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Quaternionic potentials in non-relativistic quantum mechanics

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Abstract

We discuss the Schrödinger equation in the presence of quaternionic potentials. The study is performed analytically as long as it proves possible, when not, we resort to numerical calculations. The results obtained could be useful to investigate an underlying quaternionic quantum dynamics in particle physics. Experimental tests and proposals to observe quaternionic quantum effects by neutron interferometry are briefly reviewed.

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1. Introduction

After the classical mathematical and physical works on foundations of quaternionic quantum mechanics [1–4], there has been, in recent years, a wide interest in formulating quantum theories by using the non-commutative ring of quaternions [5–12]. Some of the main results emerging from the use of *new* algebraic structures in particle physics are reviewed in the books of Dixon [13] and Gürsey and Tze [14]. For a detailed discussion of quaternionic quantum mechanics and field theory we refer to the excellent book of Adler [15].

The present paper has grown from an attempt to understand the experimental proposals [16–18] and theoretical discussions [19–21] underlying the quaternionic formulation of the Schrödinger equation. The main difficulty in obtaining quaternionic solutions of a physical problem is due to the fact that, in general, the standard mathematical methods of resolution break down. In recent years, some of these problems have been overcome. In particular, the discussion of quaternionic eigenvalue equations [22] and differential operators [23] is *now* recognized as quite satisfactory. On the other hand, physical interpretations of quaternionic solutions represent a more delicate question [15]. In discussing the Schrödinger equation what is still lacking is an understanding of the role that quaternionic potentials could play in quantum mechanics and where deviations from the standard theory would appear.

The earliest experimental proposals to test quaternionic deviations from complex quantum mechanics were made by Peres [16] who suggested that the non-commutativity of quaternionic phases could be observed in Bragg scattering by crystals made of three different atoms, in neutron interferometry and in meson regeneration. In 1984, the neutron interferometric experiment was realized by Kaiser *et al* [17]. The neutron wavefunction traversing slabs of two dissimilar materials (titanium and aluminium) should experience non-commutativity of the phase shifts when the order in which the barriers are traversed is reversed. The experimental result showed that the phase shifts commute to better than one part in 3×10^4. To explain this null result, Klein postulated [18] that quaternionic potentials act only for some of the fundamental forces and proposed an experiment for testing possible violations of the Schrödinger equation by permuting the order in which nuclear, magnetic and gravitational potentials act on neutrons in an interferometer.

The first theoretical analysis of two quaternionic potential barriers was developed by Davies and McKellar [21]. In their paper, by translating the quaternionic Schrödinger equation into a pair of coupled complex equations and solving the corresponding complex system by numerical methods, Davies and McKellar showed that, notwithstanding the presence of complex *instead* of quaternionic phases, the predictions of quaternionic quantum mechanics differ from those of the usual theory. In particular, they pointed out that in contrast to the complex quantum mechanics prediction, where the left and right transmission amplitudes, t_L and t_R, are equal in magnitude and in phase, in the quaternionic quantum mechanics only the magnitudes $|t_L|$ and $|t_R|$ are equal. So, the measurement of a phase shift should be an indicator of quaternionic effects *and* of space-dependent phase potentials. However, this conclusion leads to the embarrassing question of why there was no phase change in the experiment proposed by Peres and realized by Kaiser *et al*. To reconcile the theoretical predictions with the experimental observations, Davies and McKellar reiterated the Klein conclusion and suggested subjecting the neutron beam to different interactions in permuted order. In the final chapter of the Adler book [15], we find an intriguing question. Do the Kaiser and colleagues experiment, and the elaborations on it proposed by Klein, actually test for residual quaternionic effects? According to the non-relativistic quaternionic scattering theory developed by Adler [15], the answer is clearly no. Experiments to detect a phase shift are equivalent to detecting time-reversal violation, which so far has not been detectable in neutron-optical experiments.

In this paper, after a brief introductory discussion about probability amplitudes, anti-self-adjoint operators, stationary states and time-reversal invariance, we study the phenomenology of quaternionic one-dimensional square potentials. The j–k part of these potentials is treated as a perturbation of the complex case. We show that there are many possibilities in looking for quaternionic deviations from the standard (complex) theory. Nevertheless, in particular cases, we have to contend with quaternionic effects which minimize the deviations from complex quantum mechanics. With this paper, we would like to close the debate on the role that quaternionic potentials could play in quantum mechanics, but more realistically, we simply contribute to the general discussion.

2. Amplitudes of probability

In this section, following Adler [15], we briefly discuss what kinds of number systems can be used to *appropriately* define amplitudes of probability. Let us consider a *generic* (complex, quaternionic, biquaternionic, octonionic, etc) Hilbert space $\mathbb{V}$ whose dimensionality is specified according to the nature of the physical system under consideration. In quantum mechanics a physical state can be represented by an element in this space. With each pair of elements of $\mathbb{V}$, by a binary mapping (inner product) $\mathbb{V} \times \mathbb{V} \to \mathbb{A}$, we associate an amplitude of probability $\alpha \in \mathbb{A}$ and define a real modulus function $N(\alpha)$ such that $P = [N(\alpha)]^2$, where P is the probability of finding the system in a particular state. The first four assumptions on $N(\alpha)$ are those usually imposed for a modulus function, that is

$$N(0) = 0 \qquad N(\alpha) > 0 \qquad N(r\alpha) = |r| N(\alpha) (r \in \mathbb{R}) \qquad N(\alpha_1 + \alpha_2) \leqslant N(\alpha_1) + N(\alpha_2).$$

A last assumption is obtained by imposing that in the absence of quantum interference, probability amplitude superposition, $\alpha_{if} = \sum_n \alpha_{in}\alpha_{nf}$, should reduce to probability superposition, $P_{if} = \sum_n P_{in} P_{nf}$. Consequently, for any two elements $\alpha_{1,2}$ of the algebra $\mathbb{A}$, we get

$$N(\alpha_1\alpha_2) = N(\alpha_1)N(\alpha_2).$$

This condition implies the *division algebra* property. The only division algebras over $\mathbb{R}$ are the real, complex ($\mathbb{C}$), quaternions ($\mathbb{H}$) and octonions ($\mathbb{O}$). A simple example of a nondivision algebra is provided by complexified quaternions (or biquaternions).

As shown in [15], the associative law of multiplication (which fails for octonions) is needed to give correct completeness relations and to guarantee that anti-Hermitian time evolution operators leave invariant inner products. Thus, probability amplitude must be defined in *associative division algebras*. Nevertheless, this does *not* mean that octonionic or complexified quaternionic formulation of quantum mechanics is ruled out. In fact, it is possible to work with octonionic or complexified quaternionic states and use *complex* or *quaternionic* probability amplitudes. For example, the choice of a complex projection of inner products allows formulations of relativistic equations and gauge theories by octonions [24, 25] and complexified quaternions [26–32]. The important point to note here is the possibility of introducing translation rules [33, 34] from which we can immediately obtain octonionic or complexified quaternionic counterparts of standard (complex) theories. Our point of view is that the use of the complex projection of inner products opens the door to the use of nonassociative and nondivision algebras in physics and plays an important role in investigating *new* gauge group in unification models [35, 36]. Further investigations, i.e. octonionic and complexified quaternionic versions of physical theories based on the use of *quaternionic* probability amplitudes, could be interesting *when and if* the validity of quaternionic quantum mechanics based on quaternionic inner products is proved.

Throughout the paper, the states which represent quantum systems will be defined by vectors in quaternionic Hilbert space, $\mathbb{V}_{\mathbb{H}}$, linear under *right* multiplication [5] by quaternionic scalar and the amplitudes of probability will be defined by the binary mapping $\mathbb{V}_{\mathbb{H}} \times \mathbb{V}_{\mathbb{H}} \to \mathbb{H}$.

3. Quaternionic Schrödinger equation

In the standard formulation of nonrelativistic quantum mechanics, the complex wavefunction $\varphi(\boldsymbol{r}, t)$, describing a particle without spin subjected to the influence of a real potential $V(\boldsymbol{r}, t)$, satisfies the Schrödinger equation

$$\partial_t \varphi(\boldsymbol{r}, t) = \frac{\mathrm{i}}{\hbar} \left[\frac{\hbar^2}{2m} \nabla^2 - V(\boldsymbol{r}, t) \right] \varphi(\boldsymbol{r}, t). \tag{1}$$

In quaternionic quantum mechanics [15], the anti-self-adjoint operator

$$\mathcal{A}^V(\boldsymbol{r}, t) = \frac{\mathrm{i}}{\hbar} \left[\frac{\hbar^2}{2m} \nabla^2 - V(\boldsymbol{r}, t) \right]$$

can be generalized by introducing the complex potential $W(\boldsymbol{r}, t) = |W(\boldsymbol{r}, t)| \exp[\mathrm{i}\theta(\boldsymbol{r}, t)]$,

$$\mathcal{A}^{V,W}(\boldsymbol{r}, t) = \frac{\mathrm{i}}{\hbar}\left[\frac{\hbar^2}{2m}\nabla^2 - V(\boldsymbol{r}, t)\right] + \frac{\mathrm{j}}{\hbar}W(\boldsymbol{r}, t)$$

where the quaternionic imaginary units i, j and k satisfy the following associative but non-commutative algebra:

$$\mathrm{i}^2 = \mathrm{j}^2 = \mathrm{k}^2 = \mathrm{ijk} = -1.$$

The anti-Hermiticity is required to guarantee the time conservation of transition probabilities. As a consequence of this generalization for the anti-self-adjoint Hamiltonian operator, the quaternionic wavefunction $\Phi(\boldsymbol{r}, t)$ satisfies the following equation:

$$\partial_t \Phi(\boldsymbol{r}, t) = \left\{\frac{\mathrm{i}}{\hbar}\left[\frac{\hbar^2}{2m}\nabla^2 - V(\boldsymbol{r}, t)\right] + \frac{\mathrm{j}}{\hbar}W(\boldsymbol{r}, t)\right\}\Phi(\boldsymbol{r}, t). \tag{2}$$

Observe that $\Phi(\boldsymbol{r}, t)$ has to be multiplied by i and j from the left-hand side because we are considering quaternionic Hilbert space linear from the right multiplication by quaternionic scalars. The presence of the imaginary units on the left-hand side and not from the right also guarantees the anti-Hermiticity of $\mathcal{A}^{V,W}$. Exactly as in the case of the standard quantum mechanics, we can define a current density

$$\boldsymbol{J} = \frac{\hbar}{2m}[(\nabla\overline{\Phi})\,\mathrm{i}\Phi - \overline{\Phi}\mathrm{i}\nabla\Phi]$$

and a probability density

$$\rho = \overline{\Phi}\Phi.$$

Due to the non-commutativity nature of quaternions, the position of the imaginary unit i in the current density is fundamental to obtaining the continuity equation

$$\partial_t \rho + \nabla\cdot\boldsymbol{J} = 0. \tag{3}$$

3.1. Stationary states

The quaternionic Schrödinger equation in the presence of time-independent potentials

$$[V(\boldsymbol{r}), |W(\boldsymbol{r})|, \theta(\boldsymbol{r})]$$

reads

$$\partial_t \Phi(\boldsymbol{r}, t) = \left\{\frac{\mathrm{i}}{\hbar}\left[\frac{\hbar^2}{2m}\nabla^2 - V(\boldsymbol{r})\right] + \frac{\mathrm{j}}{\hbar}W(\boldsymbol{r})\right\}\Phi(\boldsymbol{r}, t). \tag{4}$$

The quaternionic stationary state wavefunction[4]

$$\Phi(\boldsymbol{r}, t) = \Psi(\boldsymbol{r})\exp\left[-\frac{\mathrm{i}}{\hbar}Et\right]$$

is the solution of equation (4) on the condition that $\Psi(\boldsymbol{r})$ is a solution of the time-independent Schrödinger equation

$$\left[\mathrm{i}\frac{\hbar^2}{2m}\nabla^2 - \mathrm{i}V(\boldsymbol{r}) + \mathrm{j}W(\boldsymbol{r})\right]\Psi(\boldsymbol{r}) + \Psi(\boldsymbol{r})\,\mathrm{i}E = 0. \tag{5}$$

[4] The choice of the imaginary unit i in the time exponential and as a factor in the Laplacian operator (4) guarantees the standard results in the complex limit case. Observe that we are treating the quaternionic potentials as perturbation effects on standard (complex) quantum mechanics.

Equation (5) represents a right complex eigenvalue equation on the quaternionic field [22, 37],

$$\mathcal{A}_E^{V,W}(\boldsymbol{r})\Psi(\boldsymbol{r}) = -\Psi(\boldsymbol{r})\,\mathrm{i}E.$$

The allowed energies are determined by the right complex eigenvalues $\lambda = -\mathrm{i}E$ of the quaternionic linear anti-self-adjoint operator $\mathcal{A}_E^{V,W}(\boldsymbol{r})$. The stationary state wavefunctions are particular solutions of equation (4). More general solutions can be constructed by superposition of such particular solutions. Summing over various allowed values of E, we get

$$\Phi(\boldsymbol{r}, t) = \sum_E \Psi(\boldsymbol{r}) \exp\left[-\frac{\mathrm{i}}{\hbar}Et\right] q_E \tag{6}$$

where q_E are constant quaternionic coefficients. The summation may imply an integration if the energy spectrum of E is continuous.

3.2. Time-reversal invariance

From equation (4), we can immediately obtain the time-reversed Schrödinger equation

$$\partial_t \Phi_{\mathrm{T}}(\boldsymbol{r}, -t) = -\left\{\frac{\mathrm{i}}{\hbar}\left[\frac{\hbar^2}{2m}\nabla^2 - V(\boldsymbol{r})\right] + \frac{\mathrm{j}}{\hbar}W(\boldsymbol{r})\right\}\Phi_{\mathrm{T}}(\boldsymbol{r}, -t). \tag{7}$$

In complex quantum mechanics the $*$-conjugation yields a time-reversed version of the original Schrödinger equation. In quaternionic quantum mechanics there does *not* exist a universal time-reversal operator [15]. Only a *restricted* class of time-independent quaternionic potentials, i.e.

$$W(\boldsymbol{r}) = |W(\boldsymbol{r})| \exp[\mathrm{i}\theta]$$

is time-reversal invariant. For these potentials,

$$\Phi_{\mathrm{T}}(\boldsymbol{r}, -t) = u\Phi(\boldsymbol{r}, t)\bar{u} \qquad u = k\exp[\mathrm{i}\theta]. \tag{8}$$

For complex wavefunctions, we recover the standard result $\Phi_{\mathrm{T}}(\boldsymbol{r}, -t) = \Phi^*(\boldsymbol{r}, t)$.

3.3. One-dimensional square potentials

On solving the quaternionic Schrödinger equation, a great mathematical simplification results from the assumption that the wavefunction and the potential energy depend only on the x-coordinate,

$$\mathrm{i}\frac{\hbar^2}{2m}\ddot{\Psi}(x) + [\,\mathrm{j}W(x) - \mathrm{i}V(x)]\Psi(x) + \Psi(x)\,\mathrm{i}E = 0. \tag{9}$$

We shall consider one-dimensional problems with a potential which is pieced together from a number of *constant* portions, i.e. square potentials. In the potential region

$$[V;\,|W|, \theta]$$

the solution of the second-order differential equation (9) is given by [23]

$$\Psi(x) = u^{E;|W|,\theta}\left\{\exp\left[z_-^{E;V,|W|}x\right]c_1 + \exp\left[-z_-^{E;V,|W|}x\right]c_2\right\} \\ + v^{E;|W|,\theta}\left\{\exp\left[z_+^{E;V,|W|}x\right]c_3 + \exp\left[-z_+^{E;V,|W|}x\right]c_4\right\} \tag{10}$$

where $c_{1,\ldots,4}$ are complex coefficients determined by the boundary conditions,

$$z_\pm^{E;V,|W|} = \sqrt{\frac{2m}{\hbar^2}(V \pm \sqrt{E^2 - |W|^2})} \in \mathbb{C}(1, \mathrm{i})$$

and

$$u^{E;|W|,\theta} = \left(1 - \mathrm{k}\frac{|W|\exp[\mathrm{i}\theta]}{E + \sqrt{E^2 - |W|^2}}\right) \qquad v^{E;|W|,\theta} = \left(\mathrm{j} - \frac{\mathrm{i}|W|\exp[-\mathrm{i}\theta]}{E + \sqrt{E^2 - |W|^2}}\right) \in \mathbb{H}.$$

In the free potential region, the solution reduces to

$$\Psi(x) = \exp\left[\mathrm{i}\frac{p}{\hbar}x\right]c_1 + \exp\left[-\mathrm{i}\frac{p}{\hbar}x\right]c_2 + \mathrm{j}\left\{\exp\left[\frac{p}{\hbar}x\right]c_3 + \exp\left[-\frac{p}{\hbar}x\right]c_4\right\}$$

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

$$\Psi_-(x) = \exp\left[\mathrm{i}\frac{p}{\hbar}x\right] + r\exp\left[-\mathrm{i}\frac{p}{\hbar}x\right] + \mathrm{j}\tilde{r}\exp\left[\frac{p}{\hbar}x\right] \tag{11}$$

where $|r|^2$ is the standard probability of reflection and $\left|\tilde{r}\exp\left[\frac{p}{\hbar}x\right]\right|^2$ represents an additional evanescent reflection.

4. Time-reversal invariant (TRI) potential barrier

Let us consider the TRI potential

$$[V(x); |W(x)|, \theta].$$

In equation (9), the space-independent phase θ can be removed by taking the transformation

$$\Psi(x) \to \exp\left[\mathrm{i}\frac{\theta}{2}\right]\Psi(x)\exp\left[-\mathrm{i}\frac{\theta}{2}\right]. \tag{12}$$

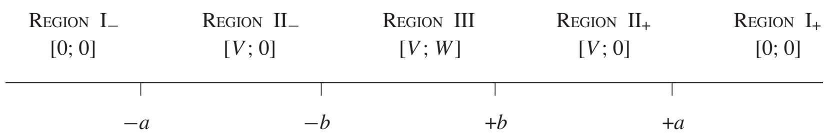
Under this transformation

$$u^{E;|W|,\theta} \to u^{E;|W|} \quad \text{and} \quad v^{E;|W|,\theta} \to v^{E;|W|}\exp[-\mathrm{i}\theta].$$

Reflection and transmission probabilities do *not* change (actually the exponential $\exp[-\mathrm{i}\theta]$ can be absorbed in the complex coefficients $c_{3,4}$). So, without loss of generality, we can discuss the quaternionic Schrödinger equation in the presence of the square potential

$$[V(x); |W(x)|]$$

which has the following shape:



The particle is free for $x < -a$, where the solution is given by equation (11), and for $x > a$, where the solution is

$$\Psi_+(x) = t\exp\left[\mathrm{i}\frac{p}{\hbar}x\right] + \mathrm{j}\,\tilde{t}\exp\left[-\frac{p}{\hbar}x\right]. \tag{13}$$

In equations (11) and (13), we have respectively omitted the complex exponential solutions $\exp\left[-\frac{p}{\hbar}x\right]$ and $\exp\left[\frac{p}{\hbar}x\right]$ because they are in conflict with the boundary condition that $\Psi(x)$ remain finite as $x \to -\infty$ and $x \to +\infty$. In order to determine the complex amplitudes r, t, $\tilde{r}$ and $\tilde{t}$, we match the wavefunction and its slope at the discontinuities of the potential (see the appendix).

By using the continuity equation, we can immediately obtain the standard relation between the transmission and reflection coefficients, t and r. In fact, equation (3) implies that the current density

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

has the same value at all points x. In the free potential regions, the probability current densities are given by $\mathcal{J}_- = \frac{p}{m}(1-|r|^2)$ and $\mathcal{J}_+ = \frac{p}{m}|t|^2$. Consequently, we find

$$|r|^2 + |t|^2 = 1. \tag{14}$$

In figure 1(a), we plot the transmission probability $|t|^2$ as a function of E (eV) for quaternionic potentials of different widths and heights (we assume that the incident particle is an electron). The presence of a quaternionic perturbation potential modifies the shape of the (complex) transmission probability curve. We have a reduction of the transmission probability. The presence of an inflection point is evident by increasing the width and the height of quaternionic potentials. Figure 1(b) shows the transmission probability for the quaternionic potential

$$V + \mathrm{j}|W| = (2.0 + \mathrm{j}1.5)\ \mathrm{eV}$$

and the complex *comparative* barrier [19]

$$Z = \sqrt{V^2 + |W|^2} = 2.5\ \mathrm{eV}.$$

The wave numbers for these potentials are

- $E > \sqrt{V^2+|W|^2}$:

$$z_-^Z = \mathrm{i}\sqrt{\frac{2m}{\hbar^2}\left(E - \sqrt{V^2+|W|^2}\right)} \in \mathrm{i}\mathbb{R}_+$$
$$z_-^{V,W} = \mathrm{i}\sqrt{\frac{2m}{\hbar^2}\left(\sqrt{E^2-|W|^2} - V\right)} \in \mathrm{i}\mathbb{R}_+$$
$$z_+^{V,W} = \sqrt{\frac{2m}{\hbar^2}\left(\sqrt{E^2-|W|^2} + V\right)} \in \mathbb{R}_+$$

- $|W| < E < \sqrt{V^2+|W|^2}$:

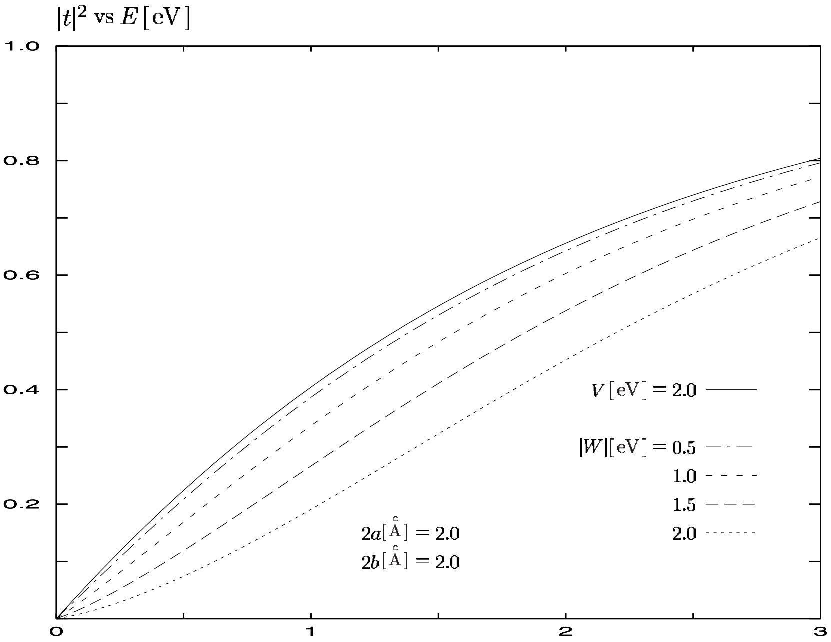
$$z_-^Z = \sqrt{\frac{2m}{\hbar^2}\left(\sqrt{V^2+|W|^2} - E\right)} \in \mathbb{R}_+$$
$$z_\pm^{V,W} = \sqrt{\frac{2m}{\hbar^2}\left(V \pm \sqrt{E^2-|W|^2}\right)} \in \mathbb{R}_+$$

- $E < |W|$:

$$z_-^Z = \sqrt{\frac{2m}{\hbar^2}\left(\sqrt{V^2+|W|^2} - E\right)} \in \mathbb{R}_+$$
$$z_\pm^{V,W} = \sqrt{\frac{2m}{\hbar^2}\sqrt{V^2+|W|^2-E^2}\,\exp[\pm\mathrm{i}\varphi]} \in \mathbb{C}$$

where $\varphi = \arctan[\sqrt{(|W|^2-E^2)/V^2}]$. For small quaternionic perturbations, the complex *comparative* barrier Z represents a good approximation of the quaternionic potential $V + \mathrm{j}|W|$. In this case,

$$Z \sim V\left(1 + \frac{1}{2}\frac{|W|^2}{V^2}\right) \quad \text{and} \quad z_-^{V,W} \sim z_-^Z.$$



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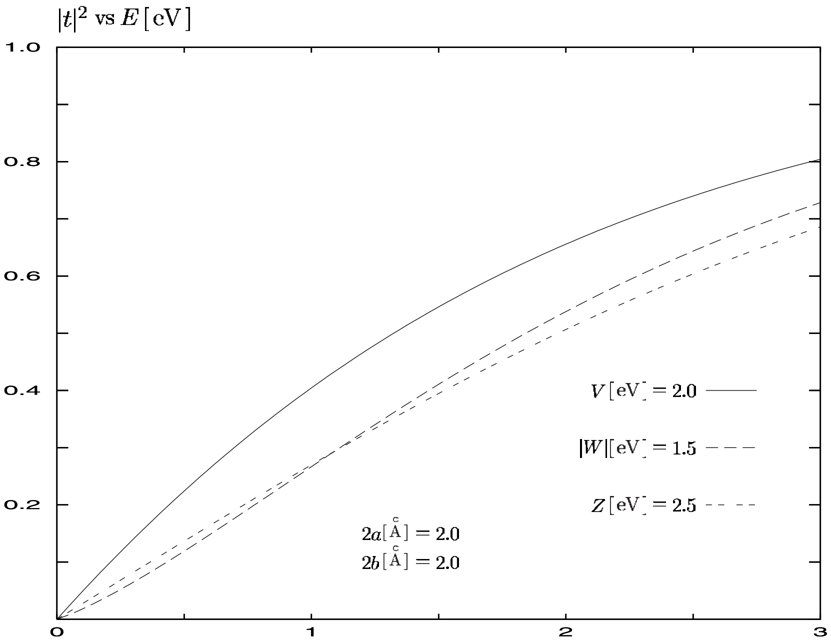

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Figure 1. Electron transmission probability, $|t|^2$, as a function of E (eV) for quaternionic time-reversal invariant potentials [40]. The full line indicates the complex quantum mechanics result for the potential barrier of width a (Å) $= 1.0$ and height V (eV) $= 2.0$. The dashed lines (drawn for a fixed width b (Å) $= 1.0$ and different values of the height $|W|$ of the potential jW) show the quaternionic perturbation effects and the transmission probability for the complex (comparative) barrier $Z = \sqrt{V^2 + |W|^2}$.

The anti-self-adjoint operators corresponding to the quaternionic potential $V + \mathrm{j}|W|$ and to the complex barrier Z are respectively

$$\mathcal{A}_E^{V,W} = \mathrm{i}\left[\frac{\hbar^2}{2m}\nabla^2 - V\right] + \mathrm{j}W(\boldsymbol{r}, t) \qquad \text{and} \qquad \mathcal{A}_E^{Z} = \mathrm{i}\left[\frac{\hbar^2}{2m}\nabla^2 - \sqrt{V^2 + |W|^2}\right].$$

By using these operators, we can write down two complex wave equations

$$\left[\mathcal{A}_E^{V,W}\right]^2 \Psi(x) = -E^2\Psi(x) \qquad \text{and} \qquad \left[\mathcal{A}_E^{Z}\right]^2 \Psi(x) = -E^2\Psi(x). \quad (15)$$

The complex operators

$$\left[\mathcal{A}_E^{V,W}\right]^2 = -\left[\frac{\hbar^2}{2m}\nabla^2 - V\right]^2 - |W|^2 = -\left(\frac{\hbar^2}{2m}\right)^2 \nabla^4 + 2V\frac{\hbar^2}{2m}\nabla^2 - V^2 - |W|^2$$

and

$$\left[\mathcal{A}_E^{Z}\right]^2 = -\left[\frac{\hbar^2}{2m}\nabla^2 - \sqrt{V^2 + |W|^2}\right]^2 = -\left(\frac{\hbar^2}{2m}\right)^2 \nabla^4 + 2\sqrt{V^2 + |W|^2}\frac{\hbar^2}{2m}\nabla^2 - V^2 - |W|^2$$

can now be easily compared. The difference is due to the factor which multiplies ∇^2. Thus, complex comparative barriers only represent a first approximation to quaternionic potentials. In general, we have to consider the pure quaternionic potential, $\mathrm{j}|W|$, as a perturbation effect on the complex barrier V.

Deviations from (complex) quantum mechanics appear in the proximity of the complex barrier V when a quaternionic perturbation is turned on. Actually, in quaternionic quantum mechanics we find an additional evanescent probability of transmission, that is $|\tilde{t}|^2$. This probability as a function of E (eV) is drawn in figure 2 for different values of x.

To conclude the discussion of quaternionic one-dimensional time-invariant potentials, we analyse the transmission probability $|t|^2$ as a function of the width of complex and quaternionic potentials. In figure 3, we plot the transmission probability for critical values of E. For $E > \sqrt{V^2 + |W|^2}$, the minimum value of the transmission probability oscillation decreases when the quaternionic perturbation increases.

5. Time-reversal violating (TRV) potential barrier

Let us modify the previous potential barrier by introducing a time-reversal violating space-dependent phase $\theta(x)$. We shall consider, for region III, the following cases:

REGION III_0	REGION III_0	REGION III_θ	REGION III_θ
$[V; \lvert W\rvert, 0]$	$[V; \lvert W\rvert, 0]$	$[V; \lvert W\rvert, \theta]$	$[V; \lvert W\rvert, \theta]$
REGION III_0	REGION III_θ	REGION III_θ	REGION III_0
$[V; \lvert W\rvert, 0]$	$[V; \lvert W\rvert, \theta]$	$[V; \lvert W\rvert, \theta]$	$[V; \lvert W\rvert, 0]$
REGION III_θ	REGION III_θ	REGION III_0	REGION III_0
$[V; \lvert W\rvert, \theta]$	$[V; \lvert W\rvert, \theta]$	$[V; \lvert W\rvert, 0]$	$[V; \lvert W\rvert, 0]$

$-b$ $\quad -c \quad$ 0 $\quad +c \quad$ $+b$

As remarked in the introduction, quaternionic deviations from complex quantum mechanics could be observed by considering left and right transmissions through the same quaternionic

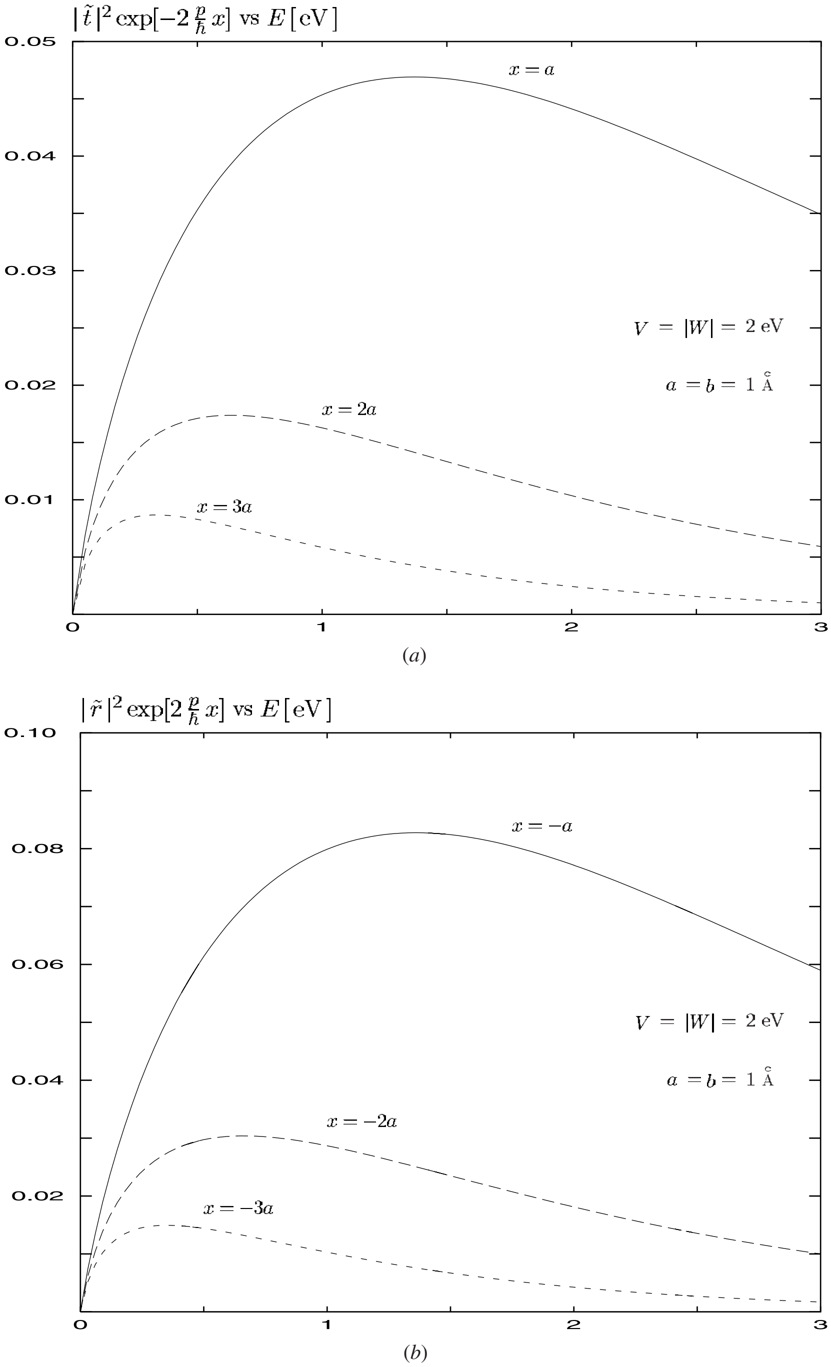


Figure 2. Additional probability of electron transmission, $|\tilde{t}|^2 \exp[-2px/\hbar]$, and reflection, $|\tilde{r}|^2 \exp[2px/\hbar]$, as a function of E (eV) for the quaternionic time-reversal invariant potential of width $a = b = 1.0$ Å and height $V = |W| = 2.0$ eV [40]. The curves show the additional probability of transmission and reflection for different values of x.

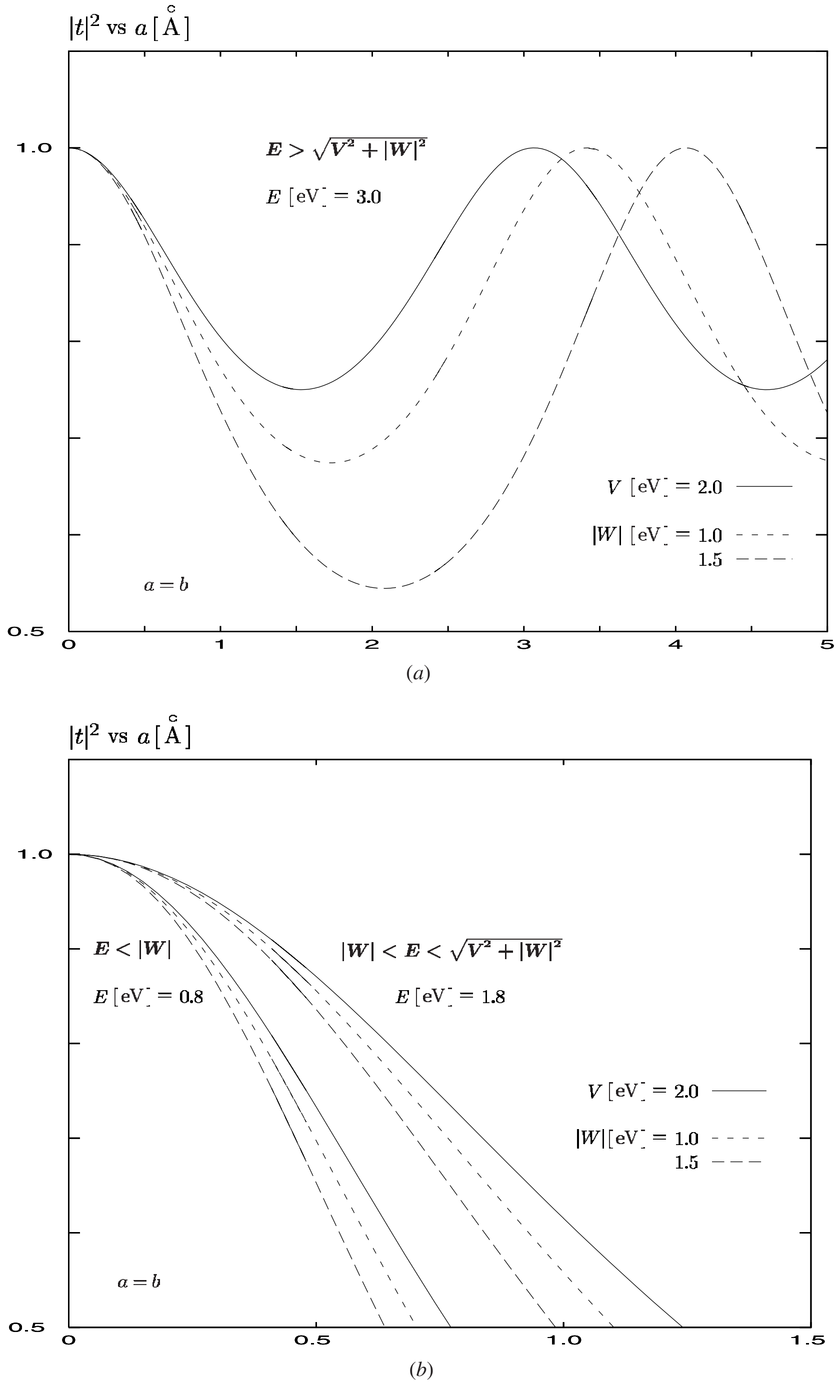
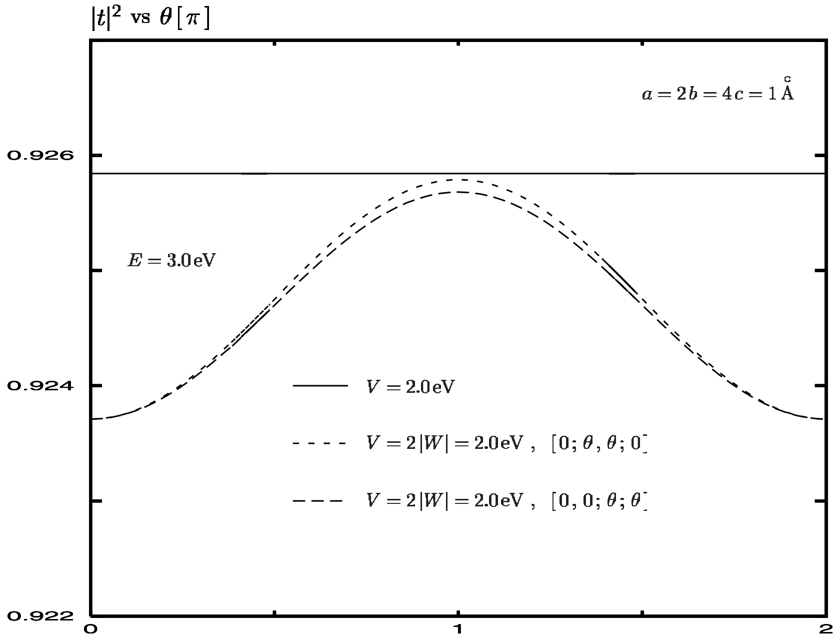


Figure 3. Electron transmission probability, $|t|^2$, as a function of a (Å) for quaternionic time-reversal invariant potentials [40]. The curves (drawn for different values of E) show the transmission probability of the complex quantum mechanics potential barrier of height V (eV) = 2.0 and of potentials of the same complex height and quaternionic height $|W|$ (eV) = 1.0 and 1.5.



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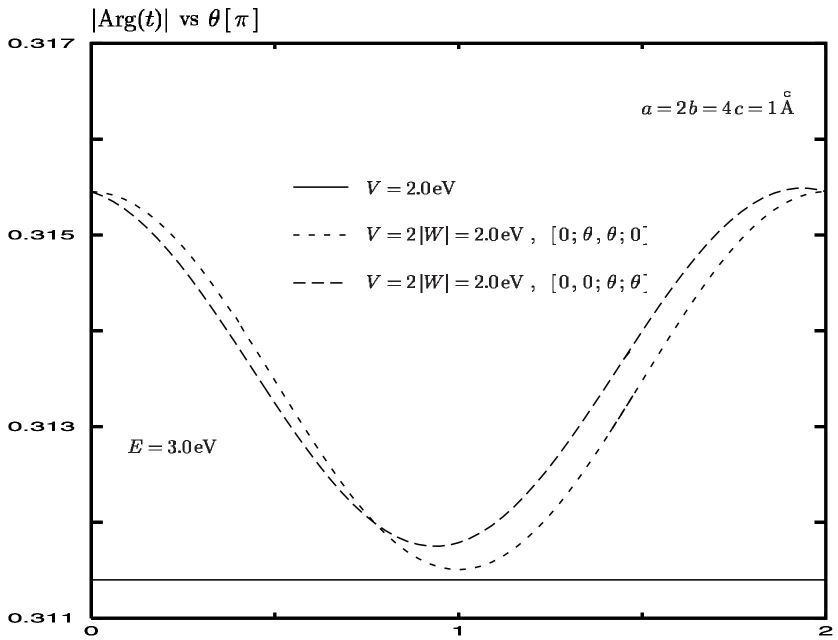

(*b*)

Figure 4. Electron transmission probability, $|t|^2$, and absolute value of the transmission coefficient argument, $|\text{Arg}(t)|$, as a function of the time-violating phase $\theta[\pi]$ for potentials of height $V = 2|W| = 2.0$ eV and width $a = 2b = 4c = 1.0$ Å [40]. The curves show that only asymmetric (time-violating) quaternionic potentials could distinguish between left and right transmissions. The value of the energy is fixed at $E = 3.0$ eV.

Table 1. Transmission probability, $|t|^2$, and transmission coefficient, t, for different values of the potential phase, θ.

$[E; V, \|W\|]$	θ	$\|t\|^2$	t
[3; 2, 0]	[0, 0; 0, 0]	0.925 842	0.915 930 − i 0.294 811
[3; 2, 1]	[0, 0; 0, 0]	0.923 710	0.913 674 − i 0.298 177
	$\left[0, 0; \frac{\pi}{6}, \frac{\pi}{6}\right]$	0.923 843	0.913 869 − i 0.297 802
[3; 2, 1]	$\left[0, \frac{\pi}{6}; \frac{\pi}{6}, 0\right]$	0.923 850	0.913 822 − i 0.297 959
	$\left[\frac{\pi}{6}, \frac{\pi}{6}; 0, 0\right]$	0.923 843	0.913 757 − i 0.298 147
	$\left[0, 0; \frac{\pi}{4}, \frac{\pi}{4}\right]$	0.924 000	0.914 057 − i 0.297 490
[3; 2, 1]	$\left[0, \frac{\pi}{4}; \frac{\pi}{4}, 0\right]$	0.924 016	0.913 998 − i 0.297 699
	$\left[\frac{\pi}{4}, \frac{\pi}{4}; 0, 0\right]$	0.924 000	0.913 898 − i 0.297 977
	$\left[0, 0; \frac{\pi}{3}, \frac{\pi}{3}\right]$	0.924 205	0.914 289 − i 0.297 122
[3; 2, 1]	$\left[0, \frac{\pi}{3}; \frac{\pi}{3}, 0\right]$	0.924 232	0.914 226 − i 0.297 360
	$\left[\frac{\pi}{3}, \frac{\pi}{3}; 0, 0\right]$	0.924 205	0.914 095 − i 0.297 718
	$\left[0, 0; \frac{\pi}{2}, \frac{\pi}{2}\right]$	0.924 699	0.914 820 − i 0.296 317
[3; 2, 1]	$\left[0, \frac{\pi}{2}; \frac{\pi}{2}, 0\right]$	0.924 753	0.914 776 − i 0.296 542
	$\left[\frac{\pi}{2}, \frac{\pi}{2}; 0, 0\right]$	0.924 699	0.914 596 − i 0.297 006
	$[0, 0; \pi, \pi]$	0.925 681	0.915 736 − i 0.295 142
[3; 2, 1]	$[0, \pi; \pi, 0]$	0.925 789	0.915 873 − i 0.294 900
	$[\pi, \pi; 0, 0]$	0.925 681	0.915 736 − i 0.295 142

$E = 3\,\text{eV}$; $V = 2|W| = 2\,\text{eV}$; $a = 2b = 4c = 1$ Å.

potential barrier. The left transmission ($x < -a$) for the quaternionic potential of height $|W|$ and phase

$$\theta(x) = \begin{cases} 0 & -b < x < 0 \\ \theta & 0 < x < b \end{cases} \tag{16}$$

is obviously equivalent to the right transmission ($x > a$) for the quaternionic potential of height $|W|$ and phase

$$\theta(x) = \begin{cases} \theta & -b < x < 0 \\ 0 & 0 < x < b \end{cases}. \tag{17}$$

By using transformation (12), we can replace the phase (17) by

$$\theta(x) = \begin{cases} 0 & -b < x < 0 \\ -\theta & 0 < x < b \end{cases}. \tag{18}$$

Thus, the plot of the transmission coefficient as a function of $\theta[\pi]$ is a valid indicator of possible deviations from complex quantum mechanics. Symmetric curves (around the point $\theta[\pi] = 1$) will imply *no* difference between left and right transmissions through the same quaternionic barrier. In figure 4, we draw the transmission probability, $|t|^2$, and the absolute value of the transmission coefficient argument, $|\text{Arg}(t)|$, as a function of the phase $\theta[\pi]$. Qualitative deviations for complex quantum mechanics appear for *asymmetric* time-violating potentials. It is also interesting to note that by increasing the phase ($\theta[\pi] \to 1$), quaternionic perturbation effects are *minimized*. For the convenience of the reader we explicitly give, see table 1, the transmission probability $|t|^2$ and the transmission coefficient t for different values of the potential phase θ and the electron energy E [38].

6. Conclusions

Difficulties in quaternionic analysis and algebra have often created (and sometimes justified) a feeling of distrust in quaternionic formulations of physical theories. Recent significant progress in quaternionic and Clifford calculus and the consequent improvement of the mathematical structures involved in the quaternionic quantum mechanics could result in a rapid development of this subject.

The usefulness of quaternions (and, more in general, Clifford algebras) to unify algebraic and geometric aspects in discussing special relativity, Maxwell and Dirac equations is universally recognized. Nevertheless, notwithstanding the substantial literature analysing quaternionic physical theories, a strong motivation forcing the use of quaternions *instead* of complex numbers is lacking. The experimental proposals of Peres [16], the theoretical analysis of Davies and McKellar [19, 21] and the detailed and systematic development of quaternionic quantum mechanics in Adler's book [15] surely represent a milestone in looking for quaternionic deviations from complex quantum mechanics.

In this paper, we have presented a complete phenomenology of the quaternionic potential barrier by discussing the time-invariant and time-violating cases. Interesting features of quaternionic perturbation effects emerge in the transmission and reflection coefficients. Various graphs show how the quantum measurement theory may be affected by changing from complex to quaternionic systems. The present work represents a preliminary step towards a significant advance in understanding quaternionic potentials and in looking for their experimental evidence. An interesting discussion about the quaternionic violations of the algebraic relationship between the six coherent cross sections of any three scatterers, taken singly and pairwise, is found in [39].

Quaternionic time-violating potentials and quaternionic perturbations (which minimize the deviations from complex quantum mechanics) could play an important role in the CP violating physics. A theoretical discussion based on the wave packet formalism will be necessary to analyse experimental tests based on kaon regeneration [16, 39]. For asymmetric potentials non-null signals of quaternionic (time violating) effects should be observed. We will try to develop the wave packet treatment in a later paper.

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Appendix. Matching conditions

A.1. TRI potential barrier

The matching conditions for the TRI potential barrier imply

$$\begin{pmatrix} 1 \\ r \\ \tilde{r} \\ \tilde{r} \end{pmatrix} = \mathcal{S}[a, b;\, E;\, V, |W|] \begin{pmatrix} t \\ t \\ \tilde{t} \\ \tilde{t} \end{pmatrix} \tag{19}$$

where

$$\mathcal{S}[a,b;\,E;\,V,|W|] = \underbrace{D_- A_-}_{\text{S[I}_-\text{]}}\,\underbrace{M^V D^V_{b-a}[M^V]^{-1}}_{\text{S[II]}}\,\underbrace{Q^{|W|}M^{V,|W|}D^{V,|W|}_{-2b}[M^{V,|W|}]^{-1}[Q^{|W|}]^{-1}}_{\text{S[III]}}$$

$$\times\,\underbrace{M^V D^V_{b-a}[M^V]^{-1}}_{\text{S[II]}}\,\underbrace{A_+ D_+}_{\text{S[I}_+\text{]}}$$

and

$$D_- = \operatorname{diag}\left\{\exp\left[\mathrm{i}\frac{p}{\hbar}a\right],\exp\left[-\mathrm{i}\frac{p}{\hbar}a\right],\exp\left[\frac{p}{\hbar}a\right],\exp\left[\frac{p}{\hbar}a\right]\right\}$$

$$A_- = \frac{1}{2}\begin{pmatrix}1 & -\mathrm{i}\frac{\hbar}{p}\\ 1 & \mathrm{i}\frac{\hbar}{p}\end{pmatrix}\oplus\begin{pmatrix}1 & 0\\ 0 & \frac{\hbar}{p}\end{pmatrix}$$

$$M^{V,|W|} = \begin{pmatrix}1 & 1\\ z_-^{E;\,V,|W|} & -z_-^{E;\,V,|W|}\end{pmatrix}\oplus\begin{pmatrix}1 & 1\\ z_+^{E;\,V,|W|} & -z_+^{E;\,V,|W|}\end{pmatrix}$$

$$M^V = M^{V,|W|\to 0}$$

$$Q^{|W|,\theta} = \begin{pmatrix}1 & [v^{E;|W|,\theta}]_{\mathbb{C}}\\ [-\mathrm{j}u^{E;|W|,\theta}]_{\mathbb{C}} & 1\end{pmatrix}\otimes\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

$$Q^{|W|} = Q^{|W|,\theta\to 0}$$

$$D^{V,|W|}_\eta = \operatorname{diag}\left\{\exp\left[z_-^{E;\,V,|W|}\eta\right],\ \exp\left[-z_-^{E;\,V,|W|}\eta\right],\ \exp\left[z_+^{E;\,V,|W|}\eta\right],\ \exp\left[-z_+^{E;\,V,|W|}\eta\right]\right\}$$

$$D^V_\eta = D^{V,|W|\to 0}_\eta$$

$$A_+ = \begin{pmatrix}1 & 0\\ 0 & \mathrm{i}\frac{p}{n}\end{pmatrix}\otimes\begin{pmatrix}1 & 0\\ 0 & -\frac{p}{n}\end{pmatrix}$$

$$D_+ = \operatorname{diag}\left\{\exp\left[\mathrm{i}\frac{p}{\hbar}a\right],\ \exp\left[\mathrm{i}\frac{p}{\hbar}a\right],\ \exp\left[-\frac{p}{\hbar}a\right],\ \exp\left[-\frac{p}{\hbar}a\right]\right\}.$$

The *complex limit* is obtained by setting $b = 0$. In this case (S[III] $= \mathbf{1}$) $\mathcal{S}[a,b;\,E;\,V,W]$ reduces to

$$\mathcal{S}[a;\,E;\,V] = D_- A_- M^V D^V_{-2a}[M^V]^{-1}A_+ D_+.$$

By matrix algebra, we easily calculate the coefficients for reflection and transmission

$$t = \exp\left[-2\mathrm{i}\frac{p}{\hbar}a\right]\left\{\cosh[2z_-^{E;\,V}a] + \frac{\mathrm{i}}{2}\chi_-\sinh[2z_-^{E;\,V}a]\right\}^{-1}$$

$$r = -\frac{\mathrm{i}}{2}\chi_+\sinh[2z_-^{E;\,V}a]t$$

$$\tilde{t} = 0$$

$$\tilde{r} = 0$$

where $\chi_\pm = \frac{\hbar}{p}z_-^{E;\,V} \pm \left(\frac{\hbar}{p}z_-^{E;\,V}\right)^{-1}$.

A.2. TRV potential barrier

The matrix $\mathcal{S}[a,b,c;\,E;\,V,|W|,\theta]$ is now expressed in terms of

$$\text{S[III]} = \begin{cases}\text{S[III}_{00\theta\theta}\text{]} : S[0,-b]\times S[\theta,-b]\\ \text{S[III}_{0\theta\theta 0}\text{]} : S[0,c-b]\times S[\theta,-2c]\times S[0,c-b]\\ \text{S[III}_{\theta\theta 00}\text{]} : S[\theta,-b]\times S[0,-b]\end{cases}$$

where

$$S[\theta,\eta] = Q^{|W|,\theta}M^{V,|W|}D^{V,|W|}_\eta\left[M^{V,|W|}\right]^{-1}\left[Q^{|W|,\theta}\right]^{-1}.$$

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