Observability of quaternionic quantum mechanics

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Beginning with the quaternionic generalization of the Schrödinger equation, we present a simple system consisting of two successive square barriers of general (quaternionic) height, and discuss situations in which the predictions of quaternionic quantum mechanics differ from those of the usual complex theory. Specifically, we show that the transmission coefficient may pick up a phase change on reversal of the barrier order. We comment on why this phase change would not necessarily be observed in experiments. Finally, we present a necessary condition for the magnitude of the transmission coefficient to change under reversal of the direction of traversal of the barrier.

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I. INTRODUCTION

The possibility of formulating quantum mechanics over a quaternionic field has been recognized since the early work of Birkhoff and Von Neumann [1]. It remains an open question whether such a generalization of the complex quantum mechanics (CQM) is required to describe nature, largely because quaternionic quantum mechanics (QQM) seems to be well hidden from experimental determination. In particular, it is not hard to show that in any scattering experiment, the asymptotic states in QQM are necessarily complex [2], while simple calculations of scattering from quaternionic square barriers show no qualitative differences from results in CQM [3].

To our knowledge there has been only one explicit proposal to look for QQM effects [4], followed by one actual experiment using neutron interferometry [5]. The rationale for that experiment was to look for noncommutative effects of reversing the order of two metal targets traversed by a split beam of neutrons. A phase change between the two transmitted beams was looked for, but not found. It was subsequently suggested [6] that the experiment does not rule out QQM, as the interaction of the neutrons with the targets, aluminum and titanium, respectively, is of the same type (strong interaction), and may, in some sense, have the same "quaternionic phase." Both the experiment and subsquent criticism appear to have been based upon the observation that the quaternion algebra is noncommutative, with an inference that the quantum mechanics will behave in a similar way. We are unaware of any calculation based on the appropriate wave equations leading to such a conclusion. It is the aim of this paper to provide such a calculation, in order to better discuss the implications of the experimental results, and to point to possible reasons for the null result even if QQM is the theory required to describe the real world. In Sec. II we briefly review simple one-dimensional calculations of scattering from square barriers in CQM and QQM. In Sec. III we discuss further the problem of scattering by two successive square barriers, highlighting the difference in the behavior of the phase of the transmission coefficient for the two theories under some circumstances. We also comment on the relevance of our results for discussion of the experiment of Ref. [5]. In Sec. IV we present the proof of a necessary condition for the amplitude of the transmission coefficient to change under reversal of barrier order in QQM, a result with no analog in CQM.

II. ONE-DIMENSIONAL SQUARE BARRIERS IN CQM AND QQM

We begin this section with some brief comments on scattering from single square barriers in CQM and QQM in one dimension. The Schrödinger equation for CQM is, in units in which $m = \frac{1}{2}$ and $\hbar = 1$ for convenience,

$$\frac{d^2}{dx^2}\Psi(x) + [E - V(x)]\Psi(x) = 0 \,. \tag{1}$$

For the case of a square barrier (that is, $V(x) = V_0 \neq 0$ only when $x \in [a,b]$), in the case of scattering of an incident beam from the left, we can write the wave function as

$$\Psi(x) = \begin{cases} e^{ik(x-a)} + Re^{-ik(x-a)}, & x < a \\ Ae^{i\mu x} + Be^{-i\mu x}, & a < x < b \\ Te^{ik(x-b)}, & b < x, \end{cases} \tag{2}$$

where $k^2 = E$, and $\mu^2 = E - V_0$. It is straightforward to match the boundary conditions at $x = a$ and b in the usual way to obtain the transfer matrix $\mathcal{T}$ for the problem. The elements of the 2×2 matrix $\mathcal{T}$ are given by

$$\begin{aligned} \mathcal{T}_{11} &= e^{-ik(b-a)}\left[\cos\theta + \frac{i}{2}\left(\frac{\mu}{k} + \frac{k}{\mu}\right)\sin\theta\right], \\ \mathcal{T}_{12} &= \frac{i}{2}\left(\frac{\mu}{k} - \frac{k}{\mu}\right)e^{-i(b+a)k}\sin\theta, \\ \mathcal{T}_{21} &= \mathcal{T}_{12}^*, \\ \mathcal{T}_{22} &= \mathcal{T}_{11}^*, \end{aligned} \tag{3}$$

where $\theta = \mu(b-a)$. From these expressions we may obtain the reflection and transmission coefficients R and T:

$$T = \frac{1}{\mathcal{T}_{11}},$$
$$R = -\frac{\mathcal{T}_{21}}{\mathcal{T}_{22}}. \tag{4}$$

If we now want to calculate the transmission coefficient for what we term a "compound square barrier"—two successive square barriers, generally of different heights V_1 and V_2 and different widths (from $x = a$ to b for V_1 and $x = b$ to c for V_2)—all we need to do is multiply together the appropriate $\mathcal{T}$ matrices and calculate R and T using Eqs. (4) and the elements of the product matrix. Presenting only the result for the transmission coefficient T for a compound barrier we find

$$T = e^{ik(c-a)} \left(\cos\theta_1 + \frac{i}{2}\Sigma_1 \sin\theta_1\right) \times \left(\cos\theta_2 + \frac{i}{2}\Sigma_2 \sin\theta_2\right), \tag{5}$$

where $\theta_1 = \mu_1(b-a)$, $\theta_2 = \mu_2(c-b)$, $\mu_i{}^2 = E - V_i$, and $\Sigma_i = \frac{\mu_i}{k} - \frac{k}{\mu_i}$, $i = 1, 2$. It is now easy to see that if we interchange $a \leftrightarrow c$, $k \leftrightarrow -k$, and $1 \leftrightarrow 2$ (in the subscripts) in Eq. (5), then the expression for T is unchanged. Such a set of substitutions is just that required to describe transmission through the barrier from the right-hand side (i.e., from the region $x > b$). This is a simple example of a general result in CQM; if the direction of incidence on a barrier of arbitrary shape is changed, the transmission coefficient T is unaltered in magnitude *and phase.* This is essentially a textbook result [7], but we shall briefly outline a proof in Sec. IV. In the remainder of this section we review the QQM $\mathcal{T}$ matrix and outline the calculation of the T and R coefficients. For background material and the basic QQM formalism the reader is referred to Refs. [2] and [3].

The one-dimensional QQM time-independent Schrödinger equation takes the form [in the same units as for Eq. (1) [2]]

$$\tilde{H}\Phi(x) = E\Phi(x)i, \tag{6}$$

where

$$\tilde{H} = -i\frac{d^2}{dx^2} + iV(x), \tag{7}$$

$V(x)$ being, in general, a quaternion-valued potential. We can avoid the noncommutative nature of quaternionic algebra in Eq. (6), by separating the equation into two coupled complex equations, writing

$$\Phi(x) = \Phi_\alpha(x) + j\Phi_\beta(x)$$

and (8)

$$V(x) = V_\alpha(x) + jV_\beta(x)$$

to obtain

$$\left(-\frac{d^2}{dx^2} + V_\alpha\right)\Phi_\alpha - V_\beta^*\Phi_\beta = E\Phi_\alpha,$$
$$\left(\frac{d^2}{dx^2} - V_\alpha\right)\Phi_\beta - V_\beta\Phi_\alpha = E\Phi_\beta. \tag{9}$$

One may solve these equations for the case of piecewise constant potentials and thus obtain in a manner analogous to the complex case the transfer matrix. Unfortunately, even for this simple case the expressions become unwieldy rather quickly. Since we will not use them explicitly here, the reader is referred to Ref. [3] for the expressions for R and T. For our purpose we will simply note that the expressions obtained in Ref. [3] can be quite easily shown to give an invariant T for the case of scattering from a single square barrier, which is to be expected on physical grounds due to the symmetry of the barrier. If we are to find a difference from CQM we obviously must look at a more complicated system. In the next section we address the scattering from a sequence of square barriers.

III. PHASE CHANGES IN THE TRANSMISSION COEFFICIENT

As mentioned in the preceding section, for a barrier of arbitrary shape in CQM, changing the direction of travel across a barrier makes no difference to the transmission coefficient, although the relection coefficient is in general phase shifted. We now turn to QQM for the case of two successive (different) square barriers. It is extremely difficult to work with analytic expressions for the T coefficient, so we turned to numerical evaluation, using the $\mathcal{T}$ matrix given in Ref. [3]. As per the CQM case of Sec. II, it is simply a matter of multiplying together the $\mathcal{T}$ matrices for the successive barriers. Our results are shown in Table I. We have in each case taken the incident energy of the asymptotically complex wave form to be ten units, and varied the heights and quaternionic phase of the barriers. At this point we observe that the condition for the incident energy to be "higher than the barrier" in the usual sense is

$$E^2 > |V_\alpha|^2 + |V_\beta|^2. \tag{10}$$

The results given in Table I are for T and T', the transmission coefficients for plane waves incident from the left and right, respectively, of the two barriers. Barrier 1 extends from $x = a$ to $x = b$, and barrier 2 from $x = b$ to $x = c$. The expressions in Ref. [3] allow arbitrary values for these parameters, but the results shown are for $a = 0$, $b = 2$, and $c = 4$, i.e., barriers of the same width. It makes no difference to our general conclusions if this is not so. We let the barriers take the most general flux conserving form:

$$V_i = V_\alpha^{(i)} + jV_\beta^{(i)}, \quad i = 1, 2 \tag{11}$$

where the $V_\alpha^{(i)}$ are real numbers (which is required to avoid the presence of sources or sinks of flux), and the

TABLE I. Representative results for the left and right incident plane-wave transmission coefficients from a compound (double) square barrier, T and T' respectively, for various values of the potentials. In each case $|T|^2 = |T'|^2$, so only $|T|^2$ is given. The energy of the incident wave is ten units, in each case higher than the total barrier height.

$V_\alpha^{(1)}$	$V_\beta^{(1)}$	$V_\alpha^{(2)}$	$V_\beta^{(2)}$	T	T'	$\|T\|^2$
5	$0+i0$	6	$0+i0$	$-0.463+i0.832$	$-0.463+i0.832$	0.907
5	$1+i0$	6	$1+i0$	$-0.421+i0.849$	$-0.421+i0.849$	0.898
5	$4+i4$	6	$4+i4$	$0.959+i0.275$	$0.959+i0.275$	0.996
5	$7+i0$	6	$0+i7$	$0.290-i0.441$	$0.131-i0.512$	0.279
5	$0+i0$	6	$0+i7$	$0.746+i0.233$	$0.746+i0.233$	0.610
0	$6+i6$	0	$7+i7$	$0.583+i0.398$	$0.583+i0.398$	0.498
0	$9+i0$	0	$0+i9$	$0.077+i0.993$	$-0.626+i0.775$	0.992

$V_\beta^{(i)}$ are complex numbers, given as an ordered pair in the table.

One may draw from the table the following inferences: (i) If the quaternionic parts of the potentials are set to zero, then the results of CQM are obtained. This is consistent with previous results, as the asymptotic complex states are completely decoupled from any quaternionic piece in the potential in this limit. (ii) If the (complex) phases of the $V_\beta^{(i)}$ are equal, then we again obtain $T = T'$, as in CQM. In this case the wave traversing the barrier does not encounter a change in phase anywhere. If we set either $V_\beta^{(i)} = 0$, then $T = T'$ as well. (iii) If the $V_\beta^{(i)}$ have different complex phases, then we will obtain, in general, a phase shifted result for T', that is, $T = e^{i\phi}T'$, with $\phi \neq 0$ a real number. This result is a new feature of QQM. Unfortunately, it is extremely difficult to explicitly see this result from the analytic expressions because of the size of the result for the compound barrier.

This result implies that there may well be observable consequences of QQM, should it be possible to arrange an experiment to look for a phase change in a beam which has traversed two barriers in different directions. This conclusion, however, begs two questions: Why was there no phase change in the experiment of Perez and what does it mean for a potential to be quaternionic? We have no clear answer to the second of these questions, other than to remark that if the underlying dynamics of nature is quaternionic it is not unreasonable to suggest that modeling the scattering of a particle from some target via a potential would require a quaternionic phase to be introduced. To discuss the experimental nonobservation of a phase change, we are led to a conclusion similar to that of Klein [6]. Since the targets used in the experiment were very many neutron wavelengths thick, it is reasonable to assume that the average of many interactions in the material may be approximated by square barriers. Then the simple analysis here suggests that the experimental results are explicable if we conclude that the (quaternionic) phases of the interactions are the same. It is therefore worth reiterating the suggestion of Klein that an improved experiment may be done by subjecting the parts of the split neutron beam to the different interactions of nature (gravitational, strong, and electromagnetic) in permuted order. This might be done, for instance, by allowing one beam to pass through a gravitational potential, followed by an electromagnetic field, and then a metal target, while the other encounters them in a different order. Such an experiment may be difficult to perform, but seems to be a better place to look for QQM than has been done before. We emphasize that these considerations have not been derived previously from the wave mechanical formalism which we have employed.

We note in passing here that the experiment of Ref. [5], although not an effective test of QQM for the reasons outlined here, remains a very elegant demonstration of the role of coherence in quantum mechanics (of either complex or quaternionic variety).

IV. CHANGE OF THE AMPLITUDE OF THE TRANSMISSION COEFFICIENT?

In this section we present an intriguing possibility. It may be possible to find a situation where the magnitude of the transmission coefficient is altered by changing the direction of travel across a potential barrier. We will derive here a necessary condition for this to occur, although it is fair to warn the reader that we do not know how to derive a sufficient condition, and we have not been able to construct an explicit example of a system exhibiting this feature.

We first show that this result cannot occur in CQM. If $u_i(x)$, $i = 1, 2$ are the two linearly independent (real) solutions of the Schrödinger equation in a finite region of nonzero potential [that is, $V(x) \neq 0$ for $a < x < b$, but vanishes elsewhere], it is straightforward to derive the result

$$R = \frac{p_2^-(b)p_1^-(a) - p_1^-(b)p_2^-(a)}{p_1^+(a)p_2^-(b) - p_1^-(b)p_2^+(a)}, \tag{12}$$

with

$$p_i^\pm(x) = u_i(x) \pm \frac{u_i'(x)}{ik}. \tag{13}$$

(It is easier to see what is going on by looking at R rather than T, but the two are of course linked by the relation $|R|^2 + |T|^2 = 1$.) Under inversion of reflection as discussed in Sec. I, $p_i^\pm(a) \leftrightarrow p_i^\mp(b)$, and R changes at most by a phase, which follows directly from Eqs. (12) and (13).

We now turn to the equivalent problem in QQM. We may use the first of the Eqs. (9) to eliminate Φ_β from the problem. We thus obtain a single fourth-order equation for Φ_α:

$$\Phi_\alpha'''' - 2\frac{(V_\beta^*)'}{V_\beta^*}\Phi_\alpha''' + 2\left[\left(\frac{(V_\beta^*)'}{V_\beta^*}\right)^2 - 2V_\alpha - \frac{(V_\beta^*)''}{V_\beta^*}\right]\Phi_\alpha''$$

$$-2\left[V_\alpha' + (E - V_\alpha)\left(\frac{(V_\beta^*)'}{V_\beta^*}\right)\right]\Phi_\alpha' + F(x,E)\Phi_\alpha = 0\,, \tag{14}$$

where

$$F(x,E) = |V_\beta|^2 + (V_\alpha)^2 - E^2 - V_\alpha'' + 2V_\alpha'\frac{\left(V_\beta^*\right)''}{V_\beta^*}$$

$$+2(E - V_\alpha)\left(\frac{\left(V_\beta^*\right)'}{V_\beta^*}\right)^2 - (E - V_\alpha)\frac{\left(V_\beta^*\right)''}{V_\beta^*}\,.$$

Finding solutions of this equation is, except for a few simple cases, obviously a difficult task. We can, however, make an observation which will be of use later; if the quantities

$$\frac{(V_\beta^*)''}{V_\beta^*}\,, \quad \frac{(V_\beta^*)'}{V_\beta^*} \tag{15}$$

are real, then the solutions of Eq. (14) are also able to be written as real functions, as all of the coefficients of the equation are real functions of x. If we write the general solution of Eq. (14) as

$$\Phi_\alpha(x) = A_1u_1(x) + A_2u_2(x) + A_3u_3(x) + A_4u_4(x)\,, \tag{16}$$

then we may write

$$\Phi_\beta(x) = A_i\frac{[E - V_\alpha(x)]u_i(x) + u_i''(x)}{-V_\beta^*(x)}. \tag{17}$$

Here there is a sum over i when it is repeated in a product, and the second equation follows from the first of Eqs. (9). Matching the boundary conditions at $x = a$ and b as before we can solve for R:

$$R = \frac{1}{2}A_ip_i^-(a)\,, \tag{18}$$

where the A_i satisfy the matrix equation

$$M\begin{pmatrix}A_1\\A_2\\A_3\\A_4\end{pmatrix} = \begin{pmatrix}p_1^+(a) & p_2^+(a) & p_3^+(a) & p_4^+(a)\\ q_1^+(a) & q_2^+(a) & q_3^+(a) & q_4^+(a)\\ p_1^-(b) & p_2^-(b) & p_3^-(b) & p_4^-(b)\\ q_1^+(b) & q_2^+(b) & q_3^+(b) & q_4^+(b)\end{pmatrix}\begin{pmatrix}A_1\\A_2\\A_3\\A_4\end{pmatrix} = \begin{pmatrix}2\\0\\0\\0\end{pmatrix}. \tag{19}$$

The p's and q's appearing in Eq. (19) are given in terms of the u_i by

$$p_i^\pm(x) = u_i(x) \pm \frac{u_i'}{ik}\,,$$

$$q_i^\pm(x) = [u_i''(x) + (E - V_\alpha)u_i(x)]\left(1 \pm \frac{(V_\beta^*)'}{V_\beta^*}\right)$$

$$\mp\frac{1}{k}\left[u_i''' + (E - V_\alpha)u_i'(x) - V_\alpha'(x)u_i(x)\right]. \tag{20}$$

Now, using Eqs. (18) and (19) it is possible to write the reflection coefficient as

$$R = \frac{-P_{12}Q_{34} + P_{13}Q_{24} - P_{14}Q_{23} - P_{23}Q_{14} + P_{24}Q_{13} - P_{34}Q_{12}}{\det M}\,, \tag{21}$$

where the quantities P_{ij} and Q_{ij} are given by

$$P_{ij} = p_i^-(a)p_j^-(b) - p_j^-(a)p_i^-(b)$$

and

$$Q_{ij} = q_i^+(a)q_j^-(b) - q_j^+(a)q_i^-(b)\,. \tag{22}$$

Under inversion $Q_{ij} \to -Q_{ij}$, but the behavior of the P_{ij} is more complicated. If we expand out the expression for the P_{ij} above in terms of the u_i we obtain

$$\begin{aligned}P_{ij} = {} & [u_i(a)u_j(b) - u_j(a)u_i(b)]\\ & +\frac{i}{k}[u_i'(a)u_j(b) + u_i(a)u_j'(b)\\ & -u_j'(a)u_i(b) - u_j(a)u_i'(b)]\\ & -\frac{1}{k^2}[u_i'(a)u_j'(b) - u_j'(a)u_i'(b)]\,.\end{aligned} \tag{23}$$

It is now obvious that, if the u_i are all real, then the swap $k \to -k$, $a \leftrightarrow b$ simply corresponds to $P_{ij} \to -P_{ij}^*$. However, the sufficient condition for the u_i to be real, namely that the quantities in (15) are real, ensures that the Q_{ij} are also real. [See the explicit expressions (20) and (22).]

Since $\det M$ is invariant under this swap, we see that R simply changes by at most a phase under inversion of reflection. Hence our result: a necessary condition for $|R|$ to change under inversion of reflection is that the imaginary part of at least one of the quantities in (15) be nonzero. Unfortunately, we can show via an example that this condition is not a sufficient one for $|R|$ to be modified in this way. We also mention that the examples explicitly worked in the literature, the square barrier [3] and the δ function [2] both have $|R|$ constant, neither satisfying our necessary condition.

We attempted to investigate the general expression for R using algebraic manipulation programs when the u_i are complex-valued functions. We found that there is no simple general transformation property of R under inversion. In particular, there is no obvious (algebraic) reason for $|R|$ to remain unchanged for a sufficiently complicated potential. However, to be sure we would have to take the most general expression for R, calculate its modulus, and then see if it is invariant. Unfortunately, the expressions obtained are too unwieldy to carry out such an analysis. (One might suggest to the contrary that one may model any potential by a sequence of square barriers of varying heights and phases. Then, since we have seen that for compound square barriers $|R|$ is a constant, this suggests that the result may be generally true. The caveat to this is of course whether the argument survives the limiting process.)

We may show by an explicit example that our necessary condition is not a sufficient one. Take $V_\alpha = 0$ and $V_\beta = V_0 e^{i\mu x}$, with μ a real constant, which produces a smoothly varying phase across the barrier. Then the fourth-order Schrödinger equation (14) takes the form

$$\Phi_\alpha'''' - 2i\mu\Phi_\alpha''' - \mu^2\Phi_\alpha'' - 2i\mu E\Phi_\alpha' + \left(V_0^2 - E^2 - \mu^2 E\right)\Phi_\alpha = 0.$$

This (complex) constant coefficient differential equation may be solved in the usual way, giving an auxilliary quartic equation. We put several such examples into a numerical routine to calculate R. We found in each case that the numerator of Eq. (21) was pure imaginary and invariant under $k \to -k, a \leftrightarrow b$. We conclude that there are some nonobvious cancellations occurring in the real part of the expression for R.

For a specific example, if we take $E = 5$ units, $V_0 = 4$, and $\mu = -1$, the auxilliary equation becomes

$$\lambda^4 + 2i\lambda^3 - \lambda^2 + 10i\lambda - 14 = 0 ,$$

which has solutions $\lambda_1 = -1.37i, \lambda_2 = 1.96i, \lambda_{3,4} = \pm 1.88 - 1.29i$. There are no linear combinations of the u_i which are real, but for any choice of a and b we found numerically that $|R|$ was invariant. If one looks at Eq. (23) it can be seen that the equation is invariant under complex conjugation and $x \to -x$, which is equivalent to time-reversal (T) and parity (P) transformations. One might thus suppose that it is this PT symmetry which is responsible for "protecting" R. To check if this is so we tried a potential of the form $V_\alpha = 0, V_\beta = V_0 e^{(\mu + i\rho)x}$, with μ and ρ real numbers. In this case there is no PT symmetry, but we find numerically for various input values of μ and ρ that $|R|$ is still invariant.

V. CONCLUSIONS

By considering simple one-dimensional models we have discussed the possibilities of experimental determination of the existence of QQM. We illustrated the interesting point that QQM allows a phase change in the transmission coefficient when the barrier is reversed, which does not occur in CQM, thus placing some previous work on a firmer mathematical footing. We also presented some work aimed towards finding a system for which the *magnitude* of the transmission coefficient might change upon reversing the barrier, proving a necessary condition for this to occur. We leave it as an open question as to whether a sufficient condition exists, or whether $|T|$ is always invariant under such a change. The algebraic complexity ensures that this is a far from simple task.

We have shown also that it is not necessarily the case that QQM is ruled out by experimental nonobservation to date, and suggest reexamination of the possibility of performing an interferometry-type experiment with different types of interactions.

Note added in proof. Since the completion of this work we have received a draft of *Quaternionic Quantum Mechanics*, by S. L. Adler (Oxford University Press, London, in press) in which a successful generalization of some of the results in this paper is presented.

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