1,0,0)$ and $\mathbf{c}=(0,0,\frac{1}{2})$ are orthogonal vectors and $\boldsymbol{\Delta}=0$. So, we find two coincident quaternionic solutions given by

$$p=-\frac{1}{2}\mathbf{h}\cdot\mathbf{a}+\mathbf{h}\cdot\mathbf{a}\times\mathbf{c}=-\frac{i+j}{2}.$$

• **(ii):** $p^2+j\,p+1-k=0, \quad \Delta>0$.

In this case, $\mathbf{a}=(0,1,0)$ and $\mathbf{c}=(0,0,-1)$ are orthogonal vectors, $c_0=1$ and $\Delta=1/4$. So,

$$p_0=0, \quad x=-\tfrac{1}{2}\pm\tfrac{1}{2}, \quad y=0, \quad z=1.$$

By observing that

$$\mathbf{h}\cdot\mathbf{a}=j, \quad \mathbf{h}\cdot\mathbf{c}=-k, \quad \mathbf{h}\cdot\mathbf{a}\times\mathbf{c}=-i,$$

we find the following quaternionic solutions:

$$p_1=-i \quad \text{and} \quad p_2=-(i+j).$$

• **(ii):** $p^2+k\,p+j=0, \quad \boldsymbol{\Delta}<0$.

We have $\mathbf{a}=(0,0,1)$, $\mathbf{c}=(0,1,0)$ and $c_0=0$. Then $\mathbf{a}\cdot\mathbf{c}=0$ and $\Delta=-3/4$. So,

$$p_0=\pm\tfrac{1}{2}, \quad x=-\tfrac{1}{2}, \quad y=\mp\tfrac{1}{2}, \quad z=\tfrac{1}{2}.$$

In this case,

$$\mathbf{h}\cdot\mathbf{a}=k, \quad \mathbf{h}\cdot\mathbf{c}=j, \quad \mathbf{h}\cdot\mathbf{a}\times\mathbf{c}=-i;$$

thus, the solutions are given by

$$p_{1,2}=\tfrac{1}{2}(\pm 1-i\mp j-k).$$

• **(iii):** $p^2+i\,p+1+i+k=0$.

We have $\mathbf{a}=(1,0,0)$, $\mathbf{c}=(1,0,1)$ and $c_0=1$. In this case $\mathbf{a}\cdot\mathbf{c}\neq 0$, so we introduce the quaternion $d_0+\mathbf{h}\cdot\mathbf{d}=1+k$, whose vectorial part $\mathbf{d}=\mathbf{c}-d_0\mathbf{a}=(0,0,1)$ is orthogonal to $\mathbf{a}$. The imaginary part of our solution will be given in terms of the imaginary quaternions,

$$\mathbf{h}\cdot\mathbf{a}=i,\quad \mathbf{h}\cdot\mathbf{d}=k,\quad \mathbf{h}\cdot\mathbf{a}\times\mathbf{d}=-j.$$

The real part of p is determined by solving the equation

$$16\,p_0^6+24\,p_0^4-3\,p_0^2-1=0.$$

The real positive solution is given by $p_0^2=\frac{1}{4}$. Consequently,

$$p_0=\pm\tfrac{1}{2},\quad x=-\tfrac{1}{2}\mp 1,\quad y=\mp\tfrac{1}{2},\quad z=\tfrac{1}{2}.$$

The quaternionic solutions are

$$p_1=\tfrac{1}{2}(1-3i-j-k)\quad\text{and}\quad p_2=-\tfrac{1}{2}(1-i+j-k).$$

APPENDIX B: QUATERNIONIC LINEAR DIFFERENTIAL EQUATIONS

We solve quaternionic linear differential equations whose characteristic equations are given by examples **(i)–(iii)** in Appendix A.

• **(i):** $\ddot{\varphi}(x)+\sqrt{2}(i+j)\dot{\varphi}(x)-[1+2\sqrt{2}(i+j)]\varphi(x)=0,\quad \varphi(0)=i,\quad \dot{\varphi}(0)=\dfrac{1+k}{\sqrt{2}}.$

The exponential $\exp[p\,x]$ is solution of the previous differential equation if and only if the quaternion p satisfies the following quadratic equation:

$$p^2+\sqrt{2}(i+j)p-1-2\sqrt{2}(i+j)=0,$$

whose solutions are given by

$$p_{1,2}=\pm\sqrt{2}-(1\mp\sqrt{2})\,\frac{i+j}{\sqrt{2}}.$$

Consequently,

$$\varphi(x)=\exp\left\{\left[\sqrt{2}-(1-\sqrt{2})\,\frac{i+j}{\sqrt{2}}\right]x\right\}c_1+\exp\left\{\left[-\sqrt{2}-(1+\sqrt{2})\,\frac{i+j}{\sqrt{2}}\right]x\right\}c_2.$$

By using the initial conditions, we find

$$\varphi(x)=\exp\left[-\frac{i+j}{\sqrt{2}}\,x\right]\cosh\left[\left(\sqrt{2}+\frac{i+j}{\sqrt{2}}\right)x\right]i.$$

• **(ii):** $\ddot{\varphi}(x)+(1+i)\dot{\varphi}(x)+\dfrac{2+i+k}{4}\,\varphi(x)=0,\quad \varphi(0)=0,\quad \dot{\varphi}(0)=-\dfrac{1+i+j}{2}.$

We look for exponential solutions of the form $\varphi(x)=\exp[q\,x]=\exp[(p-\frac{1}{2})x]$. The quaternion p must satisfy the quadratic equation,

$$p^2+i\,p+\tfrac{1}{2}k=0.$$

This equation implies

$$p_1=p_2=-\frac{i+j}{2}.$$

Thus,

$$\varphi_1(x)=\exp\left[-\frac{1+i+j}{2}x\right].$$

The second linearly independent solution is given by

$$\varphi_2(x)=(x+i)\exp\left[-\frac{1+i+j}{2}x\right].$$

By using the initial conditions, we find

$$\varphi(x)=\{\exp[qx]+(x+i)\exp[qx]i\}[1+q^{-1}(1+iq)i]^{-1},$$

where $q=-(1+i+j)/2$.

- **(ii):** $\ddot{\varphi}(x)+(2+j)\dot{\varphi}(x)+(2+j-k)\varphi(x)=0,\ \varphi(0)=\frac{1-i}{2},\ \dot{\varphi}(0)=j.$

  The exponential solution $\varphi(x)=\exp[qx]=\exp[(p-1)x]$ leads to

$$p^2+jp+1-k=0,$$

whose solutions are

$$p_1=-i \quad \text{and} \quad p_2=-(i+j).$$

Consequently,

$$\varphi(x)=\exp[-x]\{\exp[-ix]c_1+\exp[-(i+j)x]c_2\}.$$

The initial conditions yield

$$\varphi(x)=\exp[-x]\left\{\exp[-ix]\frac{3-i-2j}{2}+\exp[-(i+j)x](j-1)\right\}.$$

- **(ii):** $\ddot{\varphi}(x)+k\dot{\varphi}(x)+j\varphi(x)=0,\ \varphi(0)=i+k,\ \dot{\varphi}(0)=1.$

  The characteristic equation is

$$p^2+kp+j=0,$$

whose solutions are

$$p_{1,2}=\tfrac{1}{2}(\pm 1-i\mp j-k).$$

Thus, the general solution of our differential equation reads as

$$\varphi(x)=\exp\left[\frac{1-i-j-k}{2}x\right]c_1+\exp\left[-\frac{1+i-j+k}{2}x\right]c_2.$$

By using the initial conditions, we obtain

$$\varphi(x)=\left\{ \exp\left[\frac{1-i-j-k}{2}x\right]+\exp\left[-\frac{1+i-j+k}{2}x\right]\right\}\frac{i+k}{2}.$$

• **(iii):** $\ddot{\varphi}(x)+(i-2)\dot{\varphi}(x)+(2+k)\varphi(x)=0,\ \varphi(0)=0,\ \dot{\varphi}(0)=j.$
By substituting $\varphi(x)=\exp[q\,x]=\exp[(p+1)x]$ in the previous differential equation, we find

$$p^2+i\,p+1+i+k=0.$$

The solutions of this quadratic quaternionic equation are

$$p_1=\tfrac{1}{2}(1-3i-j-k)\quad\text{and}\quad p_2=-\tfrac{1}{2}(1-i+j-k).$$

So, the general solution of the differential equation is

$$\varphi(x)=\exp\left[\frac{1-3i-j-k}{2}x\right]c_1+\exp\left[-\frac{1-i+j-k}{2}x\right]c_2.$$

By using the initial conditions, we obtain

$$\varphi(x)=\left\{\exp\left[\frac{1-3i-j-k}{2}x\right]-\exp\left[-\frac{1-i+j-k}{2}x\right]\right\}\frac{j-i+2k}{6}.$$

APPENDIX C: DIAGONALIZATION AND JORDAN FORM

In this appendix, we find the solution of quaternionic and complex linear differential equations by using diagonalization and Jordan form.

1. Quaternionic linear differential equation

By using the discussion about quaternionic quadratic equation, it can immediately be shown that the solution of the following second order equation:

$$\ddot{\varphi}(x)+(k-i)\dot{\varphi}(x)-j\,\varphi(x)=0,$$

with initial conditions

$$\varphi(0)=\frac{k}{2},\quad \dot{\varphi}(0)=1+\frac{j}{2},$$

is given by

$$\varphi(x)=\left(x+\frac{k}{2}\right)\exp[i\,x].$$

Let us solve this differential equation by using its matrix form (47), with

$$M=\begin{pmatrix}0 & 1\\ j & i-k\end{pmatrix}.$$

This quaternionic matrix can be reduced to its Jordan form,

$$M=J\begin{pmatrix}i & 1\\ 0 & i\end{pmatrix}J^{-1},$$

by the matrix transformation

$$J=\begin{pmatrix} 1 & \frac{k}{2} \\ i & 1+\frac{j}{2} \end{pmatrix}, \quad J^{-1}=\begin{pmatrix} \frac{3+j}{4} & -\frac{i+k}{4} \\ -\frac{i+k}{2} & \frac{1-j}{2} \end{pmatrix}.$$

The solution of the quaternionic linear quaternionic differential equation is then given by

$$\begin{aligned}\varphi(x)&=J_{11}\exp[i\,x][J_{11}^{-1}\,\varphi(0)+J_{12}^{-1}\,\dot{\varphi}(0)]\\ &\quad+(x\,J_{11}+J_{12})\exp[i\,x][J_{21}^{-1}\,\varphi(0)+J_{22}^{-1}\,\dot{\varphi}(0)]\\ &=(x\,J_{11}+J_{12})\exp[i\,x]\\ &=\left(x+\frac{k}{2}\right)\exp[i\,x].\end{aligned}$$

2. Complex linear differential equations

Let us now consider the complex linear quaternionic differential equation,

$$\ddot{\varphi}(x)-j\,\varphi(x)i=0,$$

with initial conditions

$$\varphi(0)=j, \quad \dot{\varphi}(0)=k.$$

To find particular solutions, we set $\varphi(x)=q\exp[z\,x]$. Consequently,

$$q\,z^2-j\,q\,i=0.$$

The solution of the complex linear second order differential equation is

$$\varphi(x)=\tfrac{1}{2}[(i+j)\exp[-ix]+(j-i)\cosh x+(k-1)\sinh x].$$

This solution can also be obtained by using the matrix

$$M_{\mathbb{C}}=\begin{pmatrix} 0 & 1 \\ j\,R_i & 0 \end{pmatrix},$$

and its diagonal form

$$M_{\mathbb{C}}=S_{\mathbb{C}}\begin{pmatrix} -i\,R_i & 0 \\ 0 & i \end{pmatrix}S_{\mathbb{C}}^{-1},$$

where

$$S_{\mathbb{C}}=\begin{pmatrix} \frac{1-i-j-k}{2}+\frac{1-i+j+k}{2}R_i & \frac{1+i-j+k}{2}-\frac{1+i+j-k}{2}R_i \\ \frac{1+i+j-k}{2}-\frac{1+i-j+k}{2}R_i & -\frac{1-i-j-k}{2}+\frac{1-i+j+k}{2}R_i \end{pmatrix}$$

and

$$S_{\mathbb{C}}^{-1}=\frac{1}{4}\begin{pmatrix} \frac{1+i+j+k}{2}-\frac{1+i-j-k}{2}R_i & \frac{1-i-j+k}{2}+\frac{1-i+j-k}{2}R_i \\ \frac{1-i+j-k}{2}+\frac{1-i-j+k}{2}R_i & -\frac{1+i+j+k}{2}-\frac{1+i-j-k}{2}R_i \end{pmatrix}.$$

The solution of the complex linear quaternionic differential equation is then given by

$$\begin{aligned}\varphi(x)&=S_{\mathbb{C}\,11}\exp[-\,i\,R_i\,x][S_{\mathbb{C}\,11}^{-1}\,\varphi(0)+S_{\mathbb{C}\,12}^{-1}\,\dot{\varphi}(0)]\\&\quad+S_{\mathbb{C}\,12}\exp[ix][S_{\mathbb{C}\,21}^{-1}\,\varphi(0)+S_{\mathbb{C}\,22}^{-1}\,\dot{\varphi}(0)]\\&=\frac{1}{4}\{(1-i+j-k)\exp[-x]-(1+i-j-k)\exp[x]\}\\&\quad+\frac{i+j}{2}\exp[-ix].\end{aligned}$$

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