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Pseudoanti-Hermitian operators in quaternionic quantum mechanics

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Abstract

We introduce the concept of pseudoanti-Hermitian operators in quaternionic quantum mechanics and give a complete characterization of their spectra. We highlight some physical properties related to time-reversal symmetry of the pseudoanti-Hermitian quaternionic Hamiltonians.

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1. Introduction

Pseudo-Hermitian operators were introduced in the early 1940s by Dirac [1] and Pauli [2] in order to overcome certain divergence difficulties in quantum physics, by using an indefinite inner product. Later Lee and Wick [3] reassessed these operators showing that, contrary to a widely held belief, the introduction of pseudo-Hermitian Hamiltonians in the theory leads to a unitary *S*-matrix, provided that certain conditions are satisfied.

The question concerning pseudo-Hermitian operators has recently gained importance [4, 5], starting from a study of Bender and Boettcher [6] on certain non-Hermitian Hamiltonians with real spectra. In [4, 5], the spectrum of pseudo-Hermitian operators has been suitably characterized and it has been proved that all non-Hermitian Hamiltonians with real spectra belong to a subclass of pseudo-Hermitian Hamiltonians.

Many interesting physical properties of pseudo-Hermitian operators, connected with time-reversal invariance, are examined in [7], where the existence of an antilinear involutory operator which commutes with such operators is proved.

This last result clarifies the conjecture due to Bender and Boettcher [6] on the connection between the reality of the spectrum of some non-Hermitian Hamiltonians and their PT-invariance.

However, in a recent systematic study of quantum mechanics in quaternionic Hilbert space [8], the issue of whether there is a quaternionic analogue of pseudo-Hermitian Hamiltonians was left open; the object of the present paper is to fill this gap.

When we approach the problem of introducing this concept in quaternionic Hilbert space we must be careful. In fact, pseudo-Hermitian operators generalize standard Hermitian observables in complex Hilbert space, but there is an important difference between the structure of an observable in complex and quaternionic quantum mechanics. In complex quantum mechanics, any anti-Hermitian operator can be made Hermitian (and vice versa) by multiplying by i. In quaternionic quantum mechanics, in contrast, an anti-Hermitian operator cannot be trivially converted to a Hermitian one by multiplying by a *c*-number; in this context in fact, to obtain such a conversion one needs a 'phase' operator [8], so that standard observables (in particular, Hamiltonians) are represented by anti-Hermitian quaternionic operators. Hence, a definition of pseudoanti-Hermitian quaternionic operators (given in section 4) is needed in order to generalize standard quaternionic observables.

After introducing basic notation and mathematical tools in section 2, a complete biorthonormal eigenbasis for diagonalizable (non-Hermitian) quaternionic linear operators is derived in section 3. Then, in section 4, a complete characterization of pseudoanti-Hermitian quaternionic operator spectra is given and some of their properties are examined. In section 5, the commutant of a quaternionic diagonalizable linear operator is obtained and a connection between the pseudoanti-Hermiticity condition on a quaternionic operator and its invertible anticommutant (i.e. the set of invertible linear quaternionic operators which anticommutes with it) is recovered; more precisely the existence of a linear operator which anticommutes with any pseudoanti-Hermitian quaternionic operator will be proved, and conversely we will prove that if a quaternionic linear operator admits a linear operator which anticommutes with it, then it is pseudoanti-Hermitian. This fact allows one to conclude that any time-reversal invariant quaternionic Hamiltonian must necessarily be pseudoanti-Hermitian. In section 6, further properties and characterizations of the pseudoanti-Hermitian quaternionic operators are discussed. In section 7, a subclass of the pseudoanti-Hermitian quaternionic operators admitting an involutory linear operator which anticommutes with it is suitably characterized. To this subclass belongs any time-reversal invariant quaternionic Hamiltonian which describes fermionic quantum systems. On the basis of the previous characterization, the celebrated Kramers' theorem (stating that all energy levels of a system containing an odd number of electrons must be doubly degenerate regardless of how low the symmetry is, provided that there are no magnetic fields that remove the time-reversal symmetry), which also holds when unitary dynamics are considered in quaternionic quantum mechanics [8, 9], is recovered for the more general class of dynamics described by any time-reversal invariant quaternionic Hamiltonian with an imaginary spectrum.

2. Basic tools

A quaternion is usually expressed as

$$q = q_0 + q_1 i + q_2 j + q_3 k$$

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

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

$$q \to q^Q = q_0 - q_1 i - q_2 j - q_3 k.$$

One can verify that

$$\forall p, q \in Q \qquad (pq)^Q = q^Q p^Q.$$

Every non-zero quaternion is invertible, and the unique inverse is given by $1/q = q^Q/|q|$, where the quaternionic norm $|q|$ is defined by

$$|q|^2 = qq^Q.$$

The norm of two quaternions q and p satisfies the following property:

$$|qp| = |pq| = |p||q|.$$

Two quaternions q and p belong to the same class when the following relation is satisfied:

$$q = s^{-1}ps \qquad s \in Q. \tag{1}$$

The real part and the norm of two quaternions belonging to the same class are the same, hence also the norms of their imaginary parts coincide. Moreover, we can always assume $|s| = 1$ [10].

In a (right) finite-dimensional vector space V over Q, every linear operator is associated in a standard way with a square matrix acting on the left [11]. A necessary and sufficient condition for a quaternionic matrix to be invertible is given, for instance, in [11].

The relation

$$\langle\psi|\varphi\rangle = \sum_i \psi_i^Q \varphi_i$$

(where ψ_i, φ_i are the components in V of the vectors $|\psi\rangle$, $|\varphi\rangle$) defines a scalar product in V.

By analogy with the case of linear operators on complex vector space, one can define the Hermitian conjugate $A^\dagger = A^{TQ}$ of a matrix (A^T denotes, as usual, the transpose of A), and introduce the concepts of unitarity, Hermiticity and so on. The properties of normal operators, on quaternionic Hilbert space, have also been investigated [12].

3. Biorthonormal eigenbasis

The right eigenvalue equation for a quaternionic linear operator, H, is written as

$$H|\psi_l\rangle = |\psi_l\rangle q_l \tag{2}$$

where $|\psi_l\rangle \in V$ and $q_l \in Q$ are the quaternionic eigenvectors and their corresponding quaternionic eigenvalues. The mathematical methods to solve quaternionic eigenvalue problems can be found, for instance, in [10], where a necessary and sufficient condition is given for the diagonalizability (on finite-dimensional vector spaces) of quaternionic operators. According to [10], we can 'rephase' each eigenvector in equation (2) by means of a suitable unitary quaternion s, so that the corresponding eigenvalue, E_l (which must belong to the same class of q_l), is a complex number with positive imaginary part. Performing such rephasing, the eigenvalue equation reads

$$H|\psi_n, a\rangle = |\psi_n, a\rangle E_n \qquad E_n \in C \quad \mathrm{Im}\, E_n \geqslant 0 \tag{3}$$

where a degeneracy label a has been introduced: $a = 1, 2, \ldots, d_n$, and d_n denotes the eigenvalue degeneracy, i.e. the number of linearly independent eigenvectors associated with the eigenvalue E_n.

Let us now derive a complete biorthonormal eigenbasis for the diagonalizable quaternionic linear operators. In this paper, we limit ourselves to the study of discrete spectra only.

If H is diagonalizable, an invertible quaternionic similarity transformation S exists, such that

$$HS = S\Lambda \tag{4}$$

where Λ is the complex eigenvalue matrix. Comparing equations (3) and (4), one can easily see that the columns of S (which is in general non-unitary) must coincide with the eigenvectors $|\psi_n, a\rangle$ of H.

Multiplying the adjoint of equation (4) on the left-hand side and on the right-hand side by $S^{-1\dagger}$, we obtain

$$H^\dagger S^{-1\dagger} = S^{-1\dagger}\Lambda^* \tag{5}$$

where $*$ denotes the complex conjugation.

Denoting by $|\phi_n, a\rangle$ the ordered columns of $S^{-1\dagger}$ and looking at the previous equation column by column, the eigenvalue equation for $H^\dagger$ follows:

$$H^\dagger|\phi_n, a\rangle = |\phi_n, a\rangle E_n^*. \tag{6}$$

Note that, H not being anti-Hermitian, the state vectors $|\psi_n, a\rangle$ and $|\phi_n, a\rangle$ are, in general, different.

Moreover, the set of vectors $\{|\psi_n, a\rangle, |\phi_n, a\rangle\}$ constitutes a complete biorthonormal eigenbasis of H; indeed, from equations (4) and (5) one easily obtains

$$S^{-1}S = \mathbf{1} \quad \Leftrightarrow \quad \langle\phi_m, b|\psi_n, a\rangle = \delta_{mn}\delta_{ba} \tag{7}$$

$$S^{-1\dagger}S^\dagger = \sum_n \sum_{a=1}^{d_n} |\phi_n, a\rangle\langle\psi_n, a| = SS^{-1} = \sum_n \sum_{a=1}^{d_n} |\psi_n, a\rangle\langle\phi_n, a| = \mathbf{1}. \tag{8}$$

By using equation (8), the spectral representation of H is immediately obtained,

$$H = H\mathbf{1} = \sum_n \sum_{a=1}^{d_n} |\psi_n, a\rangle E_n \langle\phi_n, a|.$$

Finally, we observe that, if an arbitrary quaternionic choice of the spectrum is made (see equation (2)), the biorthonormal basis $\{|\psi_l\rangle, |\phi_l\rangle\} \equiv \{|\psi_n, a\rangle s(n, a), |\phi_n, a\rangle s(n, a)\}(l = 1, \ldots, \sum_n d_n)$ is obtained where $s(n, a)$ are suitable unitary quaternions (which depend on the discrete indices n and a) satisfying the following conditions:

$$s^Q(n, a)E_n s(n, a) = q_l.$$

The spectral representation of H reads, in this case,

$$H = \sum_n \sum_{a=1}^{d_n} |\psi_n, a\rangle s^Q(n, a)E_n s(n, a)\langle\phi_n, a| = \sum_l |\psi_l\rangle q_l \langle\phi_l|.$$

4. Pseudoanti-Hermitian quaternionic operators and their spectrum

In this section, a complete characterization of pseudoanti-Hermitian quaternionic operators spectra is given, and some of their properties are discussed.

Definition 1. *A quaternionic linear operator H is said to be pseudoanti-Hermitian if a linear invertible operator η exists, such that*

$$\eta H \eta^{-1} = -H^\dagger. \tag{9}$$

Note that in what follows we will prove that a Hermitian operator η always exists which fulfils condition (9). Moreover, whenever $\eta = \mathbf{1}$, $H = -H^\dagger$, so that the above definition clearly generalizes the concept of anti-Hermiticity, and the anti-Hermitian operators constitute a subclass in the larger class of pseudoanti-Hermitian operators.

The next proposition gives a complete characterization of pseudoanti-Hermitian quaternionic operator spectra.

Proposition 1. *Let H be a diagonalizable quaternionic operator. Then the following conditions are equivalent:*

(1) H is pseudoanti-Hermitian;
(2) the complex (non-imaginary) eigenvalues of H occur in pairs $(E_n, -E_n^*)$ and for each pair the degeneracy of both the eigenvalues is the same.

Proposition 1 can be easily proved by merely paraphrasing a proof given in [7] of a similar statement which holds for complex operators. We prefer to write it down again, for the benefit of the reader and also in order to fix our notation.

Proof. Let us first derive the implication (2) $\Rightarrow$ (1). Given a diagonalizable quaternionic operator H,

$$H = \sum_m |\psi_m\rangle E_m \langle\phi_m| = \sum_n \sum_{a=1}^{d_n} |\psi_n, a\rangle E_n \langle\phi_n, a|$$

where the index n (in the last term) denotes the distinct eigenvalues of H, if $\{|u_m\rangle\}$ is any complete orthonormal basis in our space, let us pose

$$O = \sum_m |\psi_m\rangle\langle u_m| \qquad \text{hence} \qquad O^{-1} = \sum_m |u_m\rangle\langle\phi_m|.$$

It is easy to show that

$$O^{-1}HO = \sum_m |u_m\rangle\langle\phi_m| \sum_{m'} |\psi_{m'}\rangle E_{m'} \langle\phi_{m'}| \sum_{m''} |\psi_{m''}\rangle\langle u_{m''}| = \sum_m |u_m\rangle E_m \langle u_m|.$$

Moreover, one easily obtains

$$(OO^\dagger)H^\dagger(OO^\dagger)^{-1} = \sum_m |\psi_m\rangle E_m^* \langle\phi_m|. \tag{10}$$

Let us now assume that condition (2) holds. We use (whenever it is necessary) the subscript '0' to denote imaginary eigenvalues and the corresponding eigenvectors, and the subscript '$\pm$' to denote the complex eigenvalues with positive or negative real parts and the same imaginary parts, respectively, and the corresponding eigenvectors. Condition (2) allows us to define a suitable operator T as follows:

$$T|\psi_{n_\pm}, a\rangle = |\psi_{n_\mp}, a\rangle \qquad T|\psi_{n_0}, a\rangle = |\psi_{n_0}, a\rangle. \tag{11}$$

Note that $T^2 = \mathbf{1}$; moreover $T = \mathbf{1}$ if and only if the spectrum of H is imaginary. Furthermore,

$$\begin{aligned} T = T\mathbf{1} = T &\left(\sum_{n_0} \sum_{a=1}^{d_{n_0}} \big|\psi_{n_0}, a\big\rangle\big\langle\phi_{n_0}, a\big| + \sum_{n_+} \sum_{a=1}^{d_{n_+}} |\psi_{n_+}, a\rangle\langle\phi_{n_+}, a| + \sum_{n_-} \sum_{a=1}^{d_{n_-}} |\psi_{n_-}, a\rangle\langle\phi_{n_-}, a| \right) \\ &= \sum_{n_0, a} \big|\psi_{n_0}, a\big\rangle\big\langle\phi_{n_0}, a\big| + \sum_{n_+, n_-, a} (|\psi_{n_-}, a\rangle\langle\phi_{n_+}, a| + |\psi_{n_+}, a\rangle\langle\phi_{n_-}, a|) \end{aligned}$$

hence,

$$\langle\phi_{n_\pm}, a|T = \langle\phi_{n_\mp}, a| \qquad \big\langle\phi_{n_0}, a\big| T = \big\langle\phi_{n_0}, a\big|. \tag{12}$$

Then, by simple calculations, one has

$$THT = -\sum_n |\psi_n\rangle E_n^* \langle\phi_n| \tag{13}$$

and finally, comparing equations (10) and (13), condition (1) follows at once, where

$$\eta = (OO^{\dagger})^{-1}T = \sum_{n_0,a} \big|\phi_{n_0}, a\big\rangle\big\langle\phi_{n_0}, a\big| + \sum_{n_+,n_-,a} (|\phi_{n_+}, a\rangle\langle\phi_{n_-}, a| + |\phi_{n_-}, a\rangle\langle\phi_{n+}, a|) = \eta^{\dagger} \tag{14}$$

and, obviously,

$$\eta^{-1} = \sum_{n_0,a} \big|\psi_{n_0}, a\big\rangle\big\langle\psi_{n_0}, a\big| + \sum_{n_+,n_-,a} (|\psi_{n_+}, a\rangle\langle\psi_{n_-}, a| + |\psi_{n_-}, a\rangle\langle\psi_{n+}, a|).$$

Let us now derive the implication (1) $\Rightarrow$ (2). According to equations (9) and (5)

$$H\eta^{-1}|\phi_n, a\rangle = -\eta^{-1}H^{\dagger}|\phi_n, a\rangle = \eta^{-1}|\phi_n, a\rangle(-E_n^*)$$

hence $\eta^{-1}|\phi_n, a\rangle \neq 0$ is an eigenvector of H associated with the eigenvalue $-E_n^*$. More generally, η^{-1} maps the eigensubspace associated with E_n to that associated with $-E_n^*$ so that, being η invertible, both the subspaces have the same dimension.

Moreover, let us observe that, if one further assumes $\eta = \eta^{\dagger}$, it is always possible to choose the eigenbasis in such a way that

$$\eta|\psi_{n_\pm}, a\rangle = |\phi_{n_\mp}, a\rangle \qquad \eta\big|\psi_{n_0}, a\big\rangle = \big|\phi_{n_0}, a\big\rangle \tag{15}$$

thus re-obtaining equation (14). □

We conclude, on the basis of the above analysis, that one can always assume that, if H is pseudoanti-Hermitian, a Hermitian operator η exists that fulfils condition (1), and which has the form given in equation (14).

Finally, recalling that in the case of the imaginary spectrum $T = \mathbf{1}$ and considering equation (10), the following statement holds:

Proposition 2. *The (complex) spectrum of a quaternionic diagonalizable pseudoanti-Hermitian operator is imaginary if and only if* $\eta = (OO^{\dagger})^{-1}$.

To conclude this section, let us consider a quantum system in a right quaternionic Hilbert space V endowed with a quaternionic scalar product, and with a (possibly non-anti-Hermitian) Hamiltonian $H = H(t)$ in general, time dependent. The quaternionic Schrödinger equation reads

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = -H|\psi\rangle. \tag{16}$$

Proposition 3. *Let* η *be a Hermitian time-independent operator in* V*. Then, the indefinite inner product* $\langle\,|\,\rangle_\eta$ *defined by*

$$\langle\psi|\varphi\rangle_\eta := \langle\psi|\eta|\varphi\rangle \qquad \forall|\psi\rangle, |\varphi\rangle \in V \tag{17}$$

is invariant under the time translation generated by the Hamiltonian H *if and only if* H *and* η *satisfy equation (9) (i.e.* H *is pseudoanti-Hermitian).*

Proof. Using the Schrödinger equation (16) and equation (17), one obtains for any two evolving state vectors $|\psi(t)\rangle$ and $|\varphi(t)\rangle$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(t)|\varphi(t)\rangle_\eta = \left(\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi|\right)\eta|\varphi\rangle + \langle\psi|\eta\frac{\mathrm{d}}{\mathrm{d}t}|\varphi\rangle = \langle\psi|(\eta H + H^{\dagger}\eta)|\varphi\rangle.$$

Therefore, $\langle\psi(t)|\varphi(t)\rangle_\eta$ is constant if and only if equation (9) holds. □

We recall that for $\eta = \mathbf{1}$ equation (9) reduces to the condition of the anti-Hermiticity of the Hamiltonian H. Hence pseudoanti-Hermitian dynamics are a generalization of unitary dynamics in Hilbert spaces.

5. Pseudoanti-Hermitian quaternionic operators and their anticommutant

In this section, we discuss the connection between the pseudoanti-Hermiticity condition and the invertible anticommutant of H (i.e. the set of invertible linear quaternionic operators which anticommute with it). This connection is highlighted by means of proposition 6 proved later in this paper. As a preliminary step, we state the following two propositions on quaternionic diagonalizable linear operators.

Proposition 4. *Let H be a diagonalizable quaternionic linear operator that admits the biorthonormal eigenbasis $\{|\psi_n, a\rangle, |\phi_n, a\rangle\}$. Then all quaternionic linear operators Δ such that*

$$\Delta H = H\Delta \tag{18}$$

are given by

$$\Delta = \sum_n \sum_{a=1}^{d_n} \sum_{b=1}^{d_n} |\psi_n, a\rangle \Delta(n; a, b) \langle \phi_n, b|$$

where

- *$\Delta(n; a, b)$ are arbitrary complex numbers if E_n is complex;*
- *$\Delta(n; a, b)$ are arbitrary quaternions if E_n is real.*

Proof. Equation (18) implies the following relations between matrix elements:

$$\langle \phi_m, b|\Delta H|\psi_n, a\rangle = \langle \phi_m, b|H\Delta|\psi_n, a\rangle.$$

By using equations (3) and (6), it is easy to obtain

$$\langle \phi_m, b|\Delta|\psi_n, a\rangle E_n = E_m \langle \phi_m, b|\Delta|\psi_n, a\rangle. \tag{19}$$

Hence if $\langle \phi_m, b|\Delta|\psi_n, a\rangle$ is different from zero, E_n and E_m must belong to the same class; but E_n and E_m are real or complex numbers with positive imaginary parts and their class can be the same only if $n = m$.

Moreover, $\Delta(n; a, b) \equiv \langle \phi_n, b|\Delta|\psi_n, a\rangle$ is necessarily complex if $\mathrm{Im}\, E_n \neq 0$, whereas it can be quaternionic only if $\mathrm{Im}\, E_n = 0$. □

Proposition 5. *Let H be a diagonalizable quaternionic linear operator. Then the set $\boldsymbol{\omega}$, of all quaternionic invertible linear operators ω such that*

$$\omega H \omega^{-1} = H^\dagger \tag{20}$$

is non-void, and is given by

$$\boldsymbol{\omega} = \rho \mathbf{G}$$

where ρ is anti-Hermitian and $\mathbf{G}$ is the invertible commutant of H.

Proof. Let $\{|\psi_n, a\rangle, |\phi_n, a\rangle\}$ be a complete biorthonormal eigenbasis associated with H,

$$H = \sum_n \sum_{a=1}^{d_n} |\psi_n, a\rangle E_n \langle \phi_n, a| \tag{21}$$

and let us consider the following operator:

$$\rho = -\sum_n \sum_{a=1}^{d_n} |\phi_n, a\rangle j \langle \phi_n, a| \qquad \text{hence} \qquad \rho^{-1} = \sum_n \sum_{a=1}^{d_n} |\psi_n, a\rangle j \langle \psi_n, a|. \tag{22}$$

Then by a simple calculation

$$\rho H \rho^{-1} = H^{\dagger}. \tag{23}$$

Hence the anti-Hermitian operator ρ belongs to $\boldsymbol{\omega}$. Moreover

$$\omega H = H^{\dagger}\omega = \rho H \rho^{-1}\omega$$

that is

$$\rho^{-1}\omega H = H\rho^{-1}\omega$$

therefore $\rho^{-1}\omega \in \mathbf{G}$, and the thesis follows at once. □

Furthermore, by analogy with the case of orthonormal basis [8], we give the following definition.

Definition 2. *Let $\mathcal{E} = \{|\psi_m\rangle, |\phi_m\rangle\}$ be a biorthonormal basis in a quaternionic Hilbert space; we define the left acting operators $I_{\mathcal{E}}$, $J_{\mathcal{E}}$, $K_{\mathcal{E}}$ as follows:*

$$I_{\mathcal{E}} := \sum_m |\psi_m\rangle i \langle\phi_m| \qquad J_{\mathcal{E}} := \sum_m |\psi_m\rangle j \langle\phi_m| \qquad K_{\mathcal{E}} := \sum_m |\psi_m\rangle k \langle\phi_m|. \tag{24}$$

The algebra is clearly isomorphic to the quaternion algebra: $I_{\mathcal{E}}^2 = J_{\mathcal{E}}^2 = K_{\mathcal{E}}^2 = -\mathbf{1}$, $I_{\mathcal{E}} J_{\mathcal{E}} = -J_{\mathcal{E}} I_{\mathcal{E}} = K_{\mathcal{E}}$.

Let us now prove our main result.

Proposition 6. *A quaternionic diagonalizable linear operator H is pseudoanti-Hermitian if and only if a linear invertible quaternionic operator $\widehat{\Omega}$ exists such that $\{H, \widehat{\Omega}\} = 0$.*

Proof. Let H be a pseudoanti-Hermitian operator. By using equations (9) and (23) one immediately obtains

$$\eta H \eta^{-1} = -\rho H \rho^{-1}.$$

Hence, the linear operator $\Omega = \rho^{-1}\eta$ anticommutes with H:

$$\Omega H + H\Omega = 0.$$

The explicit form of Ω is easily obtained from equations (14) and (22),

$$\begin{aligned}\Omega = \rho^{-1}\eta &= \sum_{n_0,a} \left|\psi_{n_0}, a\right\rangle j \left\langle\phi_{n_0}, a\right| + \sum_{n_+,n_-,a} (|\psi_{n_+}, a\rangle j \langle\phi_{n_-}, a| + |\psi_{n_-}, a\rangle j \langle\phi_{n_+}, a|) \\ &= T J_{\mathcal{B}} = J_{\mathcal{B}} T.\end{aligned} \tag{25}$$

Then Ω coincides with the product $T J_{\mathcal{B}}$, where T is the operator defined in the proof of proposition 1 and $J_{\mathcal{B}}$ is defined in equation (24), with $\mathcal{B} = \{|\psi_n, a\rangle, |\phi_n, a\rangle\}$. Finally, let us note that $\Omega^2 = -\mathbf{1}$.

In order to prove the converse implication, let us assume that an invertible operator $\widehat{\Omega}$ exists such that

$$\widehat{\Omega} H + H\widehat{\Omega} = 0.$$

Then by using proposition 5, the previous equation implies

$$(\rho\widehat{\Omega})H = -H^{\dagger}(\rho\widehat{\Omega})$$

therefore, according to definition 1 (with $\eta = \rho\widehat{\Omega}$), H is pseudoanti-Hermitian. □

As a consequence of the previous statement, it can be immediately shown that any operator which anticommutes with H has the form

$$\widehat{\Omega} = \Omega g \qquad g \in \mathbf{G} \tag{26}$$

where Ω is given by equation (25).

Moreover, the following statement holds:

Proposition 7. *A quaternionic diagonalizable pseudoanti-Hermitian operator H has imaginary spectrum if and only if it anticommutes with $J_{\mathcal{B}}g$ ($g \in \mathbf{G}$).*

Proof. Recalling that in the case of imaginary spectrum $T \equiv \mathbf{1}$, and using equation (25) the proof immediately follows. □

We conclude this section by observing that proposition 6 has an interesting physical interpretation in quaternionic quantum mechanics. Indeed, whenever H is the Hamiltonian of some physical system, it establishes a link between the properties of H and the symmetries of the physical system described by it. Since the time-reversal symmetry is associated in quaternionic quantum mechanics with a linear unitary operator with the remarkable property that it must anticommute with the Hamiltonian [8]. Hence, whenever a quaternionic quantum system admits such a symmetry (or else, more generally, it is invariant under the combined action of the time-reversal operator times a geometrical symmetry operator), the anticommutant of its Hamiltonian must be non-void, then H is a pseudoanti-Hermitian operator.

6. Further properties of the pseudoanti-Hermitian operators

In this section, a useful characterization of the pseudoanti-Hermitian quaternionic operators is obtained and some of their properties are derived.

Let us first observe that the operator Ω given in equation (25) and the operator $\Omega' = T K_{\mathcal{B}}$, where T is the operator defined in the proof of proposition 1 and $K_{\mathcal{B}}$ is given in equation (24) with $\mathcal{B} = \{|\psi_n, a\rangle, |\phi_n, a\rangle\}$, are diagonalizables and a biorthonormal eigenbasis associated with them can be easily obtained.

In fact, posing

$$\{|v_m\rangle\} = \left\{ \big|\psi_{n_0}, a\big\rangle, \frac{1}{\sqrt{2}}(|\psi_{n_+}, a\rangle + |\psi_{n_-}, a\rangle), \frac{1}{\sqrt{2}}(|\psi_{n_+}, a\rangle - |\psi_{n_-}, a\rangle)\,\mathrm{i} \right\}$$

and

$$\{|w_m\rangle\} = \left\{ \big|\phi_{n_0}, a\big\rangle, \frac{1}{\sqrt{2}}(|\phi_{n_+}, a\rangle + |\phi_{n_-}, a\rangle), \frac{1}{\sqrt{2}}(|\phi_{n_+}, a\rangle - |\phi_{n_-}, a\rangle)\,\mathrm{i} \right\}$$

it is easy to check that the set of vectors, $\mathcal{T} = \{|v_m\rangle, |w_m\rangle\}$, is a biorthonormal basis. Moreover

$$\Omega = \sum_m |v_m\rangle j \langle w_m| \tag{27}$$

and

$$\Omega' = \sum_m |v_m\rangle k \langle w_m|. \tag{28}$$

The next proposition provides us with the 'imaginary' form of the pseudoanti-Hermitian quaternionic operators.

Proposition 8. *A quaternionic diagonalizable linear operator H is pseudoanti-Hermitian if and only if a basis exists in which it assumes the form $H = \mathrm{i}H_1$ where H_1 is a suitable real matrix.*

Proof. Let H be pseudoanti-Hermitian. Then two operators Ω and Ω' given in equations (27) and (28) always exist which anticommute with it. Let $\mathcal{T} = \{|v_m\rangle, |w_m\rangle\}$ be the biorthonormal eigenbasis associated with Ω and Ω' (of course, the case of an orthonormal basis is obtained by setting $v = w$ in the following formulae), and let us consider the matrix elements of H in such a basis:

$$\begin{aligned}\langle w_i|H|v_k\rangle &= \langle w_i|\sum_n |\psi_n\rangle E_n\langle\phi_n|v_k\rangle = \langle w_i|\Omega H\Omega|v_k\rangle \\ &= \langle w_i|\sum_m |v_m\rangle j\langle w_m|\sum_n |\psi_n\rangle E_n\langle\phi_n|\sum_{m'}|v_{m'}\rangle j\langle w_{m'}|v_k\rangle \\ &= \sum_{m,m',n}\delta_{im} j\langle w_m|\psi_n\rangle E_n\langle\phi_n|v_{m'}\rangle j\delta_{m'k} = j\langle w_i|\sum_n |\psi_n\rangle E_n\langle\phi_n|v_k\rangle j \\ &= j\langle w_i|H|v_k\rangle j.\end{aligned}$$

By the same calculations, with Ω' in place of Ω, one obtains

$$\langle w_i|H|v_k\rangle = \langle w_i|\Omega' H\Omega'|v_k\rangle = k\langle w_i|H|v_k\rangle k = j\langle w_i|H|v_k\rangle j$$

so that necessarily $\langle w_i|H|v_k\rangle = \mathrm{i}h_1$, $h_1 \in R$.

In order to prove the converse implication, let $H = \mathrm{i}H_1$ (where H_1 is a real matrix) be given. Then the operator $\Omega = j\mathbf{1}$ (or $\Omega' = k\mathbf{1}$) anticommutes with it. Hence by proposition 6, H is pseudoanti-Hermitian. □

Finally, we give the following definition in order to obtain an interesting property of the pseudoanti-Hermitian quaternionic operators.

Definition 3. *A quaternionic linear operator U is said to be ζ-pseudounitary if a Hermitian invertible operator ζ exists such that*

$$\zeta^{-1}U^\dagger\zeta = U^{-1}.$$

One easily recognizes that the operators Ω and Ω', given in equations (27) and (28), are η-pseudounitary. Indeed, by a straightforward calculation

$$\eta^{-1}\Omega^\dagger\eta = -\Omega = \Omega^{-1}$$

($\Omega^2 = -\mathbf{1}$), and the same happens for Ω'. Then, also the operator

$$U(\theta) = \cos\theta\,\Omega + \sin\theta\,\Omega' \qquad \theta \in R \tag{29}$$

is η-pseudounitary and anticommutes with H, so that we can conclude: *for any pseudoanti-Hermitian quaternionic operator, H, a one-parameter family of η-pseudounitary quaternionic operators $U(\theta)$ exists, (with $U^2(\theta) = -\mathbf{1}$) which anticommutes with it.*

This last statement generalizes a standard result that holds for anti-Hermitian quaternionic operators [8] to the more general case of the pseudoanti-Hermitian ones.

7. Pseudoanti-Hermiticity and Kramers' degeneracy

As we said at the end of section 5, when time-reversal invariant physical systems are considered in quaternionic quantum mechanics, the Hamiltonian H must be pseudoanti-Hermitian. The time-reversal operator, t, is unitary with the remarkable property that $t^2 = \pm\mathbf{1}$ when fermionic or bosonic quantum systems are respectively considered [8, 9] (note that the sign of t^2 in the fermionic and bosonic systems is opposite in quaternionic quantum mechanics with respect to that in complex quantum mechanics). Moreover, as we have underlined in the introduction, Kramers' theorem also holds when quaternionic time-reversal invariant unitary dynamics of the fermionic systems are considered [8, 9].

In order to discuss the time-reversal invariance of the fermionic systems and the Kramers degeneracy in the context of the non-unitary quaternionic dynamics (i.e. when non-anti-Hermitian Hamiltonians are taken into account), we give now the following proposition that allows one to characterize a subclass of pseudoanti-Hermitian operators which admits an involutory linear operator which anticommutes with it.

Proposition 9. *Let H be a quaternionic diagonalizable linear operator. Then the following conditions are equivalent:*

(i) a linear involutory operator, Θ, exists such that $\{H, \Theta\} = 0$;
(ii) H is pseudoanti-Hermitian and the degeneracy, d_{n_0}, of its imaginary eigenvalues is even.

Proof. Let us assume that condition (i) holds; then by proposition 6, H is pseudoanti-Hermitian.

Let us now prove that d_{n_0} must be even. Recall that any operator which anticommutes with H must have the form $\Theta = \Omega h$ ($h \in \mathbf{G}$) where Ω is given by equation (25). Now, Θ being involutory and $\Omega^2 = -\mathbf{1}$,

$$h\Omega h = -\Omega. \tag{30}$$

Furthermore, the explicit form of the commutant given in proposition 4 and equation (24) implies the following constraints on the matrix elements of h and Ω, respectively:

$$\langle\phi_n|h|\psi_{n'}\rangle = 0 \qquad \text{whenever} \quad n \neq n'$$

and

$$\langle\phi_n|\Omega|\psi_{n'}\rangle = 0 \qquad \text{unless}\, n = n' = n_0 \quad \text{or} \quad n = n_\pm \text{ and } n' = n_\mp.$$

Therefore, we can study equation (30) limiting ourselves to considering the eigensubspaces associated with each distinct imaginary eigenvalue E_{n_0}, and the subspaces associated with the eigenvalue pairs (E_{n_+}, E_{n_-}), separately.

Denoting by D the invertible complex matrix (see proposition 4) associated with h in the eigensubspace corresponding to the imaginary eigenvalue E_{n_0}, equation (30) reads

$$Dj\mathbf{1}_{d_{n_0}}D = -j\mathbf{1}_{d_{n_0}}$$

where $\mathbf{1}_{d_{n_0}}$ denotes the identity matrix of dimension d_{n_0}. Then one obtains

$$D^*D = -\mathbf{1}_{d_{n_0}}. \tag{31}$$

Hence

$$0 < (\det D)^* \det D = \det(D^*D) = (-1)^{d_{n_0}}$$

which implies that d_{n_0} must be even.

In order to prove the converse implication, let us assume that H is pseudoanti-Hermitian with d_{n_0} even. Then, choosing an opportune element $h \in \mathbf{G}$ given by

$$h = \sum_{n_0} \sum_{a=1}^{d_{n_0}/2} \left(\left|\psi_{n_0}, a\right\rangle\!\left\langle\phi_{n_0}, a + d_{n_0}/2\right| - \left|\psi_{n_0}, a + d_{n_0}/2\right\rangle\!\left\langle\phi_{n_0}, a\right|\right) + \sum_{n_+,a} |\psi_{n_+}, a\rangle\langle\phi_{n_+}, a| - \sum_{n_-,a} |\psi_{n_-}, a\rangle\langle\phi_{n_-}, a|$$

$$\left(h^{-1} = \sum_{n_0} \sum_{a=1}^{d_{n_0}/2} \left(-\left|\psi_{n_0}, a\right\rangle\left\langle\phi_{n_0}, a + d_{n_0}/2\right| + \left|\psi_{n_0}, a + d_{n_0}/2\right\rangle\left\langle\phi_{n_0}, a\right| \right) \right.$$

$$\left. + \sum_{n_+,a} |\psi_{n_+}, a\rangle \langle\phi_{n_+}, a| - \sum_{n_-,a} |\psi_{n_-}, a\rangle \langle\phi_{n_-}, a| \right)$$

the operator

$$\Theta = \Omega h = \sum_{n_0} \sum_{a=1}^{d_{n_0}/2} \left(\left|\psi_{n_0}, a\right\rangle j \left\langle\phi_{n_0}, a + d_{n_0}/2\right| - \left|\psi_{n_0}, a + d_{n_0}/2\right\rangle j \left\langle\phi_{n_0}, a\right| \right)$$
$$+ \sum_{n_+,n_-} \sum_{a=1}^{d_{n+}} (-|\psi_{n_+}, a\rangle\, j\, \langle\phi_{n_-}, a| + |\psi_{n_-}, a\rangle\, j\, \langle\phi_{n_+}, a|) \tag{32}$$

obviously anticommutes with H and, by a direct calculation, $\Theta^2 = \mathbf{1}$. □

As a direct consequence of the previous proposition, the following statement holds:

Proposition 10. *The eigenvalues of any diagonalizable quaternionic operator with imaginary spectrum that admits an involutory linear operator which anticommutes with it, must be at least doubly degenerate.*

Proposition 10 has an interesting physical property. In fact, if we limit ourselves to considering the time-reversal invariant fermionic systems ($t^2 = \mathbf{1}$) described by any quaternionic (not necessarily anti-Hermitian) Hamiltonian with imaginary spectrum, then its eigenvalues must be at least doubly degenerate and hence, for such systems, Kramers' theorem still holds.

Conversely, if one considers a fermionic system described by a (not necessarily anti-Hermitian) quaternionic Hamiltonian with imaginary spectrum which admits an odd degeneracy of some eigenvalue, a time-reversal violating effect can certainly be shown (see, for instance, [13], in which time-reversal violating effects are shown for a two-level fermionic system described by a quaternionic anti-Hermitian Hamiltonian).

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