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***t*-violation and quaternionic state oscillations**

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Abstract. We derive, using the quaternionic group representation theory, the possible forms of the *t*-violating Hamiltonians, and consider time evolution in a two-level system when a *t*-violating term is added to a *t*-preserving unperturbed Hamiltonian. Transition probabilities are calculated; moreover, the time evolution of a complex state is determined analytically, showing that a quaternionic component arises naturally in its evolution. Finally, some properties of the time-reversal observable are studied and a set of selection rules is obtained.

1. Introduction

In quaternion quantum mechanics (QQM) quaternionic Hilbert space dynamics underlies observational physics; then, in this context, a very relevant point concerns the possibility of a direct experimental test for quaternionic effects.

The first proposal for tests of QQM was by Peres [1], who suggested looking for residual quaternionic effect by passing a neutron beam through slabs of two different materials, and searching to see whether the phase shifts depend on the order of the slabs. A deeper analysis of such an experiment [2] shows that in one-dimensional scattering in complex quantum mechanics (CQM) (if one considers real potentials) the left and right transmission amplitudes are equal, whereas, in general, in QQM their magnitudes are always equal and, for a system with time-reversal symmetry, they must also be equal in phase, so a non-vanishing phase (when the order of the slabs is reversed) is a time-reversal violating effect [3].

Experiments to detect a phase shift are thus equivalent to experiments to detect time-reversal violation.

Actually, scattering theory in QQM provides a natural mechanism for the generation of time-reversal violation (i.e. without resorting to extra assumptions, but just taking into account the genuinely quaternionic terms in the potential) and it leads among other things to a *t*-violating effective CQM describing the scattering of asymptotic states [3]. Of course, it must be stressed that QQM does not simply reduce itself to CQM plus a time-reversal violation.

In this paper we intend to approach the problem of time-reversal violation in QQM by means of group theory techniques. More precisely, given a (finite or compact) symmetry group G which includes the time-reversal symmetry t (the representations of G were explicitly drawn out and studied elsewhere by the authors [4]), we can determine the possible forms of a quaternionic (anti-Hermitian) Hamiltonian H of a physical system which is invariant through G , and then add to them the most general quaternionic potential V_t which admits the same geometrical symmetries as H , but is *t*-violating.

To this aim, we briefly recall in section 2 some previous results on the quaternionic irreducible representations (Q -irreps) and their classification; then, we reconsider in section 3 the representations of G and deduce in section 4 the possible forms of H and V_t , while in section 5 an analogous discussion is carried out for the complete symmetry group of a relativistic, massive physical system.

Thus, in section 6, the knowledge of the full Hamiltonian \tilde{H} is used to study the oscillations of an eigenvector of the unperturbed Hamiltonian H ; in particular, we derive explicitly (and without any resort to perturbative or approximate techniques) the transition probabilities and the time evolution of a complex superposition of eigenvectors of H , showing that a quaternionic component naturally comes out.

In section 7 the oscillations of an eigenvector of V_t (and hence, of t) are studied.

Finally, since in the realm of QQM an observable can always be associated with the time-reversal operator t , we devote section 8 to illustrating some of its properties, and, in particular, a set of selection rules are obtained, which are associated with the parity under time reversal.

2. Basic notation and tools

We recall here some basic notation and previous results.

A quaternion is usually expressed as

$$q = q_0 + q_1i + q_2j + q_3k$$

where $q_i \in R$ ($i = 0, 1, 2, 3$), $i^2 = j^2 = k^2 = -1$, $ij = -ji = k$.

The quaternion skew-field Q is an associative algebra of rank 4 over R , non-commutative and endowed with an involutory anti-automorphism (*conjugation*) such that

$$q \rightarrow q^Q = q_0 - q_1i - q_2j - q_3k.$$

In a (right) n -dimensional vector space Q^n over Q , every linear operator is associated in a standard way with an $n \times n$ matrix acting on the left [5].

In analogy with the case of complex group representations, one can introduce the concepts of unitarity, Hermiticity and so on. Moreover, if G is a finite (or a compact) group, reducibility implies complete reducibility even in the case of unitary Q -representations $D(G)$, and every Q -representation is equivalent to a unitary one [6, 7].

We have shown elsewhere [8] that all Q -irreps $D(G)$ of a finite (or compact) group G fall into three classes (*generalized Frobenius–Schur, or FS, classification*): *potentially real or of type R* (i.e. a basis exists in which D is real), *potentially complex or of type C* (i.e. a basis exists in which it has a complex but never real form), (*purely*) *quaternionic or of type Q* (i.e. in no basis does it have a complex form). Indeed, they can *all* be obtained from the irreducible complex group representations (C -irreps), in the sense that any C -irrep of class +1 or 0, according to the standard FS classification, is itself a Q -irrep of type R or C , respectively, while it reduces [6] to two equivalent Q -irreps of type Q when it is of class -1 (or ‘pseudeoreal’), and no further Q -irrep exists in addition to those generated (in the above sense) by the C -irreps.

Moreover, on the basis of some general theorems on Q -irreps [6, 8] we studied the representations $D(H)$ of all the minimal extensions $G' = G + aG$ of a finite (or compact) group G by a linear operator a , and classified them into three types (*generalized Wigner classification*) [4], according to the properties of the Q -irrep $\Delta(G)$ from which they come:

I $D(G) = \Delta(G)$, i.e. the restriction $D(G)$ of D to the subgroup G is irreducible;

II $D(G)$ is reducible and has the form

$$D(G) = \begin{pmatrix} \Delta(G) & 0 \\ 0 & \bar{\Delta}(G) \end{pmatrix} \quad D(a) = \begin{pmatrix} 0 & \Delta(a^2) \\ \mathbf{1} & 0 \end{pmatrix}$$

where $\bar{\Delta}(g) \equiv \Delta(a^{-1}ga)$ is a Q -irrep of G of the same FS class as Δ , but inequivalent to it;

III $D(G)$ is reducible and has the above form, with Δ equivalent to $\bar{\Delta}$ ($\Delta \cong \bar{\Delta}$).

Crossing the generalized Wigner and Frobenius–Schur classifications, ten different cases arise, according to the FS classes of $\Delta(G)$ and $D(G')$, but only five of them can be associated with factorizable groups. (We recall that a magnetic group $G' = G + aG$ is said to be factorizable if and only if an element $t \in aG$ exists which commutes with all elements in G). We denoted every case by a couple of letters, for instance, C/R , to point out that in this case ‘ $D(G')$ is of type C (or $D(G') \sim C$) and $D(G) \sim R$ ’.

Finally, we recall that a generalized Schur’s lemma [3, 4] holds for Q -irreps, which asserts that any linear operator commuting with a given Q -irrep D has the form $T = q\mathbf{1}$, where $q \in R, C, Q$ when D is of type Q, C, R , respectively (in the latter two cases the form of T refers to the basis in which D has a complex or a real form, respectively).

3. Q -irreps of the symmetry groups containing t

Let us consider the Q -irreps of a group G' obtained by extending a given (finite or compact) group G of geometrical symmetries by the time-reversal operator t , which is a linear operator in QQM and commutes with all spatial symmetries (hence, the extended group G' is a factorizable group [4]).

Let us then consider firstly a fermionic system, and recall that in such a case $D(t^2) = \mathbf{1}$; whenever $\Delta(G) \sim R, C$ or Q , only the cases $R/R, C/C$ and Q/Q , respectively, can occur. By the condition $[\Delta(G), D(t)] = 0$, using the generalization of Schur’s lemma, the unitarity of the representations and the constraint $D(G') \sim R, C$ or Q we easily obtain in all cases

$$D(G) = \Delta(G) \quad D(t) = \pm \mathbf{1} \tag{1}$$

and the two Q -irreps corresponding to the \pm sign will be inequivalent.

It must be stressed, however, that a representation having the previous form cannot correspond to a symmetry group. Indeed, just by definition of geometrical symmetry, the elements of G must commute with a Hamiltonian operator, which in turn must anticommute with the time-reversal operator [3, 4]. In the cases $R/R, C/C, Q/Q$, all anti-Hermitian operators commuting with $D(G)$ assume the form $(h_1i+h_2j+h_3k)\mathbf{1}, h_1i\mathbf{1}$ and $h_0\mathbf{1}$, respectively, where $h_l \in R$ ($l = 0, 1, 2, 3$), so that they all commute with the time-reversal operator $D(t)$ (in the former two cases, these forms refer to the bases in which $D(G)$ has a real or complex form, respectively); in other words, no non-zero Hamiltonian can be associated with our system. Hence, reducible representations must be taken into account to describe G' and the simplest ones are given by a sum of two representations of the form (1), which must be chosen as necessarily inequivalent

$$D'(G) = \begin{pmatrix} \Delta(G) & 0 \\ 0 & \Delta(G) \end{pmatrix} \quad D'(t) = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}. \tag{2}$$

In order to obtain the proper commutation relations with $D'(G)$, H must have the following form in the case R/R :

$$H = \begin{pmatrix} 0 & (h + h_1i + h_2j + h_3k)\mathbf{1} \\ (-h + h_1i + h_2j + h_3k)\mathbf{1} & 0 \end{pmatrix} \tag{3}$$

where $h, h_l \in R$ ($l = 1, 2, 3$), and a $q \in Q$ always exists such that

$$qHq^{-1} = \begin{pmatrix} 0 & (h+h'i)\mathbf{1} \\ (-h+h'i)\mathbf{1} & 0 \end{pmatrix} \quad (4)$$

where $h^2 = h_1^2 + h_2^2 + h_3^2$.

Analogously one obtains for the case C/C

$$H = \begin{pmatrix} 0 & \alpha\mathbf{1} \\ -\alpha^*\mathbf{1} & 0 \end{pmatrix} \quad \alpha \in C \quad (5)$$

and for the case Q/Q

$$H = \begin{pmatrix} 0 & h\mathbf{1} \\ -h\mathbf{1} & 0 \end{pmatrix} \quad h \in R. \quad (6)$$

Let us now consider a bosonic system and recall that in this case $D(t^2) = -\mathbf{1}$ (i.e. t is anti-Hermitian). The corresponding representations can be obtained by the same techniques adopted in [9] and are given by

$$D(G) = \Delta(G) \quad D(t) = i\mathbf{1} \quad (\text{case } C/R) \quad (7)$$

$$D(G) = \Delta(G) \quad D(t) = \pm i\mathbf{1} \quad (\text{case } C/C) \quad (8)$$

$$D(G) = \begin{pmatrix} \Delta(G) & 0 \\ 0 & \Delta(G) \end{pmatrix} \quad D(t) = \begin{pmatrix} 0 & -\mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix} \quad (\text{case } C/2Q). \quad (9)$$

By the same arguments we expressed above for fermionic systems, also in some bosonic cases, reducible representations must be used. Indeed, in the cases C/C and $C/2Q$, in the bases in which $D(G)$ assumes a complex form, all anti-Hermitian operators commuting with $D(G)$ are real multiples of $i\mathbf{1}$, so that they all mutually commute (whereas in the case C/R , any operator of the form $H = j\alpha\mathbf{1}$, $\alpha \in C$, anticommutes with t and then can be chosen to represent the Hamiltonian). Therefore, except for the case $\Delta \sim R$, reducible representations arise to describe G' , and the simplest ones are given, when $\Delta \sim C$, by a sum of two inequivalent representations of the form (8):

$$D'(G) = \begin{pmatrix} \Delta(G) & 0 \\ 0 & \Delta(G) \end{pmatrix} \quad D'(t) = i \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix} \quad (10)$$

which satisfies the proper commutation relations with the anti-Hermitian operator

$$H = \begin{pmatrix} 0 & \alpha\mathbf{1} \\ -\alpha^*\mathbf{1} & 0 \end{pmatrix} \quad \alpha \in C \quad (11)$$

and by a sum of two equivalent representations of the previous form (9) when $\Delta \sim Q$:

$$D'(G) = \begin{pmatrix} \Delta(G) & 0 & 0 & 0 \\ 0 & \Delta(G) & 0 & 0 \\ 0 & 0 & \Delta(G) & 0 \\ 0 & 0 & 0 & \Delta(G) \end{pmatrix} \quad D'(t) = \begin{pmatrix} 0 & -\mathbf{1} & 0 & 0 \\ \mathbf{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\mathbf{1} \\ 0 & 0 & \mathbf{1} & 0 \end{pmatrix}. \quad (12)$$

In this case H must have the following form:

$$H = \begin{pmatrix} 0 & 0 & c\mathbf{1} & d\mathbf{1} \\ 0 & 0 & d\mathbf{1} & -c\mathbf{1} \\ -c\mathbf{1} & -d\mathbf{1} & 0 & 0 \\ -d\mathbf{1} & c\mathbf{1} & 0 & 0 \end{pmatrix} \quad c, d \in R. \quad (13)$$

4. The *t*-violation in QQM

Suppose that the dynamics at the quaternionic level are governed by a quaternionic Schrödinger equation with Hamiltonian \tilde{H} , and that the asymptotic state dynamics is described by an effective Hamiltonian H which is time-reversal conserving [3], where the possible forms of H are given in the previous section.

According to this scenario, we can proceed in the study of the cases listed above, considering the Hamiltonian \tilde{H} which admits the same geometrical symmetry group G as H but violates time reversal. We can obtain \tilde{H} by using the same technique developed in the previous section to determine H , but simply omitting the condition $\{t, \tilde{H}\} = 0$, which would imply a time-reversal symmetry. In doing so we obtain the explicit form of \tilde{H} for each case, corresponding to fermionic and bosonic systems. In particular, for the fermionic cases $R/R, C/C, Q/Q$ we have, respectively,

$$\tilde{H} = H + \begin{pmatrix} (v_1\mathbf{i} + v_2\mathbf{j} + v_3\mathbf{k})\mathbf{1} & 0 \\ 0 & (u_1\mathbf{i} + u_2\mathbf{j} + u_3\mathbf{k})\mathbf{1} \end{pmatrix} \quad (14)$$

$$\tilde{H} = H + \begin{pmatrix} v\mathbf{i}\mathbf{1} & 0 \\ 0 & u\mathbf{i}\mathbf{1} \end{pmatrix} \quad (15)$$

and

$$\tilde{H} = \begin{pmatrix} 0 & h\mathbf{1} \\ -h\mathbf{1} & 0 \end{pmatrix} = H. \quad (16)$$

(All the h s, u s and v s above are real parameters.)

We immediately remark that if a fermionic system is invariant by a geometrical symmetry group G , its states associated with a Q -irrep $D(G)$ of type Q cannot violate time reversal. On the contrary, in all other cases a non-vanishing, t -violating interacting potential $V_t = \tilde{H} - H$ can exist.

By analysing analogously the bosonic cases $C/R, C/C, C/2Q$, we obtain

$$\tilde{H} = H + v\mathbf{i}\mathbf{1} \quad (17)$$

$$\tilde{H} = H + \begin{pmatrix} v\mathbf{i}\mathbf{1} & 0 \\ 0 & u\mathbf{i}\mathbf{1} \end{pmatrix} \quad (18)$$

and

$$\tilde{H} = \begin{pmatrix} 0 & b\mathbf{1} & c\mathbf{1} & d\mathbf{1} \\ -b\mathbf{1} & 0 & e\mathbf{1} & f\mathbf{1} \\ -c\mathbf{1} & -e\mathbf{1} & 0 & g\mathbf{1} \\ -d\mathbf{1} & -f\mathbf{1} & -g\mathbf{1} & 0 \end{pmatrix} \quad (19)$$

respectively, where $u, v, b, c, d, e, f, g \in R$.

We note that in equations (14)–(18) the residual term $V_t = \tilde{H} - H$ commutes with t , as one can easily verify. In the case of equation (19), by a suitable choice of the parameters ($e = -d, f = c$), we obtain $\tilde{H} = H + V_t$, where again $[V_t, t] = 0$, so that in all cases a potential V_t can exist which shares with t a common basis of eigenvectors.

To conclude this section, we note that in all the above cases the subspace associated with an H -degenerate eigenvalue decomposes into two subspaces belonging to different eigenvalues when the term V_t is switched on and the full Hamiltonian \tilde{H} is taken into account.

The eigenvalues and the eigenvectors of the full Hamiltonian \tilde{H} can be calculated by resorting to the methods outlined in [10], and using (if necessary) a software package of

symbolic computation. For instance, one obtains in the case of equation (15) (see also equation (4)) that the eigenvalues of the complex matrix H are $\pm i\sqrt{h^2 + h'^2}$ (recall that in QQM only their modulus is relevant, due to the possibility of a quaternionic rephasing of the eigenvectors [3]), so that a degeneracy arises, while the (distinct) eigenvalues of \tilde{H} are

$$i\frac{u+v}{2} \pm i\sqrt{h^2 + h'^2 + \frac{1}{4}(u-v)^2}.$$

Then if the invariance group of the Hamiltonian is reduced by the introduction of an additional interaction which does not respect the full symmetry, the new energy levels are classified by the representations of the reduced group, according to the standard group representations theory [11].

5. The complete group and parity violation

The techniques and the concepts of the previous section can be extended to explore parity violation (equivalently, t -violation) in a relativistic physical system.

To do this we can consider the quaternionic complete symmetry group of a massive physical system that we studied in a previous paper [9], i.e. the group obtained by extending the connected Poincaré group and the internal symmetry group G by means of the CPT and the generalized parity operators (Θ and \mathcal{P} , respectively; more precisely, we use $\Theta_0 = \Theta e^{-i\pi J_y}$ in place of Θ , so that $\Theta_0^2 = -\mathbf{1}$ both for fermionic as for bosonic systems [9]).

The particle multiplets (i.e. the Q -representations of the complete group) have been obtained and classified in 14 cases; we consider here only the six cases in which all internal symmetry operators commute with \mathcal{P} (and hence with t).

Following the same methods as in section 4, we obtain that only in two cases can a t -violating Hamiltonian \tilde{H} exist; we denote them by the symbols $Q//R$ ($D(G) \sim R$, while the double extension $D(G') \sim Q'$) and $C//2C$ ($D(G)$ is the direct sum of two equivalent Q -irreps of type C , and $D(G') \sim C'$). Their explicit forms in the internal variables space are, for the case $Q//R$ (recall that Θ_0 , \mathcal{P} and all operators in G are diagonal in the spin and momentum spaces [9]):

$$\mathcal{D}(G) = \Delta(G) \quad \mathcal{D}(\Theta_0) = i\mathbf{1} \quad \mathcal{D}(\mathcal{P}) = j e^{i\theta} \mathbf{1} \quad (20)$$

for some $\theta \in R$, and the Hamiltonians H and \tilde{H} are given by

$$H = j h_1 e^{i\theta} \mathbf{1} \quad \tilde{H} = j \alpha \mathbf{1} \quad (h_1 \in R, \alpha \in C).$$

Moreover, a potential term $V_t = \tilde{H} - H$ can exist which anticommutes with \mathcal{P} (hence, it commutes with t (see section 4)):

$$V_t = k h_2 e^{i\theta} \mathbf{1} \quad h_2 \in R.$$

Analogously we have for the case $C//2C$

$$\begin{aligned} \mathcal{D}(G) &= \begin{pmatrix} \Delta(G) & 0 \\ 0 & \Delta(G) \end{pmatrix} & \mathcal{D}(\Theta_0) &= \begin{pmatrix} i\mathbf{1} & 0 \\ 0 & -i\mathbf{1} \end{pmatrix} & \mathcal{D}(\mathcal{P}) &= \begin{pmatrix} 0 & e^{i\theta} \mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix} \\ H &= ih \begin{pmatrix} 0 & e^{i\theta/2} \mathbf{1} \\ e^{-i\theta/2} \mathbf{1} & 0 \end{pmatrix} & \tilde{H} &= \begin{pmatrix} 0 & \alpha \mathbf{1} \\ -\alpha^* \mathbf{1} & 0 \end{pmatrix} & & (21) \\ V_t &= h' \begin{pmatrix} 0 & e^{i\theta/2} \mathbf{1} \\ -e^{-i\theta/2} \mathbf{1} & 0 \end{pmatrix} \end{aligned}$$

where $h, h' \in R, \alpha \in C$.

When the generalized parity symmetry is violated, in contrast to the cases analysed in section 4, a direct calculation of energy levels shows that in the cases considered in the present section the additional term V_t implies a mere shift of the levels but no splitting.

For a more detailed description of all cases, see [12].

6. Two-level systems

We have explicitly shown in section 4 the possible forms of the Hamiltonians which preserve (or not) the time-reversal symmetry; we emphasize that the above results arise from a purely group-theoretical approach and, while some of these representations assume a complex form, we derived all of them in a genuinely quaternionic approach (as, we assumed the linearity of the t operator).

The knowledge of the quaternionic Hamiltonian operator allows one to exactly determine the evolution of a state vector and to investigate, for instance, what happens when a perturbation V_t (which violates t -symmetry) is added to a Hamiltonian H which preserves the time reversal. (A very similar problem were discussed by Adler [13, 14], resorting to perturbation techniques, in some papers concerning t -violation in the K-meson decays.)

We will show in this section that some amusing features arise in doing so. We choose as our ‘laboratory’ a two-level system, which in many physical situations can describe, to a good approximation, a more involved system. We avoid for the moment discussion of the more complicated case given by equation (19) and the simpler case given by equation (17). Moreover, we will restrict ourselves to a genuinely quaternionic case, because the calculations in the cases of equations (15) and (18), in which the Hamiltonians are complex, follow in an easy manner from the analogous discussions in CQM.

Let us consider then the two-dimensional case

$$H = \begin{pmatrix} 0 & h + ih' \\ -h + ih' & 0 \end{pmatrix} \quad V_t = j \begin{pmatrix} v & 0 \\ 0 & v \end{pmatrix} \quad \tilde{H} = H + V_t \quad (22)$$

that can be obtained from equation (14) by a suitable choice of the parameters and imposing $\Delta(G) \equiv 1$.

The unperturbed complex Hamiltonian H admits the two eigenvectors

$$|\psi'_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} i e^{i\eta} \\ 1 \end{pmatrix} \quad |\psi'_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -i e^{i\eta} \\ 1 \end{pmatrix} \quad (23)$$

where $\tan \eta = \frac{h'}{h}$, belonging to the eigenvalues $-i\varepsilon = -i\sqrt{h^2 + h'^2}$ and $i\varepsilon$, respectively.

By rephasing them (in particular, the first one), one obtains the two orthogonal eigenvectors

$$|\psi_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} i e^{i\eta} \\ 1 \end{pmatrix} j = |\psi'_1\rangle j \quad |\psi_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -i e^{i\eta} \\ 1 \end{pmatrix} = |\psi'_2\rangle \quad (24)$$

both belonging to the eigenvalue $i\varepsilon$.

The degeneracy of ε can be removed by adding the perturbation (time-independent) term V_t which, as we remarked above, commutes with t so that in QQM it violates t -symmetry.

One obtains in this case that the eigenvalues and the (orthogonal) eigenvectors of \tilde{H} ,

$$\tilde{H} |\Phi_{\pm}\rangle = |\Phi_{\pm}\rangle iE_{\pm}$$

are given by

$$E_{\pm} = \sqrt{h'^2 + (h \pm v)^2} \quad (25)$$

$$|\Phi_{\pm}\rangle = \frac{1}{2} \begin{pmatrix} \pm 1 - j e^{i\phi_{\pm}} \\ \pm e^{i\phi_{\pm}} + j \end{pmatrix} \quad (26)$$

where $\tan \phi_{\pm} = \frac{h_{\pm}v}{h}$. The evolution operator $U = e^{-\tilde{H}t}$ can be obtained, in the easiest way, by introducing the matrix S which diagonalizes \tilde{H} :

$$S\tilde{H}S^{-1} = i \begin{pmatrix} E_+ & 0 \\ 0 & E_- \end{pmatrix}$$

and which is given by [10]

$$S = \begin{pmatrix} \Phi_{+,1} & \Phi_{-,1} \\ \Phi_{+,2} & \Phi_{-,2} \end{pmatrix}^{-1}$$

where we have denoted by $\Phi_{\pm,l}$ the l th component of $|\Phi_{\pm}\rangle$.

Then,

$$U \equiv e^{-\tilde{H}t} = S^{-1} \begin{pmatrix} e^{-iE_+t} & 0 \\ 0 & e^{-iE_-t} \end{pmatrix} S$$

$$= \frac{1}{2} \left(\begin{array}{c|c} \cos E_+t + \cos E_-t & -j(\cos E_+t - \cos E_-t) \\ -k(e^{i\phi_+} \sin E_+t - e^{i\phi_-} \sin E_-t) & -i(e^{-i\phi_+} \sin E_+t + e^{-i\phi_-} \sin E_-t) \\ \hline j(\cos E_+t - \cos E_-t) & \cos E_+t + \cos E_-t \\ -i(e^{i\phi_+} \sin E_+t + e^{i\phi_-} \sin E_-t) & +k(e^{-i\phi_+} \sin E_+t - e^{-i\phi_-} \sin E_-t) \end{array} \right). \quad (27)$$

The matrix elements $\langle \psi_l | e^{-\tilde{H}t} | \psi_m \rangle$, or briefly U'_{lm} , are

$$U'_{11} = \cos E_+t + \cos E_-t - i(\sin(\phi_+ + \eta) \sin E_+t + \sin(\phi_- + \eta) \sin E_-t) - k e^{-i\eta} (\cos(\phi_+ + \eta) \sin E_+t - \cos(\phi_- + \eta) \sin E_-t) \quad (28)$$

$$U'_{12} = -i e^{i\eta} (\cos E_+t - \cos E_-t) - e^{i\eta} (\sin(\phi_+ + \eta) \sin E_+t - \sin(\phi_- + \eta) \sin E_-t) + j (\cos(\phi_+ + \eta) \sin E_+t + \cos(\phi_- + \eta) \sin E_-t) \quad (29)$$

$$U'_{21} = i e^{-i\eta} (\cos E_+t - \cos E_-t) + e^{-i\eta} (\sin(\phi_+ + \eta) \sin E_+t - \sin(\phi_- + \eta) \sin E_-t) + j (\cos(\phi_+ + \eta) \sin E_+t + \cos(\phi_- + \eta) \sin E_-t) \quad (30)$$

$$U'_{22} = \cos E_+t + \cos E_-t - i(\sin(\phi_+ + \eta) \sin E_+t + \sin(\phi_- + \eta) \sin E_-t) + k e^{i\eta} (\cos(\phi_+ + \eta) \sin E_+t - \cos(\phi_- + \eta) \sin E_-t) \quad (31)$$

where

$$\cos(\phi_{\pm} + \eta) = \mp \frac{h'v}{\varepsilon E_{\pm}}. \quad (32)$$

Let us now consider a state vector which coincides, at $t = 0$, with an eigenvector of H , say $|\psi_1\rangle$, and compute the probability of finding the system in the state $|\psi_2\rangle$ at time t . By using the previous results, we easily obtain

$$P_{12}(t) = |\langle \psi_1 | e^{-\tilde{H}t} | \psi_2 \rangle|^2 = \frac{1}{2} \{1 + \cos(\phi_+ + \phi_- + 2\eta) \sin E_+t \sin E_-t - \cos E_+t \cos E_-t\} = P_{21}(t) \quad (33)$$

and the above expression differs from the familiar Rabi formula [15] for CQM by the v -dependent factor

$$\cos(\phi_+ + \phi_- + 2\eta) = - \frac{v^2 (h'^2 - h^2) + (h^2 + h'^2)^2}{(h^2 + h'^2) \sqrt{(h^2 + h'^2 + v^2)^2 - 4h^2v^2}}. \quad (34)$$

Analogous calculations yield

$$P_{11}(t) \equiv |\langle \psi_1 | e^{-\tilde{H}t} | \psi_2 \rangle|^2 = P_{22}(t) = 1 - P_{12}(t). \quad (35)$$

We note that the above probabilities do not depend on the sign of the time; this feature occurs whenever (in a two-level system) a transition probability between orthogonal states is considered, and disappears when a different choice of states is made (see section 7).

A deeper investigation can be performed by considering the time evolution of a state vector. Let us choose, as an example, a complex superposition of the eigenstates of the Hamiltonian H , which constitutes the most general eigenvector of H belonging to the eigenvalue $i\varepsilon$, as one can easily verify. Let

$$|\omega(0)\rangle = |\psi_1\rangle \alpha + |\psi_2\rangle \beta$$

(where $|\alpha|^2 + |\beta|^2 = 1$, $\alpha, \beta \in C$) be such a vector. Then,

$$\begin{aligned} |\omega(t)\rangle &= e^{-\tilde{H}t} |\omega(0)\rangle = e^{-\tilde{H}t} |\psi_1\rangle \alpha + e^{-\tilde{H}t} |\psi_2\rangle \beta \\ &= |\psi_1\rangle [U'_{11}\alpha + U'_{12}\beta] + |\psi_2\rangle [U'_{21}\alpha + U'_{22}\beta]. \end{aligned}$$

Hence, a quaternionic component of $|\omega(t)\rangle$ arises in time; moreover, recalling the form of the U'_{lm} s (see equations (28)–(31)) it is easy to single out the complex parts of the coefficients in the above expansion, thus obtaining the ‘complex’ component $|\omega(t)\rangle_C$ of $|\omega(t)\rangle$. A somewhat cumbersome calculation yields the norm of $|\omega(t)\rangle_C$, that is

$$\| |\omega(t)\rangle_C \|^2 = 1 - \frac{1}{2} \{ (1 - a) \cos^2(\phi_+ + \eta) \sin^2 E_+ t + (1 + a) \cos^2(\phi_- + \eta) \sin^2 E_- t \} \quad (36)$$

where $a = 2 \operatorname{Im}(\alpha\beta^* e^{-i\eta})$ (note that $0 \leq a \leq 1$).

Thus, we can conclude that the purely quaternionic component of $|\omega(t)\rangle$ oscillates in time and does not vanish asymptotically.

7. Oscillations of the *t*-eigenstates

Let us now consider a different example, i.e. the oscillations of the eigenstates of V_t , which are simultaneously eigenstates of the time-reversal observable t (see equation (2)).

We denote by $|\chi_{\pm}\rangle$ the eigenstates of the degenerate Hamiltonian V_t , which are

$$|\chi_+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} i + j \\ 0 \end{pmatrix} \quad |\chi_-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ i + j \end{pmatrix} \quad (37)$$

both belonging to the eigenvalue iv .

Let us then consider the time evolution of a state vector which coincides, at $t = 0$, with $|\chi_+\rangle$, and compute the probability $P'_{12}(t)$ of finding the system in the state $|\chi_-\rangle$ at time t . Recalling the form of the evolution operator (see equation (27)), by a straightforward calculation one obtains

$$\begin{aligned} P'_{12}(t) &= |\langle \chi_+ | e^{-\tilde{H}t} | \chi_- \rangle|^2 \\ &= \frac{1}{2} \{ 1 + \cos E_+ t \cos E_- t - \cos(\phi_+ - \phi_-) \sin E_+ t \sin E_- t \} = P'_{21}(t). \end{aligned} \quad (38)$$

Analogously,

$$P'_{11}(t) = P'_{22}(t) = 1 - P'_{12}(t). \quad (39)$$

We again obtain a formula which is very similar to equation (33) and which differs from Rabi's formula by the term

$$\cos(\phi_+ - \phi_-) = \frac{h^2 + h^2 - v^2}{\sqrt{(h^2 + h^2 + v^2)^2 - 4h^2v^2}}. \quad (40)$$

In the same manner we can finally calculate the transition probability between the states $|\chi_+\rangle$ and $|\psi_1\rangle$:

$$|\langle\psi_1|U|\chi_+\rangle|^2 = \frac{1}{2} \{1 + \cos(\phi_+ + \eta) \sin E_+t \cos E_-t + \cos(\phi_- + \eta) \sin E_-t \cos E_+t\}. \quad (41)$$

(Note that in this last case the probability changes when $t \rightarrow -t$.)

8. The time-reversal observable

Since the time-inversion operator is associated in quaternion quantum mechanics with a Hermitian or an anti-Hermitian operator, an observable can always be associated with it in our theory [3], which inherits all the well known properties of observables. Then, it can be useful to extend and apply some familiar concepts explicitly to t .

8.1. Fermionic systems

We remember that for a fermionic system one has

$$t^2 = \mathbf{1} \quad t^\dagger = t. \quad (42)$$

The operators

$$P_\pm = \frac{1}{2}(\mathbf{1} \pm t) \quad (43)$$

project the states of a quaternionic Hilbert space into two subspaces associated with the eigenvalues $+1$ and -1 , respectively, of t .

Indeed, by the previous definition it is easy to check that

$$P_\pm^2 = P_\pm = P_\pm^\dagger \quad (44)$$

$$P_+P_- = P_-P_+ = 0 \quad (45)$$

$$P_+ + P_- = \mathbf{1} \quad (46)$$

and

$$tP_\pm = \pm P_\pm. \quad (47)$$

Then, for any state $|\chi\rangle$,

$$|\chi\rangle = (P_+ + P_-)|\chi\rangle = P_+|\chi\rangle + P_-|\chi\rangle = |\chi_+\rangle + |\chi_-\rangle \quad (48)$$

and the vectors $|\chi_\pm\rangle = P_\pm|\chi\rangle$ satisfy

$$t|\chi_\pm\rangle = \pm|\chi_\pm\rangle. \quad (49)$$

8.2. *Bosonic systems*

For a bosonic system we have, in contrast with the previous case,

$$t^2 = -\mathbf{1} \quad t^\dagger = -t \tag{50}$$

then *t* is anti-Hermitian and admits the spectral representation [3]

$$t = \sum_{\tau} |\tau\rangle \tau i \langle\tau| \quad \tau = \pm 1. \tag{51}$$

Let us pose

$$I = \sum_{\tau} |\tau\rangle i \langle\tau| \tag{52}$$

then we have trivially

$$[t, I] = 0 \tag{53}$$

and *tI* is Hermitian:

$$(tI)^2 = -t^2 = \mathbf{1}. \tag{54}$$

The operators

$$P'_{\pm} = \frac{1}{2}(\mathbf{1} \pm It) \tag{55}$$

satisfy the same algebra as *P*_± (see equations (44)–(46)) and project the states of a quaternionic Hilbert space into two subspaces associated, respectively, with the eigenvalues +1 and –1 of *It*:

$$ItP'_{\pm}|\chi\rangle = \pm P'_{\pm}|\chi\rangle. \tag{56}$$

8.3. *Time-reversal selection rules*

Let us consider a fermionic system.

We say that an observable *O_e* is even under time reversal if

$$tO_e = O_et \tag{57}$$

while an observable *O_o* is odd if

$$tO_o = -O_ot. \tag{58}$$

By using equation (42), then equations (57) and (58), respectively, become

$$tO_et = O_e \tag{59}$$

$$tO_ot = -O_o \tag{60}$$

and we have

$$\langle\chi_{\pm}|O_e|\chi_{\mp}\rangle = \langle\chi_{\pm}|tO_et|\chi_{\mp}\rangle = -\langle\chi_{\pm}|O_e|\chi_{\mp}\rangle = 0 \tag{61}$$

$$\langle\chi_{\pm}|O_o|\chi_{\pm}\rangle = -\langle\chi_{\pm}|tO_ot|\chi_{\pm}\rangle = -\langle\chi_{\pm}|O_o|\chi_{\pm}\rangle = 0 \tag{62}$$

which constitute a pair of ‘time-reversal selection rules’ for a fermionic system.

For a bosonic system we say that an observable *O_e* is even under time reversal if

$$ItO_eIt = O_e \tag{63}$$

while *O_o* is odd if

$$ItO_oIt = -O_o. \tag{64}$$

By using the results of the previous subsection, we easily obtain for bosonic systems a pair of time-reversal selection rules which formally coincide with the previous ones for fermionic systems.

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