

# QUATERNIONIC POTENTIALS IN NON-RELATIVISTIC QUANTUM MECHANICS

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*June 21, 2002*

**Abstract.** We discuss the Schrödinger equation in 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.

**PACS.** 03.65.-w – 03.65.Ca – 03.65.Ta – 02.30.Jr – 02.30.Tb

## I. INTRODUCTION

After the classical mathematical and physical works on foundations of quaternionic quantum mechanics [1–4], there has been, in recent years, a widely interest in formulating quantum theories by using the non commutative ring of quaternions [5–12]. Some of the main results coming out from the use of *new* algebraic structures in particle physics are reviewed in the books of Dixon [13] and Gürsey [14]. For a detailed discussion of quaternionic quantum mechanics and field theory we quote 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 physical problem is due to the fact that, in general, the standard mathematical methods of resolution break down. In the last years, some of these problems have been overcome. In particular, the discussion of quaternionic eigenvalue equations [22] and differential operators [23] is *now* recognized 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 to understand 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 crystal made of three different atoms, in neutron interferometry and in meson regeneration. In 1984, the neutron interferometric experiment was realized by Kaiser, George and Werner [17]. The neutron wave function traversing slabs of two dissimilar materials (titanium and aluminum) should experience the 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  $3 \times 10^4$ . 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 differently from 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, George and Werner. To reconcile the theoretical predictions with the experimental observations, Davies and McKellar reiterated the Klein conclusion and suggested to subject 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 Kayser 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 detect time reversal violation, which so far has not been detectable in neutron-optical experiments.

In this paper, after a brief introductory discussion of quaternionic 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.

## II. QUATERNIONIC SCHRÖDINGER EQUATION

In the standard formulation of non-relativistic quantum mechanics, the complex wave function  $\varphi(\mathbf{r}, t)$ , describing a particle without spin subjected to the influence of a real potential  $V(\mathbf{r}, t)$ , satisfies the Schrödinger equation

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

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

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

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

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

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 wave function  $\Phi(\mathbf{r}, t)$  satisfies the following equation

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

Exactly as in the case of the standard quantum mechanics, we can define a current density

$$\mathbf{J} = \frac{\hbar}{2m} \left[ (\nabla \bar{\Phi}) i \Phi - \bar{\Phi} i \nabla \Phi \right]$$

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 obtain the continuity equation

$$\partial_t \rho + \nabla \cdot \mathbf{J} = 0 . \quad (3)$$

## A. STATIONARY STATES

The quaternionic Schrödinger equation in presence of time-independent potentials

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

reads

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

The quaternionic stationary state wave function

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

is solution of Eq. (4) on the condition that  $\Psi(\mathbf{r})$  be solution of the time-independent Schrödinger equation

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

Eq. (5) represents a right complex eigenvalue equation on the quaternionic field [22]

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

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

$$\Phi(\mathbf{r}, t) = \sum_E \Psi(\mathbf{r}) \exp\left[-\frac{i}{\hbar} E t\right] q_E , \quad (6)$$

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

## B. TIME REVERSAL INVARIANCE

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

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

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.

$$W(\mathbf{r}) = |W(\mathbf{r})| \exp[i\theta] ,$$

is time reversal invariant. For these potential,

$$\Phi_{\text{T}}(\mathbf{r}, -t) = u \Phi(\mathbf{r}, t) \bar{u} , \quad u = k \exp[i\theta] . \quad (8)$$

For complex wave functions, we recover the standard result  $\Phi_{\text{T}}(\mathbf{r}, -t) = \Phi^*(\mathbf{r}, t)$ .

### C. ONE-DIMENSIONAL SQUARE POTENTIALS

In solving the quaternionic Schrödinger equation, a great mathematical simplification results from the assumption that the wave function and the potential energy depend only on the  $x$ -coordinate,

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

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]

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

where  $c_1, \dots, c_4$  are complex coefficients determined by the boundary conditions,

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

and

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

In the free potential region, the solution reduces to

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

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

$$\Psi_-(x) = \exp[i \frac{p}{\hbar} x] + r \exp[-i \frac{p}{\hbar} x] + j \tilde{r} \exp[\frac{p}{\hbar} x] , \quad (11)$$

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

### III. TIME REVERSAL INVARIANT (TRI) POTENTIAL BARRIER

Let us consider the TRI potential

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

In Eq. (9), the space-independent phase  $\theta$  can be removed by taking the transformation

$$\Psi(x) \rightarrow \exp [i \frac{\theta}{2}] \Psi(x) \exp [-i \frac{\theta}{2}] . \quad (12)$$

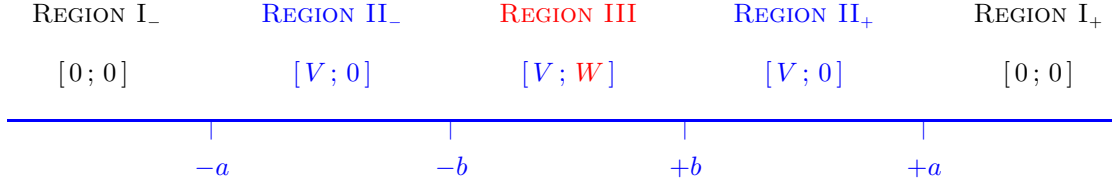
Under this transformation

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

Reflection and transmission probabilities do *not* change (actually the exponential  $\exp[-i\theta]$  can be absorbed in the complex coefficients  $c_{3,4}$ ). So, without loss of generality, we can discuss the quaternionic Schrödinger equation in 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 Eq. (11), and for  $x > a$ , where the solution is

$$\Psi_+(x) = t \exp[i \frac{p}{\hbar} x] + j \tilde{t} \exp[-\frac{p}{\hbar} x]. \quad (13)$$

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

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

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

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

$$|r|^2 + |t|^2 = 1. \quad (14)$$

In Figs.1 and 2, we plot the transmission probability  $|t|^2$  as a function of  $E[\text{eV}]$  for quaternionic potentials of different widths and heights (we assume that the incident particle is an electron). The presence of a quaternionic perturbation 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. Fig.2 shows the transmission probability for the quaternionic potential

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

and the complex *comparative* barrier [19]

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

The wave numbers for these potentials are

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

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

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

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

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

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

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

The complex operators

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

and

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

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

Deviations from (complex) quantum mechanics appear in 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  $E[\text{eV}]$  is drawn in Fig. 3 for different values of  $x$ .

To conclude the discussion of quaternionic one-dimensional time invariant potentials, we analyze the transmission probability  $|t|^2$  as a function of the width of complex and quaternionic potentials. In Fig. 4, 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. In Fig. 5, we compare complex and *pure* quaternionic potentials covering the same area,  $aV = b|W|$ . Clear deviations from complex quantum mechanics appear.

#### IV. 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 the region III, the following cases:

|                         |                         |                         |                         |
|-------------------------|-------------------------|-------------------------|-------------------------|
| REGION III <sub>0</sub> | REGION III <sub>0</sub> | REGION III <sub>θ</sub> | REGION III <sub>θ</sub> |
| [V;  W , 0]             | [V;  W , 0]             | [V;  W , θ]             | [V;  W , θ]             |
| REGION III <sub>θ</sub> | REGION III <sub>θ</sub> | REGION III <sub>θ</sub> | REGION III <sub>0</sub> |
| [V;  W , 0]             | [V;  W , θ]             | [V;  W , θ]             | [V;  W , 0]             |
| REGION III <sub>θ</sub> | REGION III <sub>θ</sub> | REGION III <sub>0</sub> | REGION III <sub>0</sub> |
| [V;  W , θ]             | [V;  W , θ]             | [V;  W , 0]             | [V;  W , 0]             |
| -b                      | -c                      | 0                       | +c                      |
|                         |                         |                         | +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 potential barrier. The left transmission ( $x < -a$ ) for the quaternionic potential of height  $|W|$  and phase

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

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

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

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

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

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  $\theta[\pi] = 1$ ) shall imply *no* difference between left and right transmission through the same quaternionic barrier. In Figs. 6, 7 and 8, we draw the transmission probability,  $|t|^2$ , and the absolute value of the transmission coefficient,  $|Arg(t)|$ , 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 ( $\theta[\pi] \rightarrow 1$ ), quaternionic perturbation effects are *minimized*. For the convenience of the reader we explicitly give (see Tables 1, 2 and 3) the transmission probability  $|t|^2$  and the transmission coefficient  $t$  for different values of the potential phase  $\theta$  and the electron energy  $E$ .

## VI. CONCLUSIONS

Very little progress in mathematical understanding of quaternionic analysis and algebra have often created (and sometimes justified) a distrust feeling to quaternionic formulations of physical theories. From our point of view, the recent increasing improvement of the mathematical structures involved in the quaternionic quantum mechanics could result in a rapid progress in 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 analyzing 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 the Adler's book [15] surely represent the 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 case. Interesting features of quaternionic perturbation effects emerge in the transmission and reflection coefficients. The 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 quaternionic violations of the algebraic relationship between the six coherent cross sections of any three scatterers, taken singly and pairwise, is found in [24].

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 [16,24]. For asymmetric potentials a non null signals of quaternionic (time violating) effects should be observed. We will try to develop the wave packet treatment in a later article.

## Acknowledgements

This work was started during the stay of S. D.Ł and G.Ć. D. at the Department of Physics, University of Lecce. The authors acknowledge INFN, CAPES and FAEP for financial support and are grateful to S. Marchiafava and P. Rotelli for helpful comments and suggestions.

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## APPENDIX. MACTHING CONDITIONS

### A. TRI POTENTIAL BARRIER

The matching conditions for the TRI potential barrier imply

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

where

$$\begin{aligned} \mathcal{S}[a, b; E; V, |W|] &= \underbrace{D_- A_-}_{\text{S[I]}} \underbrace{M^V D_{b-a}^V [M^V]^{-1}}_{\text{S[II]}} \times \\ &\quad \underbrace{Q^{|W|} M^{V,|W|} D_{-2b}^{V,|W|} [M^{V,|W|}]^{-1} [Q^{|W|}]^{-1}}_{\text{S[III]}} \times \\ &\quad \underbrace{M^V D_{b-a}^V [M^V]^{-1}}_{\text{S[II]}} \underbrace{A_+ D_+}_{\text{S[I+]}} \end{aligned}$$

and

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

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

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

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

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

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

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

$$D_\eta^V = D_\eta^{V,|W| \rightarrow 0},$$

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

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

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

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

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

$$\begin{aligned} t &= \exp \left[ -2 i \frac{p}{\hbar} a \right] \left\{ \cosh \left[ 2 z_-^{E;V} a \right] + \frac{i}{2} \chi_- \sinh \left[ 2 z_-^{E;V} a \right] \right\}^{-1}, \\ r &= -\frac{i}{2} \chi_+ \sinh \left[ 2 z_-^{E;V} a \right] t \\ \tilde{t} &= 0, \\ \tilde{r} &= 0, \end{aligned}$$

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

## B. TRV POTENTIAL BARRIER

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

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

where

$$\mathcal{S}[\theta, \eta] = Q^{|W|, \theta} M^{V, |W|} D_{\eta}^{V, |W|} [M^{V, |W|}]^{-1} [Q^{|W|, \theta}]^{-1} .$$

Table 1 [Fig. 6]

$$E = 0.5 \text{ eV}; \quad V = 2|W| = 2 \text{ eV}; \quad a = 2b = 4c = 1 \text{ \AA}$$

| $[E; V,  W ]$ | $\theta$                               | $ t ^2$  | $t$                    |
|---------------|--|----------|------------------------|
| $[0.5; 2, 0]$ | $[0, 0; 0, 0]$                         | 0.62596  | $0.618647 - i0.493189$ |
| $[0.5; 2, 1]$ | $[0, 0; 0, 0]$                         | 0.612889 | $0.605527 - i0.496212$ |
| $[0.5; 2, 1]$ | $[0, 0; \frac{\pi}{6}, \frac{\pi}{6}]$ | 0.613720 | $0.606559 - i0.495789$ |
|               | $[0, \frac{\pi}{6}; \frac{\pi}{6}, 0]$ | 0.613748 | $0.606389 - i0.496025$ |
|               | $[\frac{\pi}{6}, \frac{\pi}{6}; 0, 0]$ | 0.613720 | $0.606159 - i0.496278$ |
| $[0.5; 2, 1]$ | $[0, 0; \frac{\pi}{4}, \frac{\pi}{4}]$ | 0.614708 | $0.60763 - i0.495473$  |
|               | $[0, \frac{\pi}{4}; \frac{\pi}{4}, 0]$ | 0.614769 | $0.607413 - i0.495800$ |
|               | $[\frac{\pi}{4}, \frac{\pi}{4}; 0, 0]$ | 0.614708 | $0.607065 - i0.496165$ |
| $[0.5; 2, 1]$ | $[0, 0; \frac{\pi}{3}, \frac{\pi}{3}]$ | 0.615996 | $0.608983 - i0.495113$ |
|               | $[0, \frac{\pi}{3}; \frac{\pi}{3}, 0]$ | 0.616100 | $0.608749 - i0.495504$ |
|               | $[\frac{\pi}{3}, \frac{\pi}{3}; 0, 0]$ | 0.615996 | $0.608291 - i0.495962$ |
| $[0.5; 2, 1]$ | $[0, 0; \frac{\pi}{2}, \frac{\pi}{2}]$ | 0.619112 | $0.612155 - i0.494347$ |
|               | $[0, \frac{\pi}{2}; \frac{\pi}{2}, 0]$ | 0.619321 | $0.611982 - i0.494772$ |
|               | $[\frac{\pi}{2}, \frac{\pi}{2}; 0, 0]$ | 0.619112 | $0.611358 - i0.495332$ |
| $[0.5; 2, 1]$ | $[0, 0; \pi, \pi]$                     | 0.625369 | $0.618021 - i0.493376$ |
|               | $[0, \pi; \pi, 0]$                     | 0.625792 | $0.618478 - i0.493232$ |
|               | $[\pi, \pi; 0, 0]$                     | 0.625369 | $0.618021 - i0.493376$ |

Table 2 [Fig. 7]

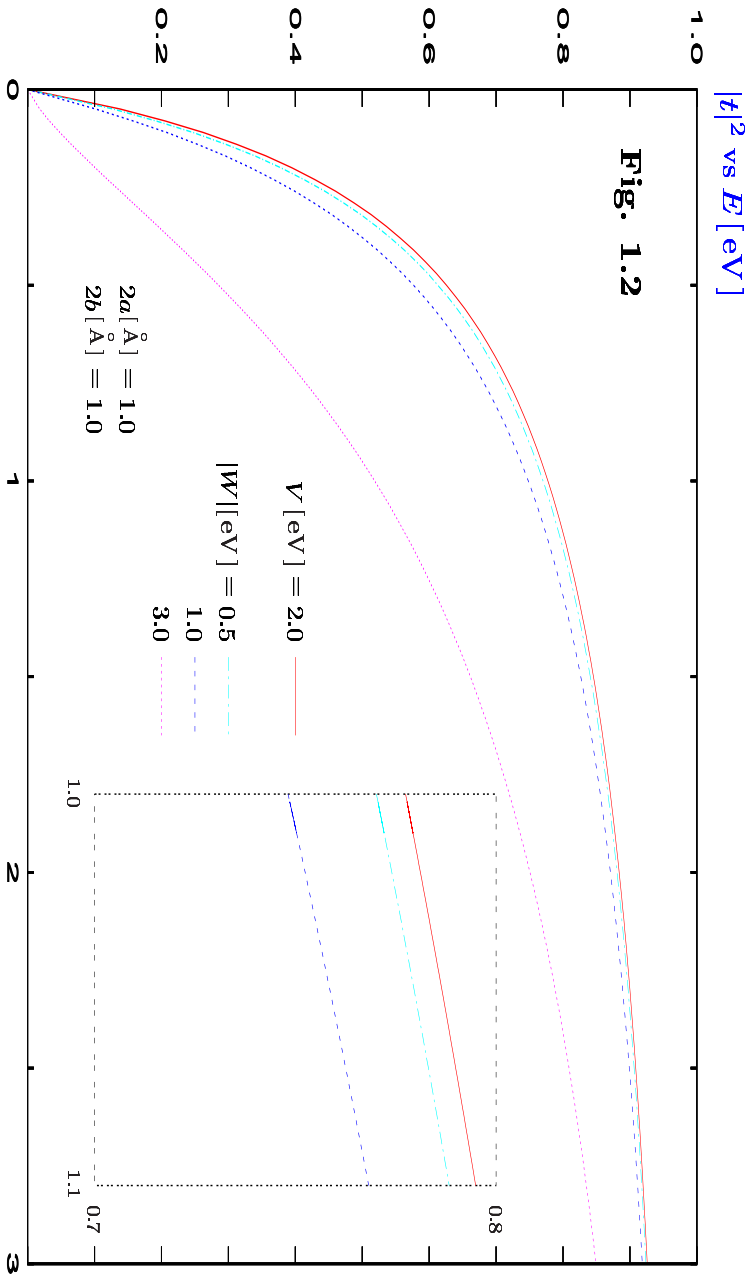
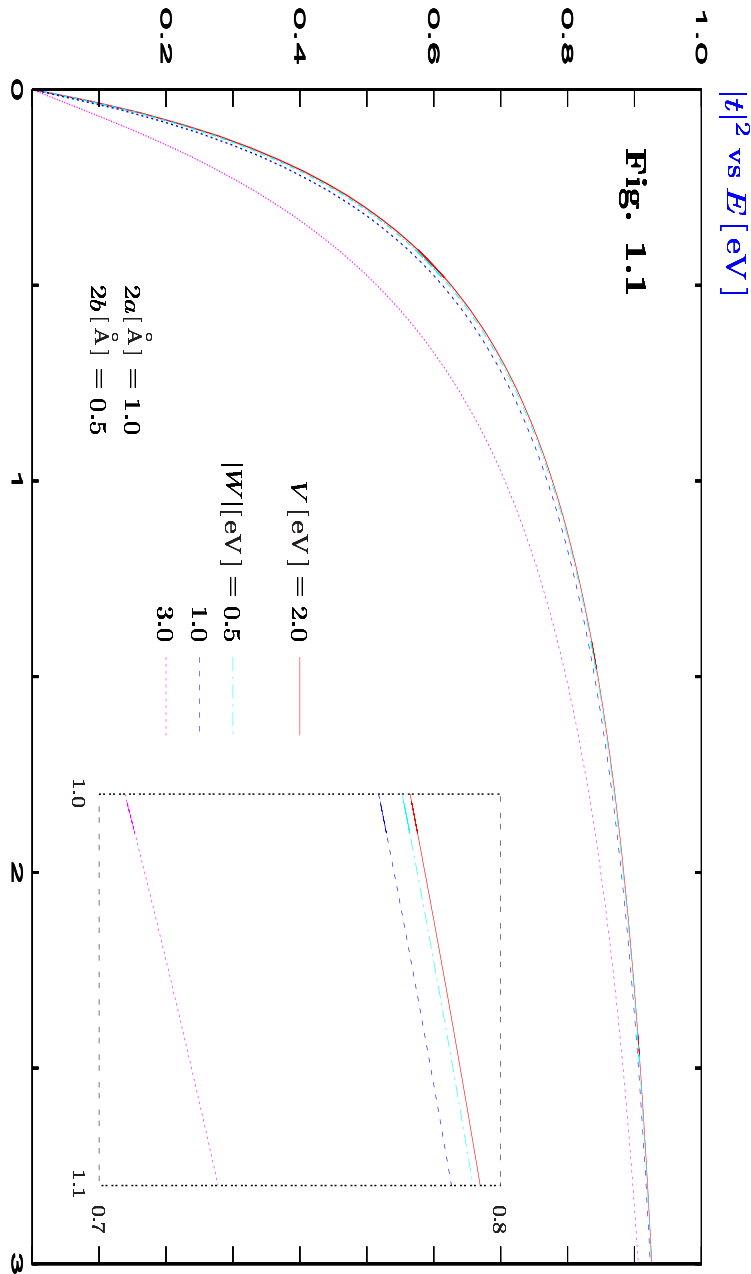
$$E = 1.5 \text{ eV}; \quad V = 2|W| = 2 \text{ eV}; \quad a = 2b = 4c = 1 \text{ \AA}$$

| $[E; V,  W ]$ | $\theta$                               | $ t ^2$  | $t$                     |
|---------------|--|----------|-------------------------|
| $[1.5; 2, 0]$ | $[0, 0; 0, 0]$                         | 0.845474 | $0.835936 - i 0.382994$ |
| $[1.5; 2, 1]$ | $[0, 0; 0, 0]$                         | 0.840310 | $0.830647 - i 0.387733$ |
| $[1.5; 2, 1]$ | $[0, 0; \frac{\pi}{6}, \frac{\pi}{6}]$ | 0.840637 | $0.831080 - i 0.387223$ |
|               | $[0, \frac{\pi}{6}; \frac{\pi}{6}, 0]$ | 0.840651 | $0.830996 - i 0.387424$ |
|               | $[\frac{\pi}{6}, \frac{\pi}{6}; 0, 0]$ | 0.840637 | $0.830877 - i 0.387660$ |
| $[1.5; 2, 1]$ | $[0, 0; \frac{\pi}{4}, \frac{\pi}{4}]$ | 0.841023 | $0.831516 - i 0.386787$ |
|               | $[0, \frac{\pi}{4}; \frac{\pi}{4}, 0]$ | 0.841055 | $0.831409 - i 0.387058$ |
|               | $[\frac{\pi}{4}, \frac{\pi}{4}; 0, 0]$ | 0.841023 | $0.831228 - i 0.387406$ |
| $[1.5; 2, 1]$ | $[0, 0; \frac{\pi}{3}, \frac{\pi}{3}]$ | 0.841526 | $0.832061 - i 0.386266$ |
|               | $[0, \frac{\pi}{3}; \frac{\pi}{3}, 0]$ | 0.841581 | $0.831948 - i 0.386580$ |
|               | $[\frac{\pi}{3}, \frac{\pi}{3}; 0, 0]$ | 0.841526 | $0.831708 - i 0.387024$ |
| $[1.5; 2, 1]$ | $[0, 0; \frac{\pi}{2}, \frac{\pi}{2}]$ | 0.842740 | $0.833323 - i 0.385115$ |
|               | $[0, \frac{\pi}{2}; \frac{\pi}{2}, 0]$ | 0.842850 | $0.833247 - i 0.385421$ |
|               | $[\frac{\pi}{2}, \frac{\pi}{2}; 0, 0]$ | 0.842740 | $0.832917 - i 0.385991$ |
| $[1.5; 2, 1]$ | $[0, 0; \pi, \pi]$                     | 0.845158 | $0.835583 - i 0.383353$ |
|               | $[0, \pi; \pi, 0]$                     | 0.845378 | $0.835836 - i 0.383087$ |
|               | $[\pi, \pi; 0, 0]$                     | 0.845158 | $0.835583 - i 0.383353$ |

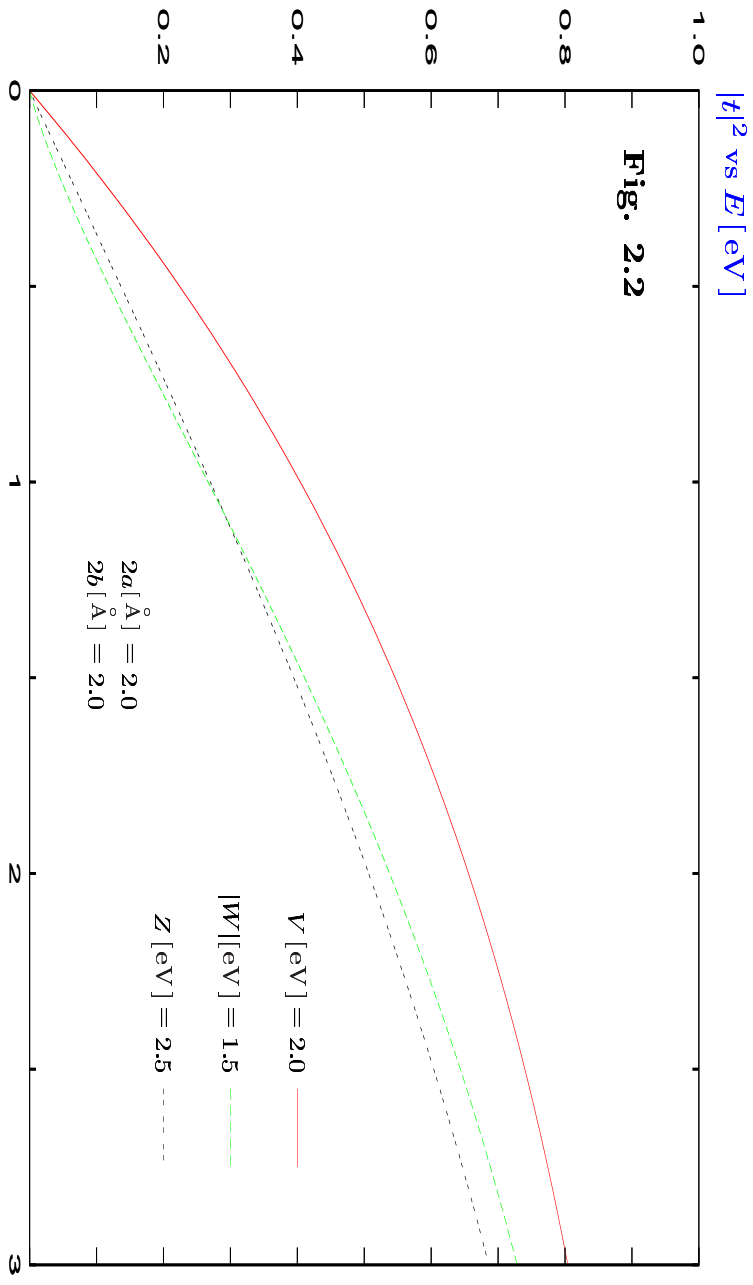
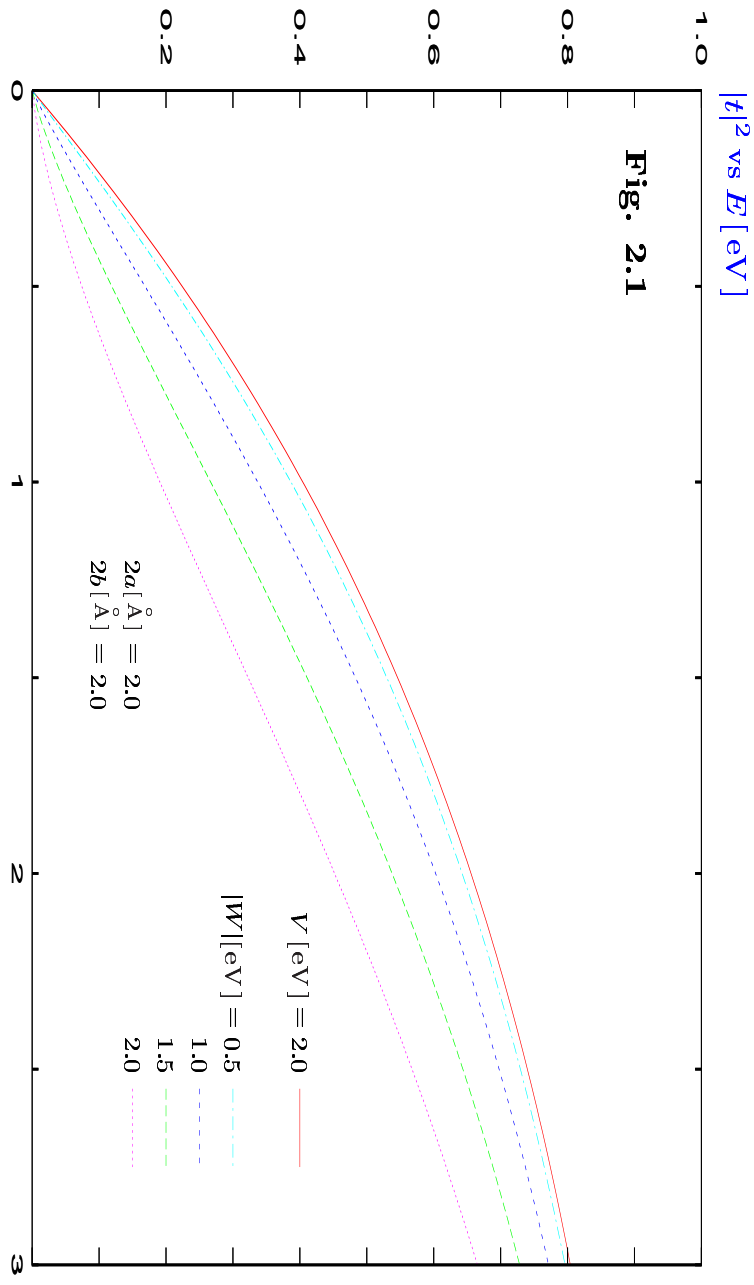
**Table 3 [Fig.8]**

$$E = 3 \text{ eV} ; \quad V = 2|W| = 2 \text{ eV} ; \quad a = 2b = 4c = 1 \text{ \AA}$$

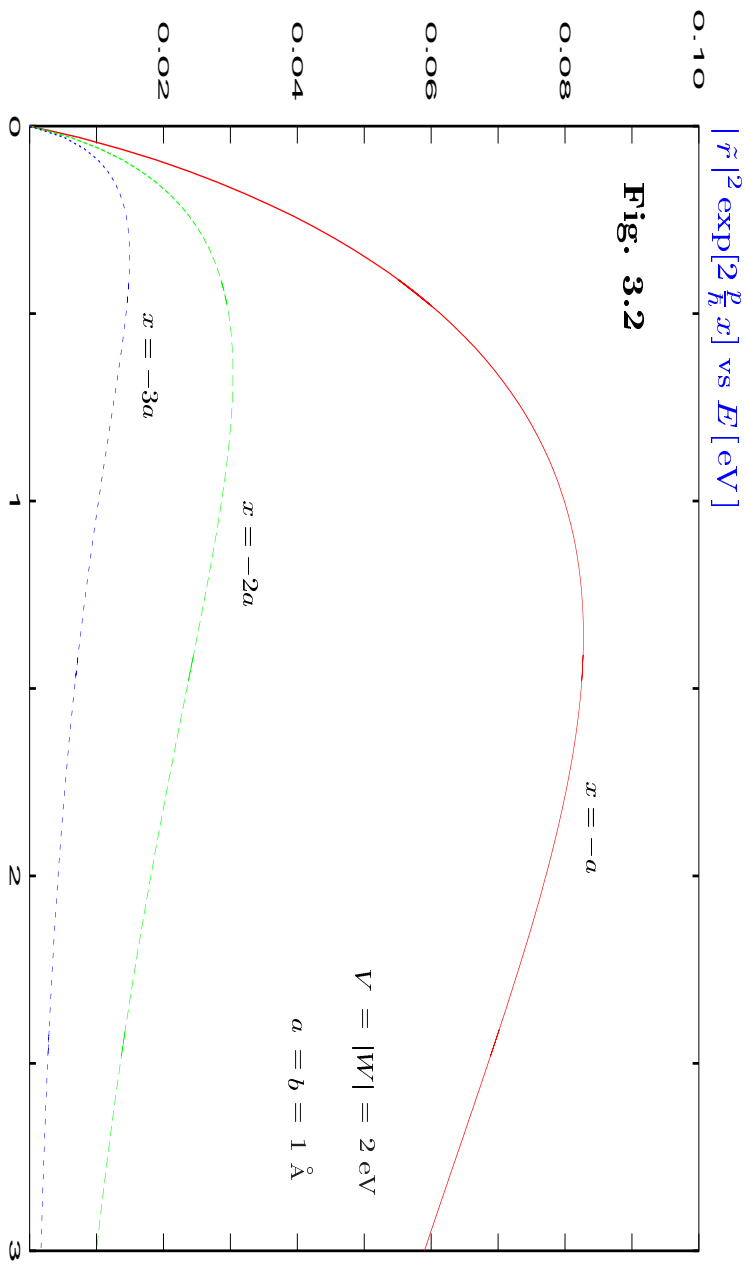
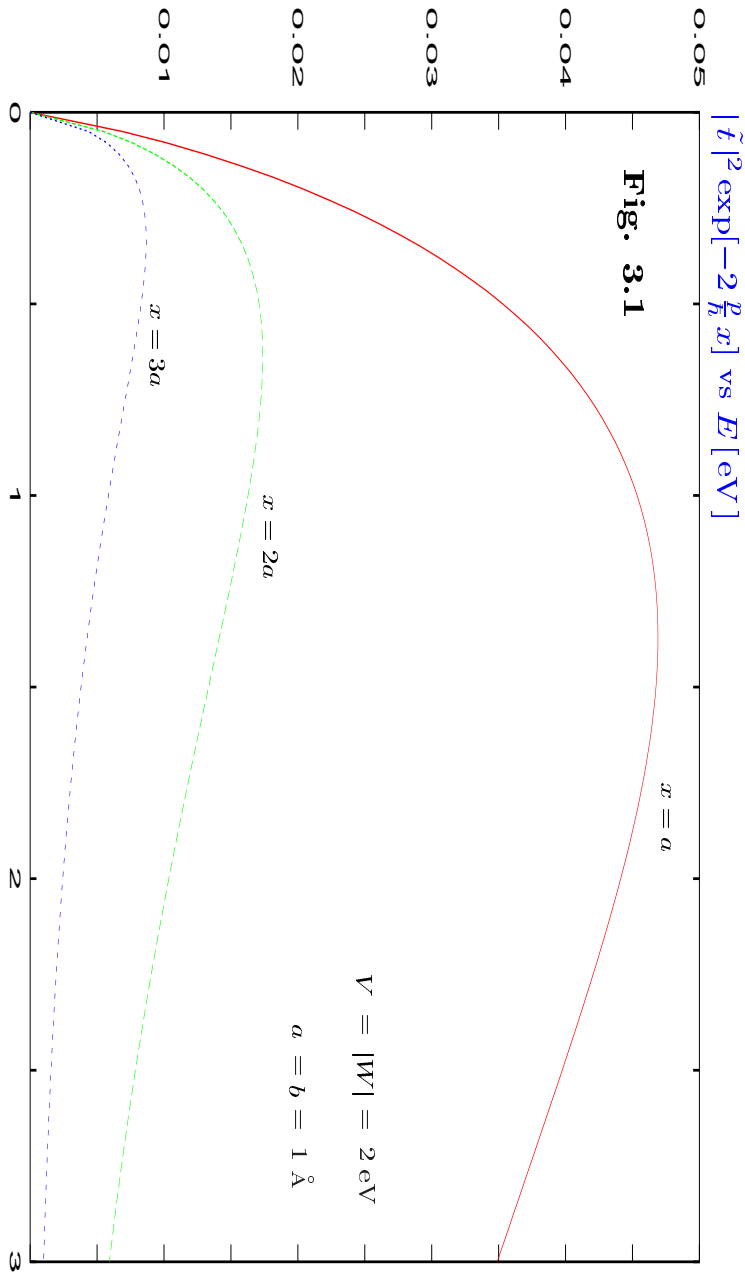
| $[E; V,  W ]$ | $\theta$                               | $ t ^2$  | $t$                    |
|---------------|--|----------|------------------------|
| $[3; 2, 0]$   | $[0, 0; 0, 0]$                         | 0.925842 | $0.915930 - i0.294811$ |
| $[3; 2, 1]$   | $[0, 0; 0, 0]$                         | 0.923710 | $0.913674 - i0.298177$ |
| $[3; 2, 1]$   | $[0, 0; \frac{\pi}{6}, \frac{\pi}{6}]$ | 0.923843 | $0.913869 - i0.297802$ |
|               | $[0, \frac{\pi}{6}; \frac{\pi}{6}, 0]$ | 0.923850 | $0.913822 - i0.297959$ |
|               | $[\frac{\pi}{6}, \frac{\pi}{6}; 0, 0]$ | 0.923843 | $0.913757 - i0.298147$ |
| $[3; 2, 1]$   | $[0, 0; \frac{\pi}{4}, \frac{\pi}{4}]$ | 0.924000 | $0.914057 - i0.297490$ |
|               | $[0, \frac{\pi}{4}; \frac{\pi}{4}, 0]$ | 0.924016 | $0.913998 - i0.297699$ |
|               | $[\frac{\pi}{4}, \frac{\pi}{4}; 0, 0]$ | 0.924000 | $0.913898 - i0.297977$ |
| $[3; 2, 1]$   | $[0, 0; \frac{\pi}{3}, \frac{\pi}{3}]$ | 0.924205 | $0.914289 - i0.297122$ |
|               | $[0, \frac{\pi}{3}; \frac{\pi}{3}, 0]$ | 0.924232 | $0.914226 - i0.297360$ |
|               | $[\frac{\pi}{3}, \frac{\pi}{3}; 0, 0]$ | 0.924205 | $0.914095 - i0.297718$ |
| $[3; 2, 1]$   | $[0, 0; \frac{\pi}{2}, \frac{\pi}{2}]$ | 0.924699 | $0.914820 - i0.296317$ |
|               | $[0, \frac{\pi}{2}; \frac{\pi}{2}, 0]$ | 0.924753 | $0.914776 - i0.296542$ |
|               | $[\frac{\pi}{2}, \frac{\pi}{2}; 0, 0]$ | 0.924699 | $0.914596 - i0.297006$ |
| $[3; 2, 1]$   | $[0, 0; \pi, \pi]$                     | 0.925681 | $0.915736 - i0.295142$ |
|               | $[0, \pi; \pi, 0]$                     | 0.925789 | $0.915873 - i0.294900$ |
|               | $[\pi, \pi; 0, 0]$                     | 0.925681 | $0.915736 - i0.295142$ |



**Fig. 1.** Electron transmission probability,  $|t|^2$ , as a function of  $E$ [eV] for quaternionic time reversal invariant potentials [25]. The full line indicates the complex quantum mechanics result for the potential barrier of width  $2a$ [Å]= 1.0 and height  $V$ [eV]= 2.0. The dashed lines (drawn for different values of the width  $2b$  and the height  $|W|$  of the potential  $jW$ ) show the quaternionic perturbation effects.

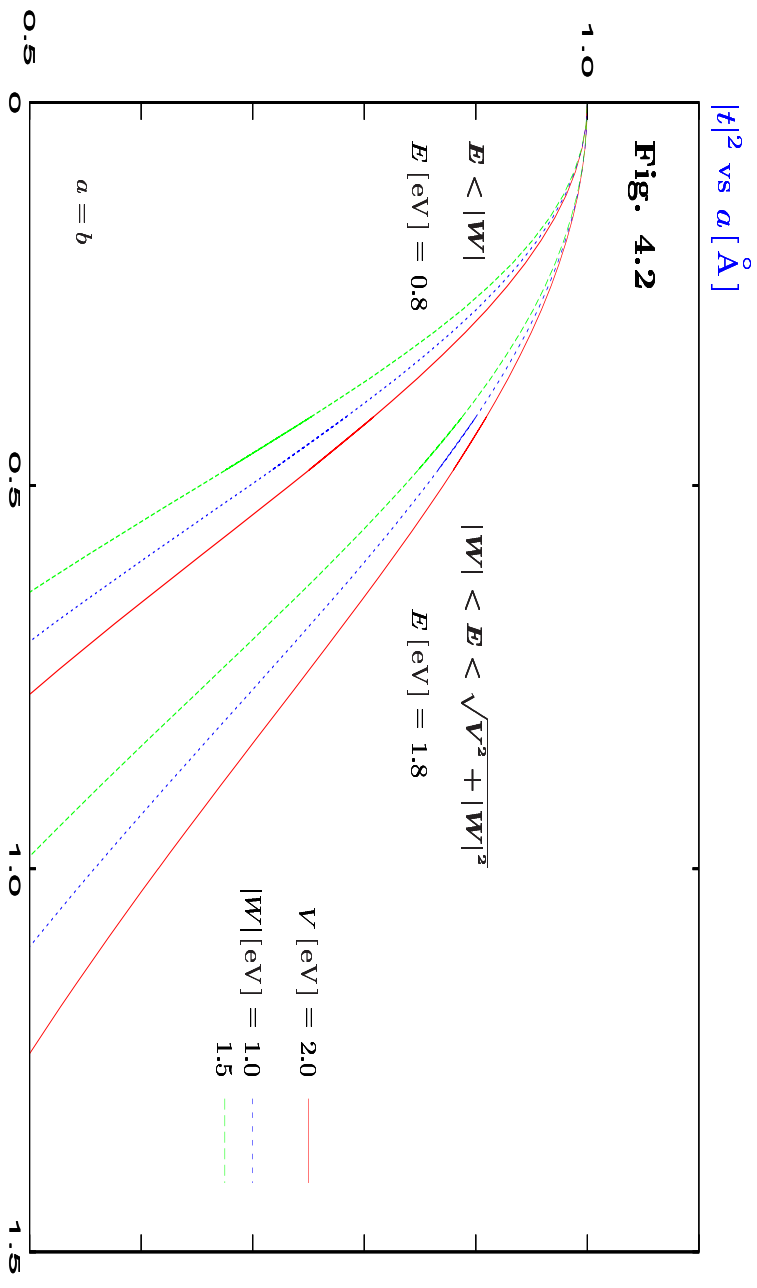
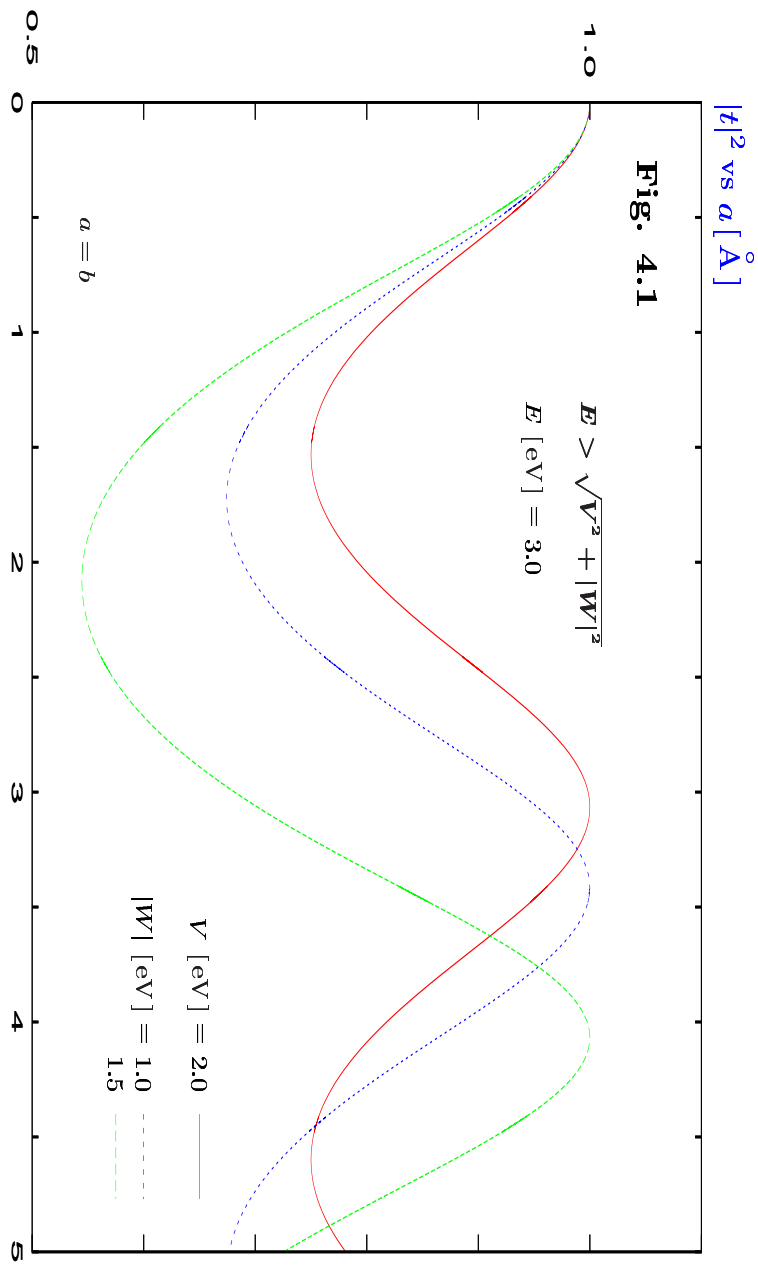


**Fig. 2.** Electron transmission probability,  $|t|^2$ , as a function of  $E$ [eV] for quaternionic time reversal invariant potentials [25]. The full line indicates the complex quantum mechanics result for the potential barrier of width  $a[\text{\AA}]=1.0$  and height  $V[\text{eV}]=2.0$ . The dashed lines (drawn for a fixed width  $b[\text{\AA}]=1.0$  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  $Z = \sqrt{V^2 + |W|^2}$ .

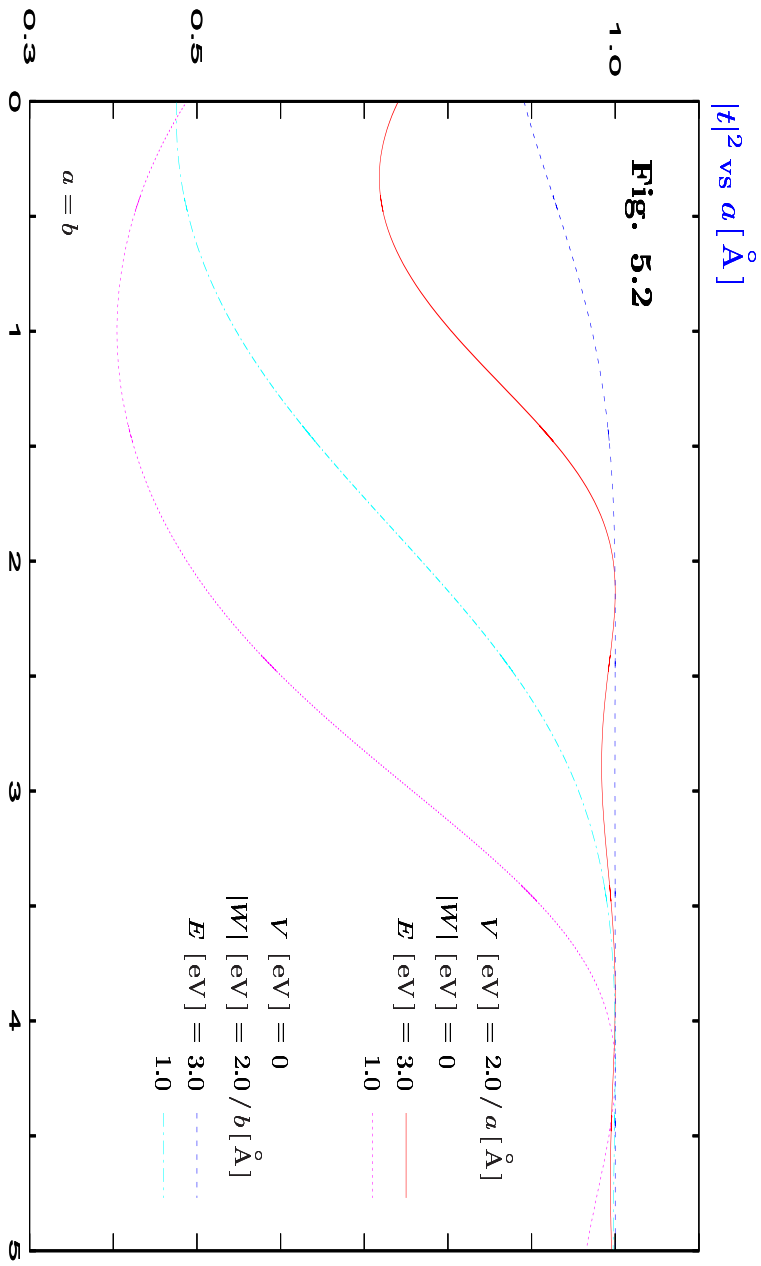
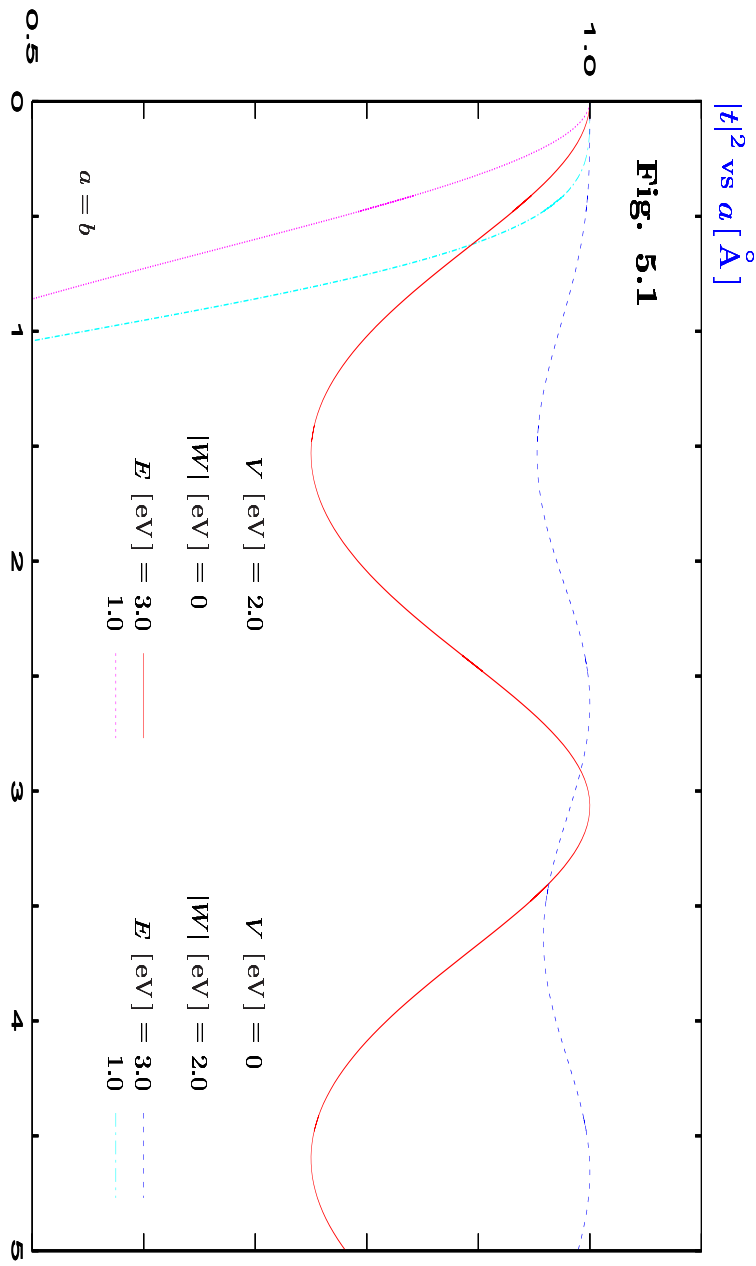


**Fig. 3.** Additional probability of electron transmission,  $|\tilde{t}|^2 \exp[-2px/\hbar]$ , and reflection,  $|\tilde{r}|^2 \exp[2px/\hbar]$ , as a function of  $E[\text{eV}]$  for the quaternionic time reversal invariant potential of width  $a = b = 1.0 \text{ \AA}$  and height  $V = |W| = 2.0 \text{ eV}$  [25]. The curves show the additional probability of transmission and reflection for different values of  $x$ .

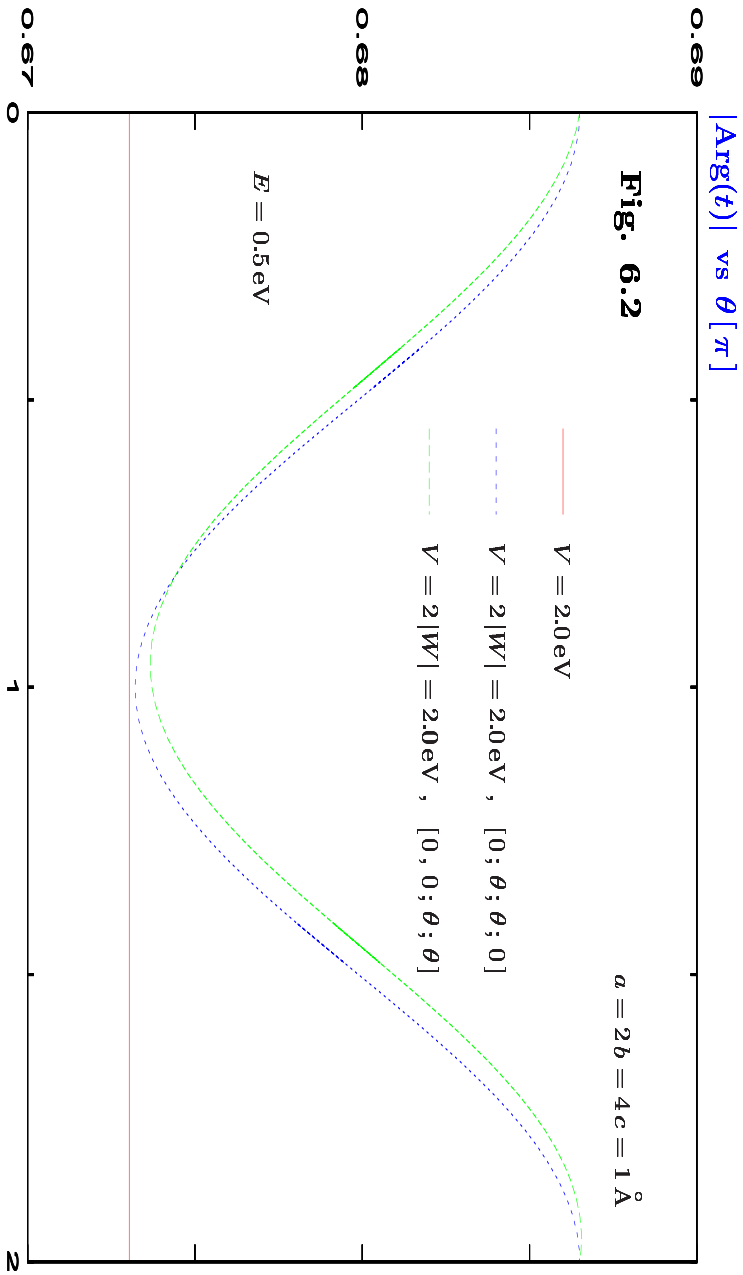
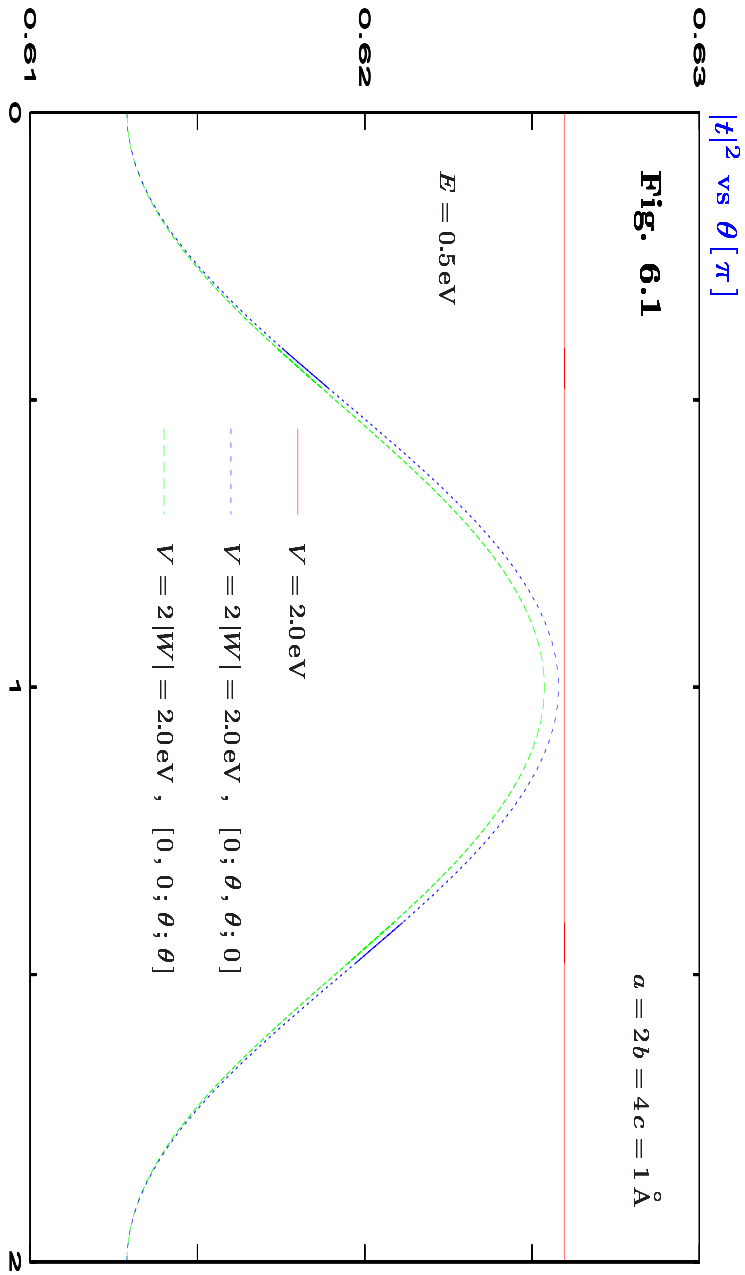




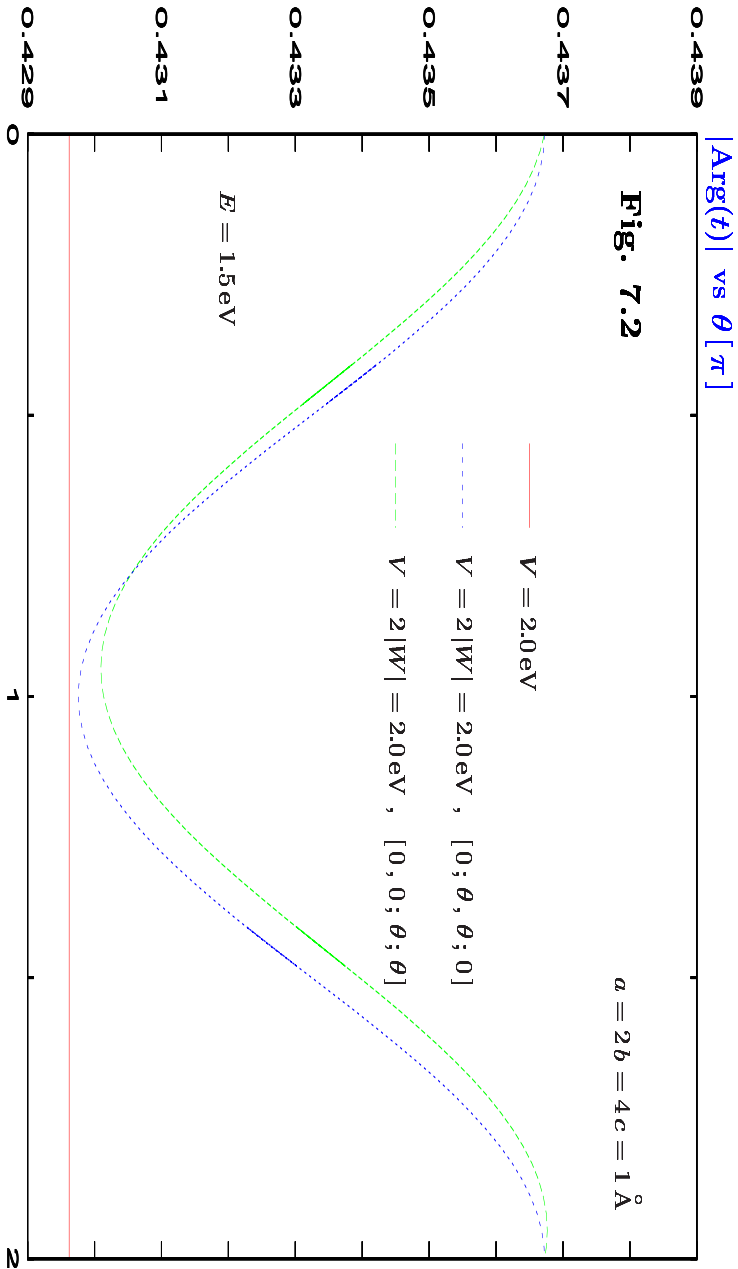
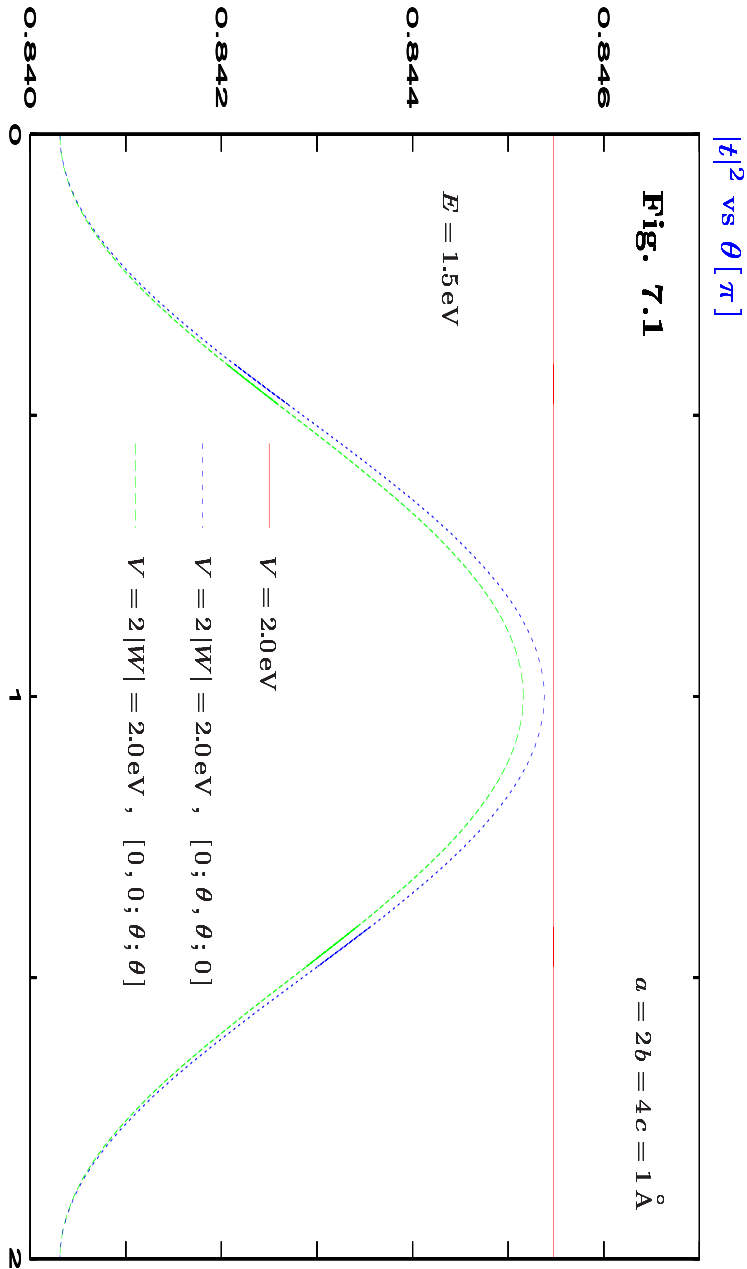
**Fig. 4.** Electron transmission probability,  $|f|^2$ , as a function of  $a[a]$  for quaternionic time reversal invariant potentials [25]. The curves (drawn for different values of  $E$ ) show the transmission probability for the complex quantum mechanics potential barrier of height  $V[\text{eV}] = 2.0$  and for potentials of the same complex height and quaternionic height  $|W|[\text{eV}] = 1.0$  and  $1.5$ .



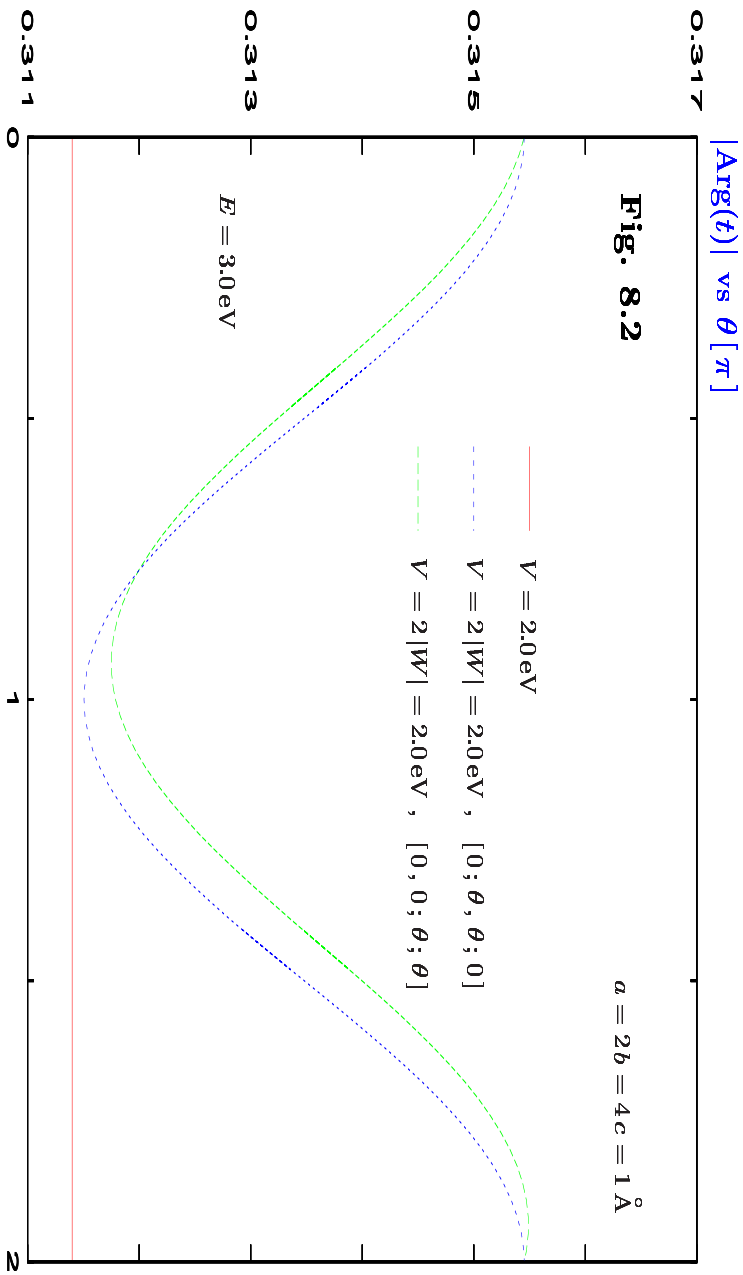
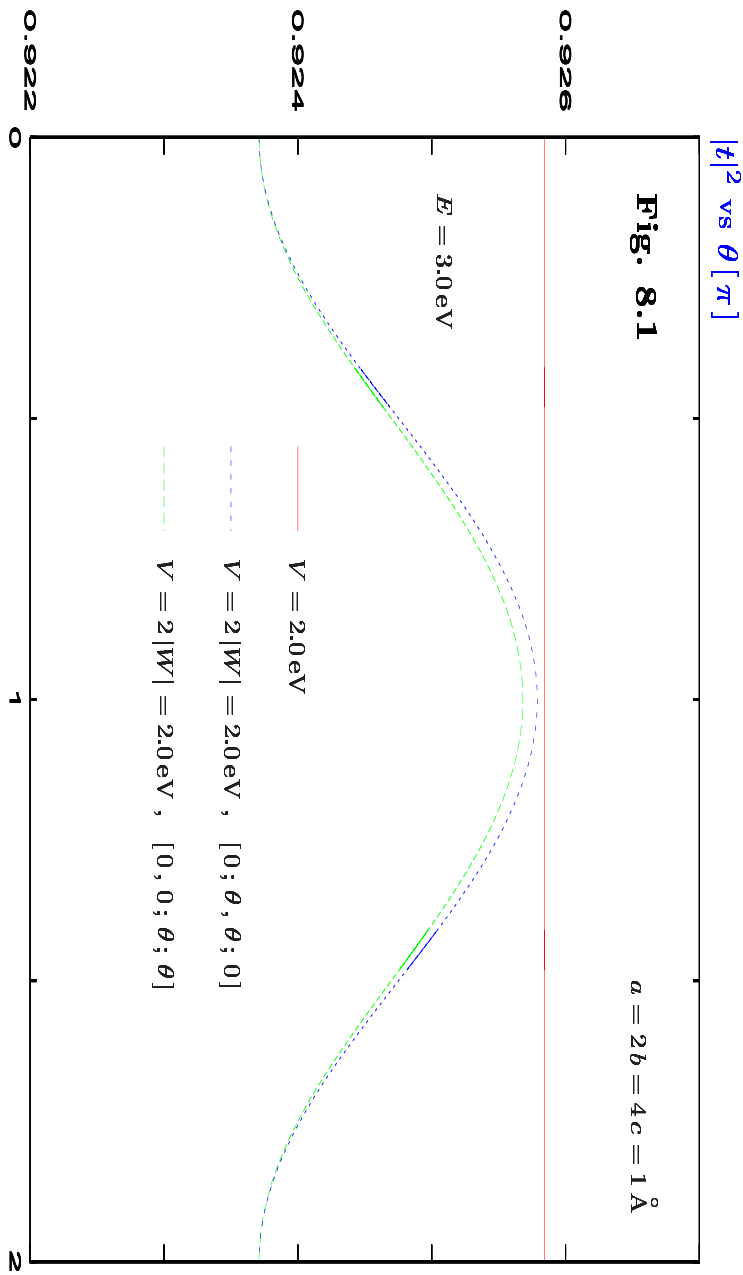
**Fig. 5.** Electron transmission probability,  $|t|^2$ , as a function of  $a$  [ $\text{\AA}$ ] for complex and *pure* quaternionic potentials with the same width and height [25]. The curves show the transmission probability for different values of  $E$ .



**Fig. 6.** Electron transmission probability,  $|f|^2$ , and absolute value of the transmission coefficient argument,  $|\text{Arg}(t)|$ , as function of the time violating phase  $\theta[\pi]$  for potentials of height  $V = 2|W| = 2.0 \text{ eV}$  and width  $a = 2b = 4c = 1.0 \text{ \AA}$  [25]. The curves show that only asymmetric (time violating) quaternionic potentials could distinguish between left and right transmission. The value of the energy is fixed to  $E = 0.5 \text{ eV}$ .



**Fig. 7.** Electron transmission probability,  $|t|^2$ , and absolute value of the transmission coefficient argument,  $|\text{Arg}(t)|$ , as function of the time violating phase  $\theta[\pi]$  for potentials of height  $V = 2|W| = 2.0 \text{ eV}$  and width  $a = 2b = 4c = 1.0 \text{ \AA}$  [25]. The curves show that only asymmetric (time violating) quaternionic potentials could distinguish between left and right transmission. The value of the energy is fixed to  $E = 1.5 \text{ eV}$ .



**Fig. 8.** Electron transmission probability,  $|t|^2$ , and absolute value of the transmission coefficient argument,  $|\text{Arg}(t)|$ , as function of the time violating phase  $\theta[\pi]$  for potentials of height  $V = 2|W| = 2.0 \text{ eV}$  and width  $a = 2b = 4c = 1.0 \text{ \AA}$  [25]. The curves show that only asymmetric (time violating) quaternionic potentials could distinguish between left and right transmission. The value of the energy is fixed to  $E = 3.0 \text{ eV}$ .