Observations of the Ramsauer–Townsend effect in quaternionic quantum mechanics

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Received: 15 February 2017 / Accepted: 13 June 2017 / Published online: 24 June 2017

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Abstract In this article, one of the well-known effects in quantum mechanics is addressed and also the extended form of quantum mechanics which is based on quaternions is presented. In the presence of this version of quantum mechanics the Ramsauer–Townsend effect has been investigated and the existence of this phenomenon is studied according to quaternionic calculations; results are presented by graphs.

1 Introduction

Scattering of an electron by square well has been one of the important problems in quantum mechanics that has been mentioned in many quantum physics books [1–6]. The Ramsauer–Townsend effect is the expression of what happens in the scattering of low energy electrons (0.1 eV) from noble gases such as neon, argon and xenon, in which there is an anomalously large transmission [1]. The importance of such an effect is that this effect only can be expressed by quantum mechanics. If we assume atoms classically to be hard spheres, the calculations for the cross section result in wrong values because there is no dependency on the incident electrons' energy. On the other hand, if we consider atoms as the cause of an attractive well, then solving the Schrödinger equation by this interaction shows that the cross section has a minimum at electron energies near 1 eV. Some of these studies are available in Refs. [7,8]. The demonstration of this effect is due to Kukolich [9]. The influence of the Ramsauer–Townsend effect on the free–free absorption coefficients of the negative argon ion at far infrared wavelengths has been addressed by John [10]. Gianturco and Willner also have studied the Ramsauer–Townsend effect for electron scattering from gaseous molecules [11]. It is instructive to see this topic in a different situation. Vahedi et al. have explored the

Ramsauer–Townsend effect in the presence of a generalized uncertainty principle [12] and even this effect has been investigated in relativistic quantum mechanics by Sin Fai Lim [13], and by Shulga and Truten [14].

Quaternionic quantum mechanics is an extended version of ordinary quantum mechanics. This form of quantum mechanics is based on quaternions. Quaternions were established by Hamilton [15,16]. Adler gave a comprehensive treatment of the rules of quaternionic quantum mechanics in [17]. Historically, the idea of using this tool to express quantum mechanics originates with work by Kaneno [18], Finkelstein et al. [19,20] and Emch [21]. Then on using the theory of a non-commutative ring of quaternions, quaternionic quantum mechanics was formulated. It is instructive to refer to work by Horwitz and Biedenharn [22], Adler [23–27] and De Leo [28–34]. Before proceeding, we would like to explain some of the physical applications of quaternions. The complete phenomenology of the quaternionic potential barrier was presented, discussing the time-invariant and time-violating cases, by De Leo. He showed how interesting features of quaternionic perturbation effects emerge in the transmission and reflection coefficients [30]. In another paper, a comprehensive discussion of quaternionic diffusion by a potential step has been presented [31]. Furthermore, an analytic solution for the stationary states of the Schrödinger considering a quaternionic step potential [32], comparison between the behavior of a wave packet in the presence of a complex and a pure quaternionic potential step [33], and the dynamics of a non-relativistic particle in presence of a quaternionic potential barrier using a matrix approach [34] are different physical topics that are studied in the quaternionic version of quantum mechanics. This version of quantum mechanics does not only exist in papers; Dixon [35] and Gürsey and Tze [36] discussed some implications of this structure in particle physics in their books. As regards exper-

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imental aspects to verify quaternionic quantum mechanics there are some proposals that seek some issues that can be expressed by quaternionic quantum mechanics. These are due to Peres [37] and Kaiser et al. [38].

In Sect. 2 we introduce the mathematical tools which are needed. Then a quaternionic form of the Schrödinger equation and the quaternionic square well are presented and solved in detail in Sect. 3. In Sect. 4 we discuss different regions of the system. The physical wave function and probability current density, reflection and transmission coefficients and also some figures are presented in order to illuminate the physical meaning of this calculation. Finally our conclusions are drawn.

2 Basic definitions and rules for quaternions

The quaternion can be defined as an extended form of complex numbers having four components. Mathematically we show it as

$$Q = q_1 + iq_2 + jq_3 + kq_4, \quad (2.1)$$

with imaginary units i, j, k and real constant q_i ($i = 1, 2, 3, 4$). There are commutation rules between these imaginary units:

$$e_a e_b = -\delta_{ab} + \varepsilon_{abc} e_c, \quad (a, b, c = 1, 2, 3). \quad (2.2)$$

We show each imaginary unit by the symbol e . δ is the Kronecker delta and ε_{abc} is the Levi-Civita symbol. Actually the meaning of Eq. (2.2) is

$$j = -ji = k, \quad jk = -kj = i, \quad ki = -ik = j. \quad (2.3)$$

These commutations allow us to write quaternions in a more familiar form, which is similar to complex numbers:

$$\begin{aligned} Q &= Q_\alpha + jQ_\beta, \\ Q_\alpha &= q_1 + iq_2, \\ Q_\beta &= q_3 - iq_4. \end{aligned} \quad (2.4)$$

This form renders the calculations easier than before. Combining Eqs. (2.3) and (2.4) produces other properties as

$$\begin{aligned} Q_\alpha j &= j\bar{Q}_\alpha, \quad jQ_\alpha = \bar{Q}_\alpha j, \\ Q_\beta j &= j\bar{Q}_\beta, \quad jQ_\beta = \bar{Q}_\beta j, \\ \bar{Q}_\alpha &= q_1 - iq_2, \\ \bar{Q}_\beta &= q_3 + iq_4. \end{aligned} \quad (2.5)$$

Similar to a complex number, the quaternion has a conjugate,

$$\bar{Q} = q_1 - iq_2 - jq_3 - kq_4. \quad (2.6)$$

They have also an inverse, defined by

$$Q^{-1} = \frac{\bar{Q}}{|Q|^2}, \quad (2.7)$$

with the modules of quaternion $|Q|^2 = q_1^2 + q_2^2 + q_3^2 + q_4^2$.

Notice that because of the commutation rules between the imaginary units, multiplication of two quaternions does not have the commutative property in general; it yields $Q_1 Q_2 \neq Q_2 Q_1$.

3 Quaternionic Schrödinger equation and quaternionic square well

In quaternionic quantum mechanics, the Schrödinger equation has the form [39]

$$\frac{\partial \Psi(x, t)}{\partial t} = -\tilde{H}\Psi(x, t), \quad (3.1)$$

where $\tilde{H}$ is an anti-Hermitian quaternionic operator and $\Psi(x, t)$ is the quaternionic wave equation. Because of our consideration for the interaction of system, we can assume the wave function to be ($\hbar = 1$)

$$\Psi(x, t) = \Phi(x)e^{-iEt} \quad (3.2)$$

with energy E . Equation (3.2) shows that Eq. (3.1) can be written as

$$\tilde{H}\Phi(x) = \Phi(x)iE. \quad (3.3)$$

We consider a one-dimensional square well of quaternionic form whose mathematical function is

$$V(x) = \begin{cases} 0, & x > a \quad \text{and } x < 0, \\ -(V_\alpha + jV_\beta), & 0 < x < a, \end{cases} \quad (3.4)$$

where $a, V_\alpha \in \mathbb{R}, V_\beta \in \mathbb{C}$ and they are constant. Graphically, we depict Eq. (3.4) in Fig. 1.

Our problem necessitates

$$\tilde{H} = -i \frac{d^2}{dx^2} + iV(x), \quad m = \frac{1}{2}. \quad (3.5)$$

In analogy with ordinary quantum mechanics, there is a continuity equation of quaternionic form,

$$\frac{\partial \rho(x, t)}{\partial t} + \frac{\partial J(x, t)}{\partial x} = 0, \quad (3.6)$$

in which

$$\rho(x, t) = \bar{\Psi}(x, t)\Psi(x, t), \quad (3.7)$$

Fig. 1 Graph of the quaternionic potential well considered

$$J(x, t) = \bar{\Psi}(x, t) i \frac{\partial \Psi(x, t)}{\partial x} - \frac{\partial \bar{\Psi}(x, t)}{\partial x} i \Psi(x, t), \quad (3.8)$$

and the presence of the imaginary unit in Eq. (3.8) is due to the non-commutative nature of multiplication of the quaternions.

4 Wave functions, probability current densities and discussions

The particles considered in this article have energy $E > \sqrt{V_\alpha^2 + |V_\beta|^2}$. For region I and III we have the same crude wave functions but after applying boundary conditions they will change. To do this first we should set $\Phi(x) = \Phi_a(x) + j\Phi_b(x)$. Using Eq. (3.3) for these regions we get

$$\frac{d^2 \Phi_a(x)}{dx^2} = -E \Phi_a(x), \quad (4.1)$$

$$\frac{d^2 \Phi_b(x)}{dx^2} = E \Phi_b(x). \quad (4.2)$$

Thus the general shape of the wave function can be obtained by solving Eqs. (4.1) and (4.2), which results in

$$\Phi(x) = z_1 e^{i\varepsilon x} + z_2 e^{-i\varepsilon x} + j(z_3 e^{\varepsilon x} + z_4 e^{-\varepsilon x}), \quad \varepsilon = \sqrt{E}. \quad (4.3)$$

In order to have wave functions that have physical meaning for different regions, we write

$$\Phi_I(x) = e^{i\varepsilon x} + r e^{-i\varepsilon x} + j(\tilde{r} e^{\varepsilon x}), \quad (4.4)$$

$$\Phi_{III}(x) = t e^{i\varepsilon x} + j(\tilde{t} e^{-\varepsilon x}). \quad (4.5)$$

Following such a method to find the wave function for region II, we write

$$\frac{d^2 \Phi_a(x)}{dx^2} + (V_\alpha + E) \Phi_a(x) - \bar{V}_\beta \Phi_b(x) = 0, \quad (4.6)$$

$$\frac{d^2 \Phi_b(x)}{dx^2} + (V_\alpha - E) \Phi_b(x) + V_\beta \Phi_a(x) = 0. \quad (4.7)$$

Inserting $\Phi_b(x)$ from Eq. (4.6),

$$\Phi_b(x) = \frac{1}{\bar{V}_\beta} \left(\frac{d^2 \Phi_a(x)}{dx^2} + (V_\alpha + E) \Phi_a(x) \right), \quad (4.8)$$

into Eq. (4.7), one obtains

$$\frac{d^4 \Phi_a(x)}{dx^4} + 2V_\alpha \frac{d^2 \Phi_a(x)}{dx^2} + (V_\alpha^2 + |V_\beta|^2 - E^2) \Phi_a(x) = 0, \quad (4.9)$$

$$\Phi_a(x) = c_1 e^{\lambda_+ x} + c_2 e^{-\lambda_+ x} + c_3 e^{i\rho x} + c_4 e^{-i\rho x}, \quad (4.10)$$

where

$$\lambda_+ = \sqrt{-V_\alpha + \sqrt{E^2 - |V_\beta|^2}}, \quad (4.11)$$

$$\rho = \sqrt{V_\alpha + \sqrt{E^2 - |V_\beta|^2}}. \quad (4.12)$$

Substituting Eq. (4.10) into Eq. (4.8) one gets

$$\begin{aligned} \Phi_b(x) = & \frac{\lambda_+^2 + V_\alpha + E}{\bar{V}_\beta} (c_1 e^{\lambda_+ x} + c_2 e^{-\lambda_+ x}) \\ & + \frac{V_\alpha + E - \rho^2}{\bar{V}_\beta} (c_3 e^{i\rho x} + c_4 e^{-i\rho x}). \end{aligned} \quad (4.13)$$

Thus the wave function for region II is

$$\begin{aligned} \Phi_{II}(x) = & (1 + jA) (c_1 e^{\lambda_+ x} + c_2 e^{-\lambda_+ x}) \\ & + (1 + jB) (c_3 e^{i\rho x} + c_4 e^{-i\rho x}). \end{aligned} \quad (4.14)$$

Here $A = \frac{\lambda_+^2 + V_\alpha + E}{\bar{V}_\beta}$ and $B = \frac{V_\alpha + E - \rho^2}{\bar{V}_\beta}$.

To find the explicit form of the coefficients in the wave functions we should utilize the boundary conditions which determine the system. They are the continuity of the wave functions and their derivatives at the boundaries. Continuity of the wave function at $x = 0$ yields

$$1 + r = c_1 + c_2 + c_3 + c_4, \quad (4.15)$$

$$\tilde{r} = A(c_1 + c_2) + B(c_3 + c_4). \quad (4.16)$$

At $x = a$, we have

$$c_1 e^{\lambda_+ a} + c_2 e^{-\lambda_+ a} + c_3 e^{i\rho a} + c_4 e^{-i\rho a} = t e^{i\varepsilon a}, \quad (4.17)$$

Fig. 2 Reflection (R) and transmission (T) coefficients and their summation plotted in terms of energy

$$A(c_1 e^{\lambda+a} + c_2 e^{-\lambda+a}) + B(c_3 e^{i\rho a} + c_4 e^{-i\rho a}) = \tilde{t} e^{-\varepsilon a}. \quad (4.18)$$

Continuity of the wave function derivatives at $x = 0$ shows

$$i\varepsilon(1-r) = \lambda_+(c_1 - c_2) + i\rho(c_3 - c_4), \quad (4.19)$$

$$\tilde{r}\varepsilon = A\lambda_+(c_1 - c_2) + B i\rho(c_3 - c_4). \quad (4.20)$$

The wave function derivatives at $x = a$ cause one to write

$$\lambda_+(c_1 e^{\lambda+a} - c_2 e^{-\lambda+a}) + i\rho(c_3 e^{i\rho a} - c_4 e^{-i\rho a}) = i\varepsilon t e^{i\varepsilon a}, \quad (4.21)$$

$$A\lambda_+(c_1 e^{\lambda+a} - c_2 e^{-\lambda+a}) + B i\rho(c_3 e^{i\rho a} - c_4 e^{-i\rho a}) = -\tilde{t}\varepsilon e^{-\varepsilon a}. \quad (4.22)$$

On the other hand the conservation law of the probability holds in this version of quantum mechanics like in ordinary quantum mechanics. To investigate this law we should eval-

uate the probability current density in region I and region III. Using Eq. (4.1) and the property that for two quaternions $\overline{q\bar{p}} = \bar{p}\bar{q}$, the probability current densities are

$$J_I = 2\varepsilon(1 - |r|^2), \quad (4.23)$$

$$J_{III} = 2\varepsilon|t|^2. \quad (4.24)$$

Thus the conservation law leaves us with

$$|r|^2 + |t|^2 = 1. \quad (4.25)$$

Equation (4.25) is depicted in Fig. 2; here one finds the quaternionic quantum mechanical Ramsauer–Townsend effect. Other treatments of the transmission coefficients in other situations are included. They verify this effect in this type of quantum mechanics.

Figure 2 verifies Eq. (4.25); as well it shows some fluctuations and the Ramsauer–Townsend effect in reflection (R) and transmission (T) coefficient in terms of energy. In Fig. 3, we have checked the transmission in terms of potential parts. In agreement with our assumptions we plotted our results in terms of $V_\beta = \beta + i\beta_i$ (Fig. 3a) in which we set $\beta_i = 0.5$, $E = 3$ and $V_\alpha, i\beta_i$ (Fig. 3b) with $\beta = 1$, $E = 3$. The reader can see that they behave alike.

In Fig. 4 we have done the same as Fig. 3 but now for the reflection coefficient.

To ensure that the elements of V_β occur symmetrically, we have plotted the transmission and reflection coefficients in terms of β and β_i with $V_\alpha = 3$, $E = 3$. The results are presented in Fig. 5. These figures show that if in laboratory we find that the transmission coefficient permits one to make a symmetrical treatment with respect to a parameter, in addition it can be candidate for a quaternionic potential.

(a) Plot of T , V_α , β .

(b) Plot of T , V_α , β_i .

Fig. 3 Treatments of the transition coefficients versus the potential parts

Fig. 4 Reflection of the transition coefficients versus the potential parts

Fig. 5 Symmetrical treatments of the imaginary part of the potential for reflection and transmission coefficients

Fig. 6 Treatments of reflection and transmission coefficients for a fixed value of the imaginary part of the potential and different energies

It can be seen in Fig. 6 that at low energies the Ramsauer–Townsend effect occurs often and clearly. We have depicted such a treatments for a fixed value of the imaginary part of the potential and for different energies.

In Fig. 7, we depict the treatments of the reflection and transmission coefficients in terms of V_α and E with V_β constant.

Figure 8 shows that by shortening the length of the well, the Ramsauer–Townsend effect happens less clearly than

Fig. 7 Reflection and transmission coefficients versus energy and real part of the potential

Fig. 8 Reflection coefficient versus energy

before. In this figure transmission vs. energy is plotted with $V_\alpha = 3$, $V_\beta = 0.5 + i0.5$.

5 Conclusions

If quaternionic quantum mechanics represents a possible way to describe nature, then it is relevant to examine how the predictions of standard theories may be affected by changing from complex to quaternionic potentials. Thus, in this article the Ramsauer–Townsend effect studied in extended form of quantum mechanics in detail. Considering three regions for our problem, we investigate the Ramsauer–Townsend effect. This effect shows up in the scattering of low energy electrons from noble gases such as neon, argon and xenon in which there is an anomalously large transmission. Therefore in the quaternionic formalism of quantum mechanics a quaternionic potential well was considered. Solving the differential equation in quaternionic quantum mechanics became simple on assuming the quaternionic wave function in a complex number representation with complex functions. After finding the wave functions and applying the boundary conditions, the physical wave function of each region was derived. Then

by computing the current density of each region, and by the definition of reflection and transmission, these coefficients were obtained. Then, in some schemes, we showed how the Ramsauer–Townsend effect worked in the considered formalism of quantum mechanics. Treatments of transmission and reflection coefficient were graphically shown in different situations. The effects of the potential parts in fix energy and vice versa and the length of the well versus energy in a fixed potential were showed graphically. In summary, besides what we expected from the Ramsauer–Townsend effect in the complex counterpart of quantum mechanics, we have seen in this study in addition some symmetrical treatments of the imaginary parts of the potential for the reflection and transmission coefficients were found.

Acknowledgements It is a great pleasure for the authors to thank the referee because of the helpful comments.

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