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ON A DECOMPOSITION THEOREM FOR DENSITY OPERATORS OF A PURE QUANTUM STATE

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Abstract

We investigate conditions for the existence of a decomposition of a hermitian projector ρ into two hermitian and time reversal invariant operators ρ_0 and χ under the form $\rho = e^{i\chi} \rho_0 e^{-i\chi}$. Sufficient conditions are given, and an explicit construction of a decomposition is performed when they are fulfilled. A stronger theorem of existence and unicity is studied. All the proofs are valid for any p-body reduced density operator of a pure state of a system of bosons as well as fermions. The decomposition studied in this work has already been used in Nuclear Physics, and may be of interest in other fields of Physics.

Introduction

The purpose of this paper is to study the following problem : given a hermitian projector ρ defined on a Hilbert space of quantal states, under what conditions (necessary or sufficient) does there exist two hermitian and time reversal invariant operators ρ_0 and χ such that

$$\rho = e^{i\chi} \rho_0 e^{-i\chi} \quad . \tag{1}$$

Such a decomposition was first introduced by Baranger and Vénéroni[1] and in the version of these authors it constitutes the starting point of the so-called "adiabatic time-dependent Hartree-Fock approximation" (ATDHF). In the framework of this formalism, the projector ρ is the reduced single-particle density operator of a system of independent spin 1/2 particles satisfying the condition $\rho^2 = \rho$, i.e. the corresponding wave-function Ψ is a Slater determinant. In the "adiabatic" limit (the collective motion is supposed to be slow compared to characteristic single-particle excitations), the decomposition (1) seems to be crucial to provide a relation between the time-dependent Hartree-Fock approximation and phenomenological descriptions of collective motion such as the Copenhagen model[2].

Indeed, as shown in Ref.1, a necessary condition for the adiabaticity is $\| \chi \| \ll 1$. The expansion of ρ given by (1), truncated at second order in χ , can then be introduced into the stationarity principle :

$$\delta \int_{t_1}^{t_2} \langle\Psi| i \frac{\partial}{\partial t} - H|\Psi\rangle \, dt = 0 \qquad , \qquad (2)$$

where "δ" stands for independent variations of Ψ and Ψ^* restricted to be Slater determinants, with fixed end points for Ψ. This procedure leads to a new expression for the integrant of (2) which exhibits exactly the same structure as the Lagrangian $\mathcal{L}_{c\ell}$ of a classical system written in terms of canonically conjugate variables :

$$\mathcal{L}_{c\ell} = \sum_i p_i \dot{q}_i - \frac{1}{2} \sum_{i,j} \left[\mathcal{M}^{-1}\right]_{ij} p_i p_j - V(q_i) \quad .$$

In this analogy, the matrix elements of ρ_0 and χ play respectively the roles of coordinates and conjugate momenta. Variations of the corresponding classical action with respect to ρ_0 and χ lead therefore to Hamilton-like equations of motion[3]. The first Hamilton equation provides mass parameters for a given "path" $\rho_0(t)$. The second equation of motion, when solved together with the first one, gives access to this collective path. Such a connexion between microscopic theories and phenomenological semi-classical models seems to be very promising for a better understanding of the nature of collective variables ; the first numerical applications of ATDHF to the calculation of mass parameters in nuclei[4] already provide some informations in this respect.

As other essential features of ATDHF formalism, we mention the following points : i) ATDHF allows the description of large amplitude collective phenomena ; in the small amplitude limit, ATDHF strictly reduces to the Random Phase Approximation. ii) Calculation of mass parameters by ATDHF is a self-consistent version of the Inglis[5] (cranking) procedure. It gives the correct mass for uniform translational motion, and furnishes the Thouless-Valatin[6] inertial parameters for rotational nuclei.

To our knowledge, decomposition (1) has been used up to now only for single-particle density operators of nuclei. Studies of its validity[7,8] have also been restricted to this particular case. The proof of existence given here is valid for the p-body reduced density matrices of systems of bosons as well as of fermions, provided they are projectors and they satisfy some conditions precised in section 2 . The stringent limitation due to the projection character of ρ excludes applications to non pure n-body states. Conditions for existence of the decomposition (1) are investigated in some details : their study has been partly neglected in the preceding works. Indeed they were focused on the ATDHF approximation, where the assumed smallness of χ makes the discussion much simpler.

The proof of the decomposition theorem given in the present work is inspired from mathematical studies of pairs of projectors which can be found for instance in Refs. 9,10. In the particular case of hermitian operators ρ , the theorem which we demonstrate is stronger than the corresponding results of these references, in the sense that we are able to impose the additional time reversal invariance for the operators χ and ρ_0.

For sake of simplicity, the proofs given below are limited to a finite N-dimensional hermitian space $\mathcal{H}$. However most of the results can be extended to infinite dimensional Hilbert spaces in the case where ρ has a finite trace. All the operators involved are linear operators defined on $\mathcal{H}$, except the antilinear time reversal operator T.

Sect. 1 is devoted to the study of some results concerning quantum time reversal which are used in sects. 2 and 3. Sect. 2 is the central part of this work ; the decomposition theorem is demonstrated there for the most general density projection operator satisfying some sufficient conditions. Finally we investigate in sect. 3 some special conditions for the existence of the decomposition (1) for the reduced single-particle density operator of a system of fermions.

1. Some useful properties of quantum time reversal

The aim of this section is to give some theorems which will be essential for the demonstration of the existence theorem of sect.2. For well known properties of time reversal, the reader is referred to Refs.11,12.

In the following the time-reversed of any linear operator A will be called A_T : $A_T = T^+AT$, and $|\bar{u}\rangle$ the time reversed of any vector $|u\rangle$: $|\bar{u}\rangle = T|u\rangle$, where T is the time reversal operator.

As well known, the operator T is antiunitary, i.e. is antilinear :

$$T(\alpha|\varphi\rangle+\beta|\Psi\rangle) = \alpha^*T|\varphi\rangle+\beta^*T|\Psi\rangle \quad ,$$

and satisfies

$$T^+T = TT^+ = 1 \ .$$

Moreover it can be shown that

$$T^2 = \pm 1 \quad . \tag{3}$$

In the latter equation, the plus sign applies to any system of bosons, or to systems containing an even number of fermions ; the minus sign applies to an odd system of fermions.

The first result to establish is a characteristic property of time reversal invariant (time-even) hermitian operators, i.e. verifying $A_T = A^+ = A$. Note that A has the following property :

if

$$A|e_i\rangle = \lambda_i|e_i\rangle \quad , \tag{4}$$

then

$$A|\bar{e}_i\rangle = \lambda_i^*|\bar{e}_i\rangle = \lambda_i|\bar{e}_i\rangle \quad . \tag{5}$$

This property is valid irrespective of the sign in Eq.(3). The following theorems, 1 and I bis, provide criteria to identify a time-even hermitian operator by its spectral representation, respectively in the cases $T^2 = 1$ and $T^2 = -1$.

Theorem 1

Let T be the time reversal operator satisfying $T^2 = 1$. A hermitian operator is time-even if and only if it is diagonable in a real[13] orthogonal basis.

Proof

a) If A is hermitian - thus diagonable - and has a complete set of real eigenvectors :

$$A = \sum_{i=1}^{N} \lambda_i |e_i\rangle\langle e_i| \ , \quad \lambda_i \in \mathbb{R} \ ,$$

$$|e_i\rangle = |\bar{e}_i\rangle \qquad i = 1,\ldots,N \ , \tag{6}$$

then

$$A_T = \sum_{i=1}^{N} \lambda_i^* |\bar{e}_i\rangle\langle \bar{e}_i| \ ,$$

and hermiticity of A together with Eq.(6) lead immediately to the time reversal invariance of A.

b) Suppose $A = A^+ = A_T$. Let $|\alpha\rangle$ be an eigenvector of A :

$$A|\alpha\rangle = \alpha|\alpha\rangle \quad .$$

One can easily verify that it is always possible to find a C-number C_α such that the vector

$$|a\rangle = C_\alpha|\alpha\rangle + C_\alpha^*|\bar{\alpha}\rangle \tag{7}$$

is normed to unity. Such a vector is clearly a real eigenvector of A. Hence it is always possible to find a real eigenvector associated with each eigenvalue. From hermiticity of A, it follows that two real eigenvectors corresponding to different eigenvalues are orthogonal.

It remains to show that each eigensubspace of A of dimensionality greater than one can be generated by real orthogonal vectors. To do this, one constructs a first real eigenvector $|a\rangle$ associated to the degenerate eigenvalue α by Eq.(7). In the eigensubspace $\mathcal{H}_\alpha$ corresponding to α, there exists a vector $|\beta\rangle$ orthogonal to $|a\rangle$. The equation $\langle a|\beta\rangle = 0$ and the time reversal invariance of $|a\rangle$ implie $\langle a|\bar{\beta}\rangle = 0$. Thus

the real eigenvector

$$|b\rangle = C_\beta|\beta\rangle + C_\beta^*|\bar{\beta}\rangle$$

is orthogonal to $|a\rangle$. By carrying on this procedure, one can find a set of real orthogonal eigenvectors spanning each eigensubspace $\mathcal{H}_\alpha$.

Theorem 1 bis

Let T be the time reversal operator satisfying $T^2 = -1$. A hermitian operator A is time-even if and only if it is diagonable in an orthogonal basis of the type $\{|e_i\rangle, |\bar{e}_i\rangle \; ; \; i=1,\ldots,\frac{N}{2}\}$ with the same eigenvalue associated to $|e_i\rangle$ and $|\bar{e}_i\rangle$:

$$A = \sum_{i=1}^{N/2} \lambda_i (|e_i\rangle\langle e_i| + |\bar{e}_i\rangle\langle\bar{e}_i|) \quad , \quad \lambda_i \in \mathbb{R} \; . \tag{8}$$

Proof

a) If Eq. (8) is satisfied, the time reversal invariance of A follows immediately.

b) Since $T^2 = -1$, there cannot exist real eigenvectors. Moreover two vectors conjugate of each other by time inversion are always orthogonal (see for instance Ref. 12 p. 574). From this remark, the recipe for construction of a complete orthogonal set of eigenvectors of A of the type $\{|e_i\rangle, |\bar{e}_i\rangle\}$ is straightforward : take one eigenvector $|e_1\rangle$ of A for the eigenvalue λ_1 ; Eqs. (4) and (5) guarantee that $|\bar{e}_1\rangle$ is also an eigenvector of A for the same eigenvalue λ_1. As already mentioned, $|\bar{e}_1\rangle$ is orthogonal to $|e_1\rangle$. If the eigensubspace corresponding to λ_1 is of dimensionality greater than two, one can find $|e_1'\rangle$ orthogonal to both $|e_1\rangle$ and $|\bar{e}_1\rangle$ such that $A|e_1'\rangle = \lambda_1|e_1'\rangle$. By Eqs. (4) and (5) one knows that $|\bar{e}_1'\rangle$ satisfies $A|\bar{e}_1'\rangle = \lambda_1|\bar{e}_1'\rangle$; furthermore, one can easily show that $|\bar{e}_1'\rangle$ is also orthogonal to $|e_1\rangle$ and $|\bar{e}_1\rangle$. Consequently, the four vectors $|e_1\rangle$, $|e_1'\rangle$, $|\bar{e}_1\rangle$, $|\bar{e}_1'\rangle$ are orthogonal to each other, and belong to the same eigensubspace of A. Proceeding further by this method, one gets the spectral decomposition of A under the form (8), where the set $\{|e_i\rangle , |\bar{e}_i\rangle; i = 1,\ldots,\frac{N}{2}\}$ is orthogonal.

As an immediate consequence, the multiplicity of any eigenvalue of a time-even hermitian operator is an even number when the time reversal operator satisfies $T^2 = -1$. When one is concerned with the Hamiltonian of an odd system of fermions, this property is known as Kramer's degeneracy.

It is now possible to set up the following properties of commuting hermitian time-even operators :

Theorem 2

Let T be the time reversal operator satisfying $T^2 = 1$. Then two hermitian time-even operators which commute have a common complete orthogonal set of real eigenvectors.

Theorem 2bis

Let T be the time reversal operator satisfying $T^2 = -1$. Then two hermitian time-even operators A and B which commute can be simultaneously diagonalized in an orthogonal basis of the type $\{|e_i\rangle, |\bar{e}_i\rangle ; i = 1,\ldots,\frac{N}{2}\}$, such that

$$A = \sum_{i=1}^{N/2} \lambda_i (|e_i\rangle\langle e_i| + |\bar{e}_i\rangle\langle\bar{e}_i|) \ , \ \lambda_i \in \mathbb{R} \ ,$$

$$B = \sum_{i=1}^{N/2} \mu_i (|e_i\rangle\langle e_i| + |\bar{e}_i\rangle\langle\bar{e}_i|) \ , \ \mu_i \in \mathbb{R} \ .$$

The proofs of these theorems are straightforward ; they follow closely those of theorems 1 and 1bis. Theorems 2 and 2 bis permit to get the last result of this section, which will be essential in the following :

Theorem 3

Let T be the time reversal operator satisfying $T^2 = \pm 1$, and let U be a unitary operator.

i) A necessary and sufficient condition for the existence of a hermitian time-even operator A satisfying

$$U = e^{iA} \tag{9}$$

is that

$$U_T = U^+ \quad . \tag{10}$$

ii) The operator A is uniquely defined if one requires that all its eigenvalues λ_i belong to a given interval :

$$\lambda_i \in [\alpha, \alpha + 2\pi[\quad . \tag{11}$$

Proof

i) The necessary condition is obvious.

Conversely, let us suppose that (10) is satisfied, and decompose U into its hermitian and antihermitian parts :

$$U = U_1 + i\, U_2 \quad ,$$

with

$$U_1 = \frac{1}{2}(U + U^+) \quad , \quad U_2 = \frac{1}{2i}(U - U^+) \quad .$$

The operators U_1 and U_2 are hermitian by definition, and time-even by virtue of (10). Moreover, the unitarity of U leads to $[U_1, U_2] = 0$. Consequently the operators U_1 and U_2 have the property stated in Theorem 2, or 2bis, according as $T^2 = 1$ or $T^2 = -1$. To any eigenvalue $e^{i\lambda}$ of U correspond the eigenvalues $\cos\lambda$ and $\sin\lambda$ of U_1 and U_2, attached to the same eigenvector of U_1 and U_2.

In other words, when $T^2 = 1$,

$$U_1 = \sum_{i=1}^{N} \cos\lambda_i |e_i\rangle \langle e_i|$$

$$U_2 = \sum_{i=1}^{N} \sin\lambda_i |e_i\rangle\langle e_i|$$

$$\lambda_i = \lambda_i^*, \quad |e_i\rangle = |\bar{e}_i\rangle \qquad i = 1,\ldots,N$$

$$\langle e_i|e_j\rangle = 0 \qquad i,j = 1,\ldots,N,$$

and when $T^2 = 1$,

$$U_1 = \sum_{i=1}^{N/2} \cos\lambda_i (|e_i\rangle\langle e_i|+|\bar{e}_i\rangle\langle\bar{e}_i|)$$

$$U_2 = \sum_{i=1}^{N/2} \sin\lambda_i (|e_i\rangle\langle e_i|+|\bar{e}_i\rangle\langle\bar{e}_i|)$$

$$\lambda_i = \lambda_i^* \qquad i = 1,\ldots,N/2,$$

$$\langle e_i|e_j\rangle=\langle e_i|\bar{e}_j\rangle= \langle\bar{e}_i|\bar{e}_j\rangle = 0 \qquad i,j = 1,\ldots,N/2.$$

Let us then define

$$A = \sum_{i=1}^{N} \lambda_i |e_i\rangle\langle e_i| \qquad \text{when } T^2 = 1$$

or

$$A = \sum_{i=1}^{N/2} \lambda_i (|e_i\rangle\langle e_i| + |\bar{e}_i\rangle\langle\bar{e}_i|) \qquad \text{when } T^2 = -1,$$

where λ_i belongs to the interval :

$$\lambda_i \in [\alpha, \alpha + 2\pi[\quad . \tag{11}$$

The operator A has real eigenvalues and is diagonable in an orthogonal basis ; thus it is hermitian. According to theorem 1, or 1bis, it is time-even, which achieves the proof of theorem 3, part i).

ii) Any operator A fulfilling (9) commutes with U, since $[A,e^{iA}] = 0$. By taking the hermitian and antihermitian parts of

$$[U,A] = 0 ,$$

one gets

$$[U_1,A] = [U_2,A] = 0 \quad .$$

Since moreover the hermitian operators U_1 and U_2 commute with each other, it is possible to find a complete set $\{|e_i\rangle\}$ of vectors which are common eigenstates of A, U_1, U_2 , and therefore of U too :

$$U|e_j\rangle = \nu_j|e_j\rangle$$

and

$$A|e_j\rangle = \lambda_j|e_j\rangle$$

with

$$e^{i\lambda_j} = \nu_j \qquad (12)$$

If all the eigenvalues λ_j of A are constrained to lie within the same interval $[\alpha,\alpha+2\pi[$, then each λ_j is uniquely defined from ν_j by eq.(12). The biunivocal correspondence between ν_j and λ_j then guarantees that all the eigenvectors of U are also eigenvectors of A (and not only those of the particular set $\{|e_j\rangle\}$). According to this property, there exists one unique hermitian operator A satisfying (11) and (9). If U fulfils (10), such an operator

A is time-even.

Theorem 3 will be the only result of this section used in sect.2. Since it has been proved in the two cases $T^2 = \pm 1$, all the results of the next section hold for systems of fermions as well as bosons.

2. The decomposition theorem

In the first part of this section, we demonstrate the existence of two hermitian and time-even operators ρ_c and χ satisfying Eq.(1), provided some conditions are fulfilled.
The proof of the existence theorem is performed by exhibiting a particular solution (ρ_c, χ), whose properties are studied in part .
Results of part B enable to obtain, in sect.2-C, a new result, the decomposition theorem, which is stronger than the existence theorem proved in sect.2-A.

A - The existence theorem

Before stating the existence theorem, it is useful to mention a preliminary result which permits to formulate the conditions for the existence of the decomposition (1) in several equivalent ways.

Preliminary result

Let ρ and ρ' be two hermitian projection operators. The following assumptions are equivalent :

(P_1) $\|\rho-\rho'\| < 1$.[14]

(P_2) The operator $(1-R)$ is regular, where

$$R = (\rho-\rho')^2 .$$

(P_3) The unitary operator

$$\tau\tau' = (2\rho-1)(2\rho'-1) \tag{13}$$

does not admit the eigenvalue $\nu = -1$.

(P_4) The projectors ρ and ρ' do not have any common eigenvector corresponding to different eigenvalues of ρ and ρ'.

The proof of these equivalences is rather straightforward, and is left to the reader.

Existence theorem

Let ρ be a hermitian projector and ρ_T its time-reversed. If ρ and ρ_T satisfy the equivalent hypothesis (P_1), there exists two operators ρ_0 and χ such that

$$\rho = e^{i\chi} \rho_0 e^{-i\chi} \tag{1}$$

$$\rho_0 = \rho_0^+ = (\rho_0)_T \tag{14}$$

$$\chi = \chi^+ = \chi_T \tag{15}$$

Lemma

Let ρ be a hermitian projector and ρ_T its time-reversed. If ρ and ρ_T satisfy the hypothesis (P_1), there exists a time-even hermitian operator χ such that

$$\rho_T = e^{-2i\chi} \rho e^{2i\chi} \quad . \tag{16}$$

Proof

The proof given here is suggested by results concerning pairs of projectors which can be found in Refs. 9,10.

Consider the hermitian and time-even operator :

$$1-R = 1-(\rho-\rho_T)^2 \quad .$$

Since ρ and ρ_T satisfie (P_1), this operator is strictly positive and one can define a hermitian inverse square root. A possible -but not unique- choice is the sum of the absolutely convergent series :

$$(1-R)^{-\frac{1}{2}} = \sum_{n=0}^{\infty} \binom{-1/2}{n} (-R)^n \quad .$$

Introducing the hermitian involution $\tau = 2\rho - 1$, one easily finds :

$$1-R = \frac{1}{4}(\tau\tau_T + \tau_T\tau + 2) \ .$$

Notice that the operator (1-R) commutes with ρ and ρ_T :

$$[1-R,\rho] = [1-R,\rho_T] = 0 \qquad (17)$$

Let us define :

$$U = [\rho\rho_T+(1-\rho)(1-\rho_T)](1-R)^{-\frac{1}{2}} = (1-R)^{-\frac{1}{2}}[\rho\rho_T+(1-\rho)(1-\rho_T)] \ , \qquad (18)$$

or, in terms of τ and τ_T :

$$U = (\tau\tau_T+\tau_T\tau+2)^{-\frac{1}{2}}(\tau\tau_T+1) = (\tau\tau_T+1)(\tau\tau_T+\tau_T\tau+2)^{-\frac{1}{2}} \ . \qquad (19)$$

We will now show that U is a unitary operator satisfying (10) and transforming ρ into ρ_T.

i) U is unitary : using the property (17), one gets

$$UU^+ = (\tau\tau_T+\tau_T\tau+2)^{-1}(\tau\tau_T+1)(\tau_T\tau+1) \ ,$$

and the involutive character of τ_T leads to $UU^+ = 1$.

ii) $U_T = U^+$. (10)

This property of U is an immediate consequence of hermiticity, time reversal invariance, and property (17) of (1-R).

iii) $\rho_T = U^+ \rho U$. (20)

To show this, let us consider

$$U\tau_T = (1-R)^{-\frac{1}{2}}(\tau\tau_T+1)\tau_T = (1-R)^{-\frac{1}{2}}(\tau+\tau_T) \quad ,$$

where we have used the involutive character of τ_T. Similarly :

$$\tau U = \tau(\tau\tau_T+1)(1-R)^{-\frac{1}{2}} = (\tau+\tau_T)(1-R)^{-\frac{1}{2}} \quad .$$

Using Eq.(17), one gets :

$$\tau U = U\tau_T \quad ,$$

or :

$$\tau_T = U^{+}\tau U \quad ,$$

which is equivalent to Eq.(20).

According to theorem 3, one can define an operator χ which satisfies :

$$U = e^{2i\chi} \quad , \qquad (21)$$

$$\chi = \chi^{+} = \chi_T \quad . \qquad (15)$$

Eq.(20), together with (15) and (21), show the lemma.

To achieve the proof of the theorem, it remains to show that the hermitian projector ρ_0 defined by

$$\rho_0 = e^{-i\chi}\,\rho\,e^{i\chi} \qquad (22)$$

is time-even. Indeed its time-reversed is

$$(\rho_0)_T = e^{i\chi}\rho_T\,e^{-i\chi} \quad , \qquad (23)$$

where we have used the time reversal invariance of χ. Replacing ρ_T by its expression (16) in (23) leads to :

$$\rho_0 = (\rho_0)_T \quad .$$

Before proceeding further, it is worth to stress the following point : we have shown the existence of a time-even hermitian operator χ satisfying (16), by invoquing theorem 3. However, such an operator χ is not yet univoquely defined, since: i) as already mentioned, the operator $(1-R)^{-1/2}$ used in the construction of U can be defined in several different ways ii) it remains to precise the interval of definition of the eigenvalues of χ . In order to remove all these ambiguities, we first note that the operator U used to define χ by Eq.(21) has the property :

$$\tau_T \tau\, U^2 = 1 \quad . \tag{24}$$

To see this, one remarks that the equation

$$\tau_T \tau (\tau\tau_T + 1)^2 = \tau\tau_T + \tau_T\tau + 2 \tag{25}$$

follows from the involution properties of τ and τ_T. Taking the square of U given by Eq.(19) :

$$U^2 = (\tau\tau_T+1)^2\ (\tau\tau_T+\tau_T\tau+2)^{-1} \quad ,$$

one obtains immediately Eq.(24), by use of Eq.(25). Eq.(24) can also be written :

$$U^2 = e^{4i\chi} = \tau\tau_T \quad . \tag{26}$$

According to theorem 3, there is a <u>unique</u> operator χ satisfying (26) and having all its eigenvalues in the interval $[\alpha, \alpha+\frac{\pi}{2}[$.

We now give the following definition of χ :

Definition

χ is defined by its action on each vector of a complete basis of eigenvectors of the diagonalizable operator $U^2 = \tau\tau_T$ in such a way that each vector $|u\rangle$ satisfying

$$\tau\tau_T|u\rangle = \nu_u|u\rangle \tag{27}$$

fulfils

$$\chi|u\rangle = \lambda_u|u\rangle \quad , \tag{28}$$

where

$$e^{4i\lambda_u} = \nu_u \quad , \tag{29}$$

$$\lambda_u \in \left]-\frac{\pi}{4} , \frac{\pi}{4}\right[\quad . \tag{30}$$

In Eq.(30), the interval of definition of λ_u is open as a consequence of condition (P_3), which excludes the eigenvalue $e^{4i\lambda_u} = -1$ for the operator $\tau\tau_T = e^{4i\chi}$.

Incidentally, we emphasize that the operator χ just defined is identical to that defined by Baranger and Vénéroni[1]. This was not apparent up to now, but is clearly illustrated by Eqs.(26) and (30). From now on, we will call the decomposition defined by such an operator χ , and the operator ρ_0 constructed from χ by Eq.(22), the "natural" decomposition , as done in Ref.1.

Notice that in the above definition of χ , conditions (P_i) are dissimulated in Eq.(30), whereas the equivalent hypothesis (P_2) was needed at the very first to define U through Eq.(18). Actually it can be easily shown (see sect. 2-C) that an operator χ defined by (27), (28), (29), and

$$\lambda_u \in \left]-\frac{\pi}{4} , \frac{\pi}{4}\right] \quad \text{or} \quad \lambda_u \in \left[-\frac{\pi}{4} , \frac{\pi}{4}\right[$$

and having at least one eigenvalue $\lambda_u = \pm\frac{\pi}{4}$ cannot fulfil Eq.(16)

For this reason, the conditions (P_i) are necessary (and sufficient) for the existence of a decomposition (1) such that the operator χ satisfies (26). (We will precise this point later on). The conditions (P_i) were not mentioned in Ref.1, whose authors were interested in the decomposition theorem for operators χ small compared to unity, i.e. verifying $\lambda_u \ll 1$. This assumption, which guarantees the fulfilment of (P_i), ensured of the existence of the decomposition (1).

B - Further properties of the "natural" decomposition

The existence theorem has just been shown by the explicit construction of a particular solution (ρ_0, χ), called "natural" decomposition . We now investigate characteristic properties of the "natural" decomposition, which will lead to a stronger theorem of existence and unicity for the decomposition (1).

To find further properties of χ , it is useful to note that if $|u\rangle$ is an eigenvector of $\tau\tau_T$ for the eigenvalue $\nu_u = e^{4i\lambda_u}$, then $\tau|u\rangle$ is also an eigenvector of $\tau\tau_T$ for the eigenvalue $\nu_u^* = e^{-4i\lambda_u}$. Indeed, the involutive character of τ and τ_T implies that if

$$\tau\tau_T|u\rangle = e^{4i\lambda_u}|u\rangle \quad , \tag{31}$$

then $\quad \tau_T\tau|u\rangle = (\tau\tau_T)^{-1}|u\rangle$

thus $\quad \tau_T\tau|u\rangle = e^{-4i\lambda_u}|u\rangle \quad . \qquad (32)$

Applying the operator τ to both members of Eq.(32) leads to :

$$\tau\tau_T(\tau|u\rangle) = e^{-4i\lambda_u}\,\tau|u\rangle \quad . \tag{33}$$

Since $\tau|u\rangle$ is always different from zero ($|u\rangle$ is different from zero as an eigenvector of $\tau\tau_T$, and τ is unitary), this shows that $\tau|u\rangle$ is eigenvector of $\tau\tau_T$. ($\tau|u\rangle$ can happen to be identical with $|u\rangle$).

By Eqs.(27), (28), (29), (30), (31) and (33), one deduces

$$\chi(\tau|u\rangle) = -\lambda_u(\tau|u\rangle) \quad ,$$

which leads to

$$(\chi\tau + \tau\chi)|u\rangle = 0 \tag{34}$$

for any eigenvector $|u\rangle$ of χ. Since relation (34) is satisfied for a complete set of vectors $|u\rangle$, then

$$\chi\tau + \tau\chi = 0 \quad . \tag{35}$$

Introducing the operator $\tau_0 = 2\rho_0 - 1$,
one has clearly :

$$\tau_0 = e^{-i\chi}\,\tau e^{i\chi} \quad ,$$

which gives

$$\chi\tau_0 + \tau_0\chi = e^{-i\chi}(\chi\tau + \tau\chi)e^{i\chi} \quad .$$

Hence the property

$$\chi\tau_0 + \tau_0\chi = 0 \tag{36}$$

is equivalent to (35).
In terms of ρ_0, Eq.(36) writes :

$$\chi\rho_0 + \rho_0\chi = \chi \quad , \tag{37}$$

which is equivalent to

$$\rho_0\chi\rho_0 = (1-\rho_0)\,\chi\,(1-\rho_0) = 0 \quad , \tag{38}$$

and the same equation holds for ρ:

$$\rho\chi\rho = (1-\rho)\chi(1-\rho) = 0 \quad . \tag{39}$$

If ρ is the one-body reduced density operator of a spin 1/2 particle system, Eq.(39) means that the operator χ has only particle-hole and hole-particle matrix elements.

C - Decomposition theorem

The equivalent properties (35) to (39) of χ which have just been established will now be used to find supplementary conditions for the unicity of the decomposition (1). We first show that, associated to Eq.(16), they completely determine the operator $e^{4i\chi}$:

Lemma

Let χ be a hermitian and time-even operator such that

$$\begin{cases} \tau_T = e^{-2i\chi}\ \tau e^{2i\chi} \\ \chi\tau + \tau\chi = 0 \end{cases} \tag{35}$$

Then χ satisfies :

$$e^{4i\chi} = \tau\tau_T \tag{40}$$

Proof

From (35) one gets obviously :

$$[\chi^{2p},\tau] = 0 \tag{41}$$

and

$$\chi^{2p+1}\tau + \tau\chi^{2p+1} = 0 \quad , \tag{42}$$

for any positive integer p. As a consequence of Eqs.(41) and (42) one obtains :

$$e^{-i\alpha\chi}\,\tau = \tau e^{i\alpha\chi} \qquad \forall\alpha \in \mathbb{R} \ ,$$

and as a particular case :

$$e^{-2i\chi}\,\tau = \tau\, e^{2i\chi} \ .$$

Hence

$$\tau\tau_T = \tau\, e^{-2i\chi}\, \tau e^{2i\chi} = \tau^2\, e^{4i\chi} = e^{4i\chi} \ .$$

Consequently, any operator χ of the decomposition (1) constrained to fulfil the supplementary condition (35) (or equivalently (37)) satisfies Eq.(40).

We can summarize the main results established up to now as follows :

i) Conditions (P_i) are sufficient conditions for the existence of a decomposition (1) of ρ into two hermitian and time-even operators ρ_0 and χ .

ii) We have constructed an explicit solution of (1), (14) and (15), the "natural" decomposition , and shown that it satisfies

$$\chi\rho_0 + \rho_0\chi = \chi \ . \qquad (37)$$

iii) It has just been proved that any decomposition (1) having the property (37) is such that the operator χ fulfils :

$$\tau\tau_T = e^{4i\chi} \ . \qquad (40)$$

iv) By reference to theorem 3, we know that there exists one unique operator χ satisfying (40) and having all its eigenvalues λ_u in the interval :

$$\lambda_u \in \left] -\frac{\pi}{4} , \frac{\pi}{4} \right[\ . \qquad (30)$$

(The two boundaries of the interval are excluded, due to conditions (P_1).) The operator χ defined in this way is shown to be time-even.

v) The operator ρ_0 constructed from χ by Eq.(22) is also time-even.

These results lead immediately to the following first version of the decomposition theorem.

Theorem 4

Let ρ_0 be a hermitian projector. If ρ and its time-reversed ρ_T satisfy the equivalent conditions (P_1), there exists a unique set of hermitian operators ρ_0 and χ such that

i) $\chi\rho_0 + \rho_0\chi = \chi$ (37)

ii) all the eigenvalues of χ lie within the interval $]-\frac{\pi}{4}, \frac{\pi}{4}[$ (30)

iii) $\rho = e^{i\chi}\, \rho_0\, e^{-i\chi}$. (1)

These two operators ρ_0 and χ are time-even, irrespective of the property $T^2 = 1$ or $T^2 = -1$ of the time reversal operator.

We will finally show that Eqs. (1) and (35) cannot be simultaneously fulfilled by an operator χ having all its eigenvalues in the interval $]-\frac{\pi}{4}, \frac{\pi}{4}]$ if the operators ρ and ρ_T do not satisfy conditions (P_1).[15]

Indeed, the violation of condition (P_3) implies for the operator $\tau\tau_T$ the existence of at least one eigenvalue $\nu_u = -1$. By the Lemma stated in 2-C, we conclude that any operator

χ fulfilling (16) and (35) has one eigenvalue $\lambda_u = \frac{\pi}{4}$: in other words, there exists a vector $|u\rangle$ such that

$$\tau\tau_T|u\rangle = -|u\rangle \quad , \tag{43}$$

$$\chi|u\rangle = \frac{\pi}{4}|u\rangle \quad .$$

Then, from Eqs.(27), (28) and (29), one gets :

$$\chi(\tau|u\rangle) = \alpha_u(\tau|u\rangle) \quad ,$$

with

$$\alpha_u \in]-\frac{\pi}{4}, \frac{\pi}{4}] \text{ and } e^{4i\alpha_u} = -1. \text{ Hence, } \alpha_u = \frac{\pi}{4} .$$

Therefore :

$$e^{-2i\chi}\,\tau e^{2i\chi}|u\rangle = \tau|u\rangle \quad .$$

But from Eq.(43), we deduce that

$$\tau_T|u\rangle = -\tau|u\rangle \quad ,$$

which leads to

$$e^{-2i\chi}\,\tau e^{2i\chi}|u\rangle \neq \tau_T|u\rangle \quad ,$$

or

$$e^{-2i\chi}\,\rho\, e^{2i\chi} \neq \rho_T$$

Since the operator χ is time reversal invariant, there cannot exist a decomposition (1) with (14). To see this, we suppose that Eqs. (1) and (14) are fulfilled. Then Eq. (23) is also satisfied. Eqs. (23), (14) and (1) implie Eq.(16), which cannot be verified if (P_3) is violated, as we have just shown.

Consequently, conditions (P_i) are not only sufficient, but also necessary for the existence of what we have called the "natural" decomposition . This result enables us to give the final formulation of the decomposition theorem :

Decomposition theorem

Let ρ be a hermitian projector, and T the time reversal antiunitary operator satisfying $T^2 = \pm 1$.

The equivalent assumptions (P_i) are necessary and sufficient conditions for the existence of a unique set of hermitian operators ρ_0 and χ such that

i) $\chi\rho_0+\rho_0\chi = \chi$

ii) all the eigenvalues of χ lie within the interval

$] -\frac{\pi}{4}, \frac{\pi}{4}]$

iii) $\rho = e^{i\chi} \rho_0 \; e^{-i\chi}$.

The two operators ρ_0 and χ are time-even, and the operator χ does not admit the eigenvalue $\lambda_u = \frac{\pi}{4}$.

3. Some implications for systems of spin 1/2 particles

Let us turn back to the existence theorem, studied in sect. 2-A. This theorem has been proved under some sufficient conditions (P_i), expressed up to now in a mathematical language. By looking at systems of spin 1/2 particles, we will now investigate necessary conditions of existence, and also get some light about their physical content.

From now on ρ will be a one-body reduced density-operator describing a system of spin 1/2 particles. Consequently the time reversal operator satisfies :

$$T^2 = -1.$$

We already noticed that to each eigenvalue of a time-even hermitian operator A is associated an even number of linearly independent eigenvectors ; if A is moreover a projector, its trace is therefore an even number. This property holds in particular for the hermitian time-even projector ρ_0 when the decomposition (1)(14)(15) exists. Since ρ is deduced from ρ_0 by a unitary transformation, we conclude that

$$\mathrm{tr}\rho = 2p \quad , \qquad p \in \mathbb{N}. \tag{44}$$

As a necessary condition for existence, Eq.(44) implies that no decomposition (1) fulfilling Eqs.(14) and (15) can be found for the reduced one-body density operator of an odd system of fermions. Property (44), which did not appear in the proof given in sect. 2-A, has just been shown "a posteriori" to be a consequence of the sufficient conditions (P_i). We directly show in an Appendix that (P_i) implie (44).

We now consider the case where the single-particle states are eigenstates of the spin operator S_z :

$$\rho = \rho^u \otimes |+\rangle\langle+| + \rho^d \otimes |-\rangle\langle-| \quad . \tag{45}$$

The operators ρ^u and ρ^d are the spatial parts of the density matrices projecting on the spin up and spin down normalized states $|+\rangle$ and $|-\rangle$:

$$S_z|\pm\rangle = \pm \frac{1}{2}|\pm\rangle$$

It might be of interest to ask under what conditions on ρ^u and ρ^d there exists a decomposition (1) satisfying (14) and (15), and such that the spin states $|\pm\rangle$ are eigenvectors of χ . Added to the requirements for χ to be hermitian and time-even, this condition constraints χ to be of the form :

$$\chi = \chi^u \otimes |+\rangle\langle+| + \chi_T^u \otimes |-\rangle\langle-| , \tag{46}$$

with

$$\chi^u = (\chi^u)^+ \quad . \tag{47}$$

We need not precise the phase convention for the time-reversed vectors $T|\pm\rangle$, because in any case $T^+|\pm\rangle\langle\pm|T = |\mp\rangle\langle\mp|$. Let n^u and n^d be the traces of ρ^u and ρ^d :

$$n^u = \mathrm{Tr}\ \rho^u \quad , \quad n^d = \mathrm{Tr}\ \rho^d \quad .$$

We will now show that the property

$$n^u = n^d \tag{48}$$

is a <u>necessary</u> condition [16] for the existence of a decomposition (1) satisfying the requirements (14),(15), (45) and (46).

This is easily seen by computing the operator $e^{2i\chi}\rho_T\, e^{-2i\chi}$, which must be equal to ρ when a decomposition (16) submitted to (46) and (47) exists. From (45) we deduce :

$$\rho_T = \rho_T^d \otimes |+><+| \; + \rho_T^u \otimes |-><-| \;,$$

and

$$e^{2i\chi} \rho_T e^{-2i\chi} = [\exp(2i\chi^u)\rho_T^d \exp(-2i\chi^u)] \otimes |+><+| \qquad (49)$$

$$+ [\exp(2i\chi_T^u)\rho_T^u \exp(-2i\chi_T^u)] \otimes |-><-| \;.$$

Equating expressions (45) and (49) of ρ , one gets :

$$\rho^u = \exp(2i\chi^u)\rho_T^d \exp(-2i\chi^u) \quad ,$$

and the conjugate equation by time reversal. From Eq.(47), the operator $\exp(2i\chi^u)$ is unitary, so that ρ^u and ρ_T^d have the same eigenvalue spectrum. Since ρ_T^d is hermitian, its trace is invariant under time reversal, and we get :

$$\mathrm{Tr}\ \rho^u = \mathrm{Tr}\ \rho_T^d = \mathrm{Tr}\ \rho^d \quad ,$$

which shows (48).

To end this section, let us see how condition (48) is contained in the assumptions (P_i) for ρ and ρ_T. We first establish the following result :

> Conditions (P_i) are satisfied for ρ and ρ_T if, and only if they are satisfied for ρ^u and ρ_T^d.

Indeed, defining

$$\tau^u = 2\rho^u - 1 \quad , \quad \tau^d = 2\rho^d - 1 \quad ,$$

and using (45), one can write the operator $\tau\tau_T$ as :

$$\tau\tau_T = \tau^u \tau_T^d \otimes |+\rangle\langle+| \quad + \quad \tau^d \tau_T^u \otimes |-\rangle\langle-| \ .$$

Under this form, it appears clearly that the operators $\tau\tau_T$ and $\tau^u \tau_T^d$ have the same eigenvalue spectrum ; it follows that if (P_3) is satisfied by one of these two operators, it is also satisfied by the other one.

From the equivalence of the conditions (P_i), we deduce that if (P_i) are satisfied by ρ and ρ_T, then

$$\| \rho^u - \rho_T^d \| < 1 \qquad .$$

As shown by Sz.-Nagy[9], this property implies (48) (see also Ref. 17). We will not demonstrate this well known result, but simply mention that it can be derived by exactly the same procedure as used in the proof of the existence theorem : using the equivalence between the conditions (P_i), the property (P_1) just shown for ρ^u and ρ_T^d allows to define

$$V = [\rho^u \rho_T^d + (1-\rho^u)(1-\rho_T^d)] \, [1-(\rho^u - \rho_T^d)^2]^{-1/2} \quad .$$

The unitary operator V is easily shown to transform ρ^u into ρ_T^d :

$$\rho_T^d = V^+ \rho^u V \quad ,$$

which leads to (48).

Summary and Comments

The essential results obtained in the present work are the existence and the decomposition theorems given in sect.2.

The first theorem states the existence of a decomposition fulfilling Eqs. (1), (14) and (15) and for any projection operator ρ which, together with its time-reversed ρ_T, satisfies the conditions (P_i). Since this result has been demonstrated by the explicit construction of a particular solution (the so-called "natural" decomposition), the conditions (P_i) appear as sufficient, but not "a priori" necessary. Investigation of necessary conditions for the existence has been made in sect.3 for the reduced one - body density operator of a system of spin 1/2 particles. We did not discuss the possible unicity of (1) submitted to (14),(15) and to the condition (11) for the eigenvalues of χ. Actually, it can be shown in some specific physical situations that such unicity is not true. A counter-example is given by the density operator obtained from a solution of the static Hartree-Fock equation by a Galilean transformation[1,7].

In order to get an existence plus unicity theorem, we have investigated characteristic properties of the "natural" decomposition ; these properties are the interval of definition (30) for the eigenvalues of χ and the relation (37). Added as supplementary conditions to Eqs.(14) and (15), they ensure unicity, and lead to the decomposition theorem.

To end up this summary of our mathematical study, we point out that the choice of a finite N-dimensional space, made here for the sake of simplicity, is not a real restriction, at least as far as the existence theorem for projection operators of finite trace is concerned. Indeed, as shown in the Appendix, the significant space to consider in this case is the linear sum $(\mathcal{R}+\mathcal{R}_T)$, which is a hermitian finite space.

Coming back to Physics, one can ask about the consequences of the non-unicity of (1) submitted to conditions (14), (15) and (11) : does it induce ambiguities in the physical results ? Does there exist any physical reason to impose the supplementary condition (37) which makes the decomposition unique ? Answers to these questions are known when the decomposition (1) is used in the framework of the ATDHF approximation. In this formalism, there are indeed some reasons to ask for condition (37). The argument goes as follows : the variation of the classical action derived from the stationarity principle (2) is submitted to the holonomic constraint $\rho_0^2 = \rho_0$; this constraint reduces the number of degrees of freedom precisely to the number of particle-hole matrix elements of χ , i.e. to the total number of matrix elements of the operator χ_n defined by the "natural" decomposition. These matrix elements play the role of classical momenta, and therefore the requirement (37) permits to take into account the constraint in a straightforward way, without need of Lagrange multipliers. In this respect the choice of the "natural" decomposition appears quite convenient. However, it is not really dictated by physical reasons[18], and the Hamilton equations can be derived for another choice of the decomposition of ρ , but with more technical difficulties[19]. In any case, this ambiguity in the choice of the decomposition is definitively removed once the adiabatic equations of motion are known. Indeed, it has been shown in Ref.1 that all the possible sets of operators (ρ_0,χ) fulfilling (1), (14) and (15) lead to equivalent dynamics ; thus condition (37) does not appear "a posteriori" as a physical limitation, and can be legitimately imposed in practical calculations, as done in Refs. 7,20.

The decomposition (1) with the conditions (14) and (15), and with, or without, the additional requirements (30) and (37), has already been used in Nuclear Physics, for the reduced one-body Hartree-Fock density of even-even nuclei. This decomposition may also be of interest in other fieldsof Physics. Indeed, the proofs of the existence and the decomposition theorems presented in this work are not restricted to one-body densities, but apply for any p-body densities of a n-body system in a pure state (provided conditions (P_i) are satisfied), and the demonstrations hold for bosons as well as fermions.

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Appendix

We restrict ourselves to a space $\mathcal{H}$ generated by the p-body states of a system of fermions and such that the time reversal operator has the property $T^2 = -1$ (i.e. p is an odd number). If $\mathcal{H}$ is a single-particle space, what follows concerns the reduced single-particle density operator used for instance in Hartree-Fock approximation.

We will show directly (another proof is given in sect. 3) that the fulfilment of conditions (P_i) for ρ and its time-reversed ρ_T requires :

$$\mathrm{tr}\ \rho = 2p \quad , \quad p \in \mathbb{N}.$$

Let $\mathcal{R}$ and $\mathcal{R}_T$ be the subspaces on to which ρ and ρ_T project :

$$\mathcal{R} = \rho(\mathcal{H}) \quad , \quad \mathcal{R}_T = \rho_T(\mathcal{H}) \quad .$$

From its definition, it is clear that the operator

$$\tau\tau_T - 1 = 4\rho\rho_T - 2(\rho+\rho_T)$$

transforms each vector of $\mathcal{H}$ into a vector of the linear sum $(\mathcal{R}+\mathcal{R}_T)$:

$$(\tau\tau_T - 1)|u\rangle = |u_1\rangle + |u_2\rangle \quad ,$$

with $|u_1\rangle \in \mathcal{R}$, $|u_2\rangle \in \mathcal{R}_T$. Hence, $(\mathcal{R}+\mathcal{R}_T)$ is an invariant subspace of $(\tau\tau_T - 1)$, and we can define the restriction Ω of the operator $(\tau\tau_T - 1)$ to the subspace $(\mathcal{R}+\mathcal{R}_T)$.

To study the spectrum of Ω , we recall that if

$$\Omega|u\rangle = (e^{4i\lambda_u} - 1)|u\rangle \quad , \tag{50}$$

then (see Eqs.(31) and (33)) :

$$\Omega(\tau|u>) = (e^{-4i\lambda_u} - 1)\tau|u> \quad . \tag{51}$$

Moreover, the time-reversed of Eq.(32) leads to :

$$\Omega|\bar{u}> = (e^{4i\lambda_u} - 1)|\bar{u}> \tag{52}$$

and the equation

$$\Omega(\tau_T|\bar{u}>) = (e^{-4i\lambda_u} - 1)\tau_T|\bar{u}> \quad . \tag{53}$$

can be deduced from (52) by a similar procedure as (51) from (50).

All the vectors $|u>$, $\tau|u>$, $|\bar{u}>$, $\tau_T|\bar{u}>$ belong clearly to $(\mathcal{R} + \mathcal{R}_T)$. The dimensionality of the subspace $\mathcal{S}_u$ generated by these four vectors (all generated from a given $|u>$) can be different in the case were $e^{4i\lambda_u}$ is real and in the opposite case :

i) if $e^{4i\lambda_u} \neq \pm 1$, these four vectors span a 4-dimensional space $\mathcal{S}_u$, since the two sets $(|u>,|\bar{u}>)$ and $(\tau|u>,\tau_T|\bar{u}>)$ correspond to different eigenvalues of Ω , and the two vectors of each set are linearly independent, as seen in sect.1

ii) the case $e^{4i\lambda_u} = -1$ cannot occur if the condition (P_3) is required

iii) if $e^{4i\lambda_u} = 1$, the four eigenvectors are associated to the same eigenvalue zero of Ω . To study the dimensionality of $\mathcal{S}_u$, we first show the following result :

<u>Lemma</u> Let ρ and ρ' be two hermitian projectors. Each vector $|u>$ satisfying :

$$\rho|u> = \rho'|u> \tag{54}$$

is a common eigenvector of ρ and ρ' :

$$\rho|u> = \rho'|u> = \mu|u> \quad .$$

Proof

Let $|u\rangle$ fulfil Eq.(54) ; we write the decomposition:

$$|u\rangle = \rho|u\rangle + |e\rangle \quad , \qquad (55)$$

and we first suppose that $\rho|u\rangle \neq 0$. Then $|u\rangle$ and $\rho|u\rangle$ belong to $(\mathcal{R} + \mathcal{R}')$, with $\mathcal{R} = \rho(\mathcal{H})$ and $\mathcal{R}' = \rho'(\mathcal{H})$. This shows that $|e\rangle \in (\mathcal{R} + \mathcal{R}')$. From Eqs.(54) and (55), it follows

$$\rho|e\rangle = \rho'|e\rangle = 0 \quad . \qquad (56)$$

The only possible vector of $(\mathcal{R} + \mathcal{R}')$ satisfying (56) is

$$|e\rangle = 0 \quad ,$$

that is :.

$$\rho|u\rangle = |u\rangle \quad .$$

In the case $\rho|u\rangle = 0$, one can give a similar proof by replacing ρ and ρ' by $(1-\rho)$ and $(1-\rho')$.

As a consequence of this lemma, all the eigenvectors of Ω associated with the eigenvalue $(e^{4i\lambda_u} - 1) = 0$ are eigenvectors of ρ and ρ_T with the eigenvalue $\mu = 1$: since τ is involutive, the equation

$$\tau\tau_T|u\rangle = |u\rangle$$

implies

$$\tau_T|u\rangle = \tau|u\rangle \quad ,$$

or equivalently

$$\rho|u\rangle = \rho_T|u\rangle \quad ,$$

and the lemma ensures that

$$\rho|u\rangle = \rho_T|u\rangle = |u\rangle \quad . \tag{57}$$

Therefore, the subspace $\mathcal{S}_u$ in the case $e^{4i\lambda_u} = 1$ is just :

$$\mathcal{S}_u = \mathcal{R} \cap \mathcal{R}_T \; .$$

This space is of dimensionality 2 or 4, since Eq.(57) implies

$$\rho_T|\bar{u}\rangle = \rho|\bar{u}\rangle = |\bar{u}\rangle \quad ,$$

with $\langle u|\bar{u}\rangle = 0$.

To summarize, we have obtained the results :

$$\dim(\mathcal{R} \cap \mathcal{R}_T) = 2n, \qquad n \in \mathbb{N} \tag{58}$$

$$\dim(\mathcal{R} + \mathcal{R}_T) = 2n + 4k \quad , \quad k \in \mathbb{N} \; . \tag{59}$$

As well known :

$$\dim(\mathcal{R} + \mathcal{R}_T) + \dim(\mathcal{R} \cap \mathcal{R}_T) = \dim \mathcal{R} + \dim \mathcal{R}_T .$$

Since

$$\dim \mathcal{R} = \dim \mathcal{R}_T \quad , \tag{60}$$

one gets from (58), (59) and (60) the final result

$$\mathrm{tr}\ \rho = \dim \mathcal{R} = 2(k + n) = 2p \quad , \quad p \in \mathbb{N} \; .$$

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13. A real vector is defined by $|e_i\rangle = |\bar{e}_i\rangle$; a real basis is composed of real vectors.

14. The norm considered is defined by $\|A\| = \sup\limits_{|u\rangle\in\mathcal{H}} \frac{\|A|u\rangle\|}{\||u\rangle\|}$

15. A similar demonstration holds for $\lambda_u \in [-\frac{\pi}{4}, \frac{\pi}{4}[$.

16. Authors of Ref.7 focused their attention on the "natural" decomposition , fulfilling condition (37). They showed that Eq.(48) is a necessary condition for the existence of this particular decomposition. One can easily see that Eqs.(37) and (15) imply (46) and (47), so that the property demonstrated here is stronger than the statement of Ref.7.

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