

ON “PARTIAL” FIDELITIES

ARMIN UHLMANN

Institut f. Theoretische Physik, Universität Leipzig,
Augustusplatz 10/11, D-04109 Leipzig, Germany
(e-mail: uhlmann@itp.uni-leipzig.de)

(Received December 21, 1999 — Revised March 20, 2000)

For pairs ω, ρ of density operators on a finite-dimensional Hilbert space of dimension d I call k -fidelity the $d - k$ smallest eigenvalues of $|\sqrt{\omega}\sqrt{\rho}|$. Representations of k -fidelities are given showing their joint concavity in ω, ρ . For $k = 0$ the known properties of fidelities and transition probabilities are reproduced. Partial fidelities characterize equivalence classes of pairs of density operators which are partially ordered in a natural way.

1. Introduction

Let us start with a short introduction to transition probability [1].

For two unit vectors, ψ and φ , of a Hilbert space the quantity $|\langle\psi, \varphi\rangle|^2$ is their transition probability. It is the squared modulus of their transition amplitude, $\langle\psi, \varphi\rangle$. Assume the state of the quantum system is $|\psi\rangle\langle\psi|$. A von Neumann’s measurement, designed to decide whether the quantum system is in the state $|\varphi\rangle\langle\varphi|$, prepares this state with probability $|\langle\psi, \varphi\rangle|^2$. Notice further that two pairs of unit vectors are unitarily equivalent iff they have equal transition probabilities.

All that becomes more complex if two density operators, ρ_1 and ρ_2 , are considered on a Hilbert space \mathcal{H} , and the quantum system is in a state, say, ρ_1 . The algebra of operators on \mathcal{H} will be called \mathcal{B} . One can choose vectors ψ_j in the direct product $\mathcal{H} \otimes \mathcal{H}$ such that

$$\mathrm{Tr} A\rho_j = \langle\psi_j, (A \otimes \mathbf{1})\psi_j\rangle, \quad A \in \mathcal{B}, \quad j = 1, 2. \quad (1)$$

The transition probability between ψ_1 and ψ_2 is not determined by the pair ρ_1, ρ_2 . But running through all the possible arrangements (1), the numbers $|\langle\psi_2, \psi_1\rangle|^2$ fill completely an interval $[0, p]$ of real numbers. The largest one, the upper bound of this interval, is called *transition probability between ρ_1 and ρ_2* and is denoted by $P(\rho_1, \rho_2)$. Thus a von Neumann’s measurement in $\mathcal{H} \otimes \mathcal{H}$ can cause a transition $\rho_1 \mapsto \rho_2$ with a probability bounded by $P(\rho_1, \rho_2)$. The bound can be reached by suitable measurements in the larger system.

Now I call attention to possibilities to characterize P intrinsically, i.e., without leaving the quantum system in question. The first one comes rather directly from

(1). Let us call *transition functional from* ρ_1 *to* ρ_2 every linear functional on \mathcal{B} of the form

$$A \longrightarrow \text{Tr } v A := \langle \psi_2, (A \otimes \mathbf{1}) \psi_1 \rangle \quad (2)$$

which arises from a setting (1). The operators v may be called *transition operators from* ρ_1 *to* ρ_2 . Generally, v is not hermitian: Exchanging the roles of ψ_1 and ψ_2 the operator v becomes its hermitian adjoint, v^* . Now (2) is a transition functional if and only if

$$|\text{Tr } A_1 v A_2^*|^2 \leq (\text{Tr } A_1 \rho_1 A_1^*) (\text{Tr } A_2 \rho_2 A_2^*), \quad A_i \in \mathcal{B}, \quad (3)$$

and it follows from the definition of P that

$$P(\rho_2, \rho_1) = \max |\text{Tr } v|^2, \quad (4)$$

where one takes the maximum over all transition operators from ρ_1 to ρ_2 . Calculating the maximum in (4) is a standard exercise with a well-known outcome. Before writing it down I would like to explain the following.

The transition probability is separately concave in every one of its arguments. However, taking the root of P , the concavity properties become dramatically enhanced: \sqrt{P} is jointly concave [2]. In the following the square root of the transition probability will be called *fidelity* and will be denoted by F , essentially following a proposal of Richard Jozsa¹. Thus

$$F(\omega, \rho) := \sqrt{P(\omega, \rho)} = \text{Tr}(\rho^{1/2} \omega \rho^{1/2})^{1/2}. \quad (5)$$

The assertion that F is jointly concave is seen from

$$F(\omega, \rho) = \frac{1}{2} \inf (\text{Tr } A \omega + \text{Tr } A^{-1} \rho), \quad A > 0, \quad A^{-1} \in \mathcal{B}, \quad (6)$$

which is the finite-dimensional version of a representation of $\sqrt{P} = F$ as an infimum of linear functionals, valid for pairs of states on von Neumann and on C*-algebras, see [3]. The representation is related to another one of equal generality estimating $P(\omega, \rho)$ from above by the product of $\text{Tr} \omega A$ and $\text{Tr} \rho A^{-1}$, with A an invertible positive operator, see [4] for a partial result and [5] for the C*-case in full generality. For finite dimensions these well-known results are reproduced by setting $k = 0$ in Eqs. (13) and (14) below.

As a matter of fact, the equality of F (or of P) for two pairs of density operators does not imply their unitary equivalence. This pleasant feature, valid for pure states, is missing for the mixed ones. Looking at (6) one may wonder whether it is not possible to get a whole series of concave invariants by taking other suitable sets of operators than the invertible positive operators in Eq. (6). To give an affir-

¹ Jozsa introduced the word *fidelity* for the transition probability. Its present usage is not unique. I think the peculiar properties of \sqrt{P} need an extra notation anyway.

mative answer belongs to the results the present paper. By the partial fidelities one gets a reasonable classification of pairs of density operators, coarser than unitary equivalence would give.

All what follows remains in finite dimensions. By modifying certain settings and by adding new arguments, Peter M. Alberti [6] was able to extend essential parts of what follows to von Neumann algebras. His results are particularly satisfactory for the type II_1 .

2. k -Fidelities

Let \mathcal{H} be a finite-dimensional Hilbert space and $d = \dim \mathcal{H}$. The *spectrum*, $\text{spec}(A)$, of an operator A is the family of roots of the polynomial $\det(A - \lambda \mathbf{1})$ counted with their correct multiplicities. If the spectrum is real we assume the set $\text{spec}(A)$ *decreasingly ordered*. This convention applies to every diagonalizable operator with real eigenvalues and in particular to every hermitian operator. Consider now

$$\text{spec}((\sqrt{\omega}\rho\sqrt{\omega})^{1/2}) = \text{spec}((\sqrt{\rho}\omega\sqrt{\rho})^{1/2}) = \{ \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_d \} \quad (7)$$

so that, according to (5), the sum of the lambdas is the fidelity. The spectrum (7) is equal to the ordered singular numbers of $\sqrt{\omega}\sqrt{\rho}$ and of $\sqrt{\rho}\sqrt{\omega}$.

I define partial fidelities simply by summing up parts of the spectrum (7).

DEFINITION. For $0 \leq k \leq d - 1$

$$F_k(\omega, \rho) := \sum_{j>k} \lambda_j, \quad k = 0, 1, \dots, d - 1. \quad (8)$$

If $k \geq d$ then $F_k = 0$. For the time being F_k will be called *k -th partial fidelity*, or simply *k -fidelity* of the pair ω and ρ .

An important point is that: I do not necessarily require that ρ and ω have trace one. Indeed, on a finite-dimensional Hilbert space (8) is naturally defined for pairs from the cone of positive operators and

$$\sqrt{c} F_k(\omega, \rho) = F_k(c\omega, \rho) = F_k(\omega, c\rho), \quad c > 0, \quad (9)$$

for positive real numbers c . Notice the properties:

- a) F_k is symmetric in its arguments,
- b) F_0 is just the fidelity F ,
- c) for pairs of pure density operators it is $F_k = 0$ for $k > 0$,
- d) if $F_k \neq 0$ then $\text{rank}(\omega) > k$ and $\text{rank}(\rho) > k$ necessarily,
- e) F_k is unitarily invariant, i.e. invariant by the simultaneous transformation $\rho \rightarrow U\rho U^*$, $\omega \rightarrow U\omega U^*$.

However, a deeper justification for the definition above is given by the following theorem.

THEOREM 1. *The partial fidelities are concave functions of the pairs $\{\omega, \rho\}$,*

$$\sum_j p_j F_k(\omega_j, \rho_j) \leq F_k\left(\sum_j p_j \omega_j, \sum_i p_i \rho_i\right) \quad (10)$$

for any probability vector p_1, p_2, \dots and arbitrary pairs $\{\omega_i, \rho_i\}$.

The theorem is a consequence of a new relation representing F_k as an infimum of linear functionals quite similar to (6). It estimates partial fidelities linearly as close as possible from above. To get the announced representation I am going to define the set PAIRS which consists of all pairs $\{A, B\}$ of positive hermitian operators, A, B , such that

$$ABA = A, \quad BAB = B. \quad (11)$$

Let $\{A, B\}$ be such a pair. It follows immediately that $(AB)^2 = AB$. Because $Q = AB$ is a product of two positive operators it is diagonalizable. On the other hand, we see that $Q^2 = Q$, so its spectrum consists of zeros and ones. Therefore, the trace of Q is equal to the rank of Q . Now (11) says that $QA = A$ and $BQ = B$ implying that the ranks of A and B cannot be larger than the rank of Q . Now $Q = AB$ shows that neither the rank of A nor the rank of B can be smaller than that of Q . Altogether we have the following result.

LEMMA 1. *For all $\{A, B\} \in \text{PAIRS}$,*

$$\text{rank}(A) = \text{rank}(B) = \text{rank}(AB) = \text{Tr } AB \quad (12)$$

is an integer called rank of the pair $\{A, B\}$.

DEFINITION. PAIRS_m consists of all pairs from PAIRS of rank m .

The promised representation of the k -th fidelities is in the following theorem.

THEOREM 2. *Let $m + k = \dim \mathcal{H}$. Then*

$$F_k(\omega, \rho) = \frac{1}{2} \inf(\text{Tr } A\omega + \text{Tr } B\rho), \quad \{A, B\} \in \text{PAIRS}_m. \quad (13)$$

One can deduce from (13) the following inequality:

$$F_k(\omega, \rho)^2 = \inf(\text{Tr } A\omega)(\text{Tr } B\rho), \quad \{A, B\} \in \text{PAIRS}_m. \quad (14)$$

The point is that with $\{A, B\}$ also $\{\lambda A, \lambda^{-1} B\}$ is contained in PAIRS_m for $\lambda > 0$. After this trivial substitution, the right-hand side of (13) is of the form $\lambda a + \lambda^{-1} b$. Taking the infimum over λ results in $2\sqrt{ab}$, and (14) is derived from (13). Eq. (14), suitably reformulated, is known for C^* -algebras if $k = 0$, see [5].

Theorem 1 is a consequence of Theorem 2. We shall prove Theorem 2 in the next section, at first assuming ρ invertible (which would be sufficient for Theorem 1). Then, by continuity arguments, we can allow for all ω and ρ . However, before going into the proof, we have to look at a “hidden” symmetry of the k -fidelities.

3. The symmetry group of the k -fidelities

Let us denote by Γ the multiplicative group of all invertible operators acting on \mathcal{H} . With $X \in \Gamma$ we define the X -transform of a pair $\{\omega, \rho\}$ by

$$\{\omega, \rho\}^X := \{X\omega X^*, (X^{-1})^* \rho X^{-1}\}. \quad (15)$$

The transformations create orbits of Γ in the set of pairs. Two pairs, $\{\omega, \rho\}$ and $\{\omega', \rho'\}$, are called Γ -equivalent iff there is $X \in \Gamma$ such that $\{\omega', \rho'\}$ is the X -transform of $\{\omega, \rho\}$.

LEMMA 2. *The k -fidelities of Γ -equivalent pairs are equal for every k .*

$$F_k(\omega, \rho) = F_k(\omega', \rho') \text{ if } \{\omega', \rho'\} = \{\omega, \rho\}^X \quad (16)$$

Proof: For the proof we start with the identity

$$(X\omega X^*)(X^{-1})^* \rho X^{-1} = X\omega\rho X^{-1}$$

saying that the spectrum of $\omega\rho$ is an invariant for Γ -equivalent pairs. It suffices to show that

$$\text{spec}(\omega\rho) = \text{spec}(\rho\omega) = \{\lambda_1^2, \lambda_2^2, \dots, \lambda_d^2\} \quad (17)$$

follows from (7). By $\sqrt{\rho}(\omega\rho)(\sqrt{\rho})^{-1} = \sqrt{\rho}\omega\sqrt{\rho}$ this is true for invertible ρ . The assumption of invertibility can be removed by continuity. \square

Substituting in (15) $\rho = X^*\tau X$ we may rewrite (16) as

$$F_k(\omega, X^*\tau X) = F_k(X\omega X^*, \tau) \quad (18)$$

In (18), by continuity, also X need not be invertible.

Only for the purpose of the following proof we abbreviate the right-hand-side of (13) by $G_k(\omega, \rho)$,

$$G_k(\omega, \rho) := \frac{1}{2} \inf(\text{Tr } A\omega + \text{Tr } B\rho), \quad \{A, B\} \in \text{PAIRS}_m.$$

We observe that also G_k allows for the Γ -invariance. Indeed, with a pair $\{A, B\}$ its transform

$$\{A, B\}_X := \{X^*AX, X^{-1}B(X^{-1})^*\} \quad (19)$$

is also in PAIRS_m , and we get the trace identities

$$\text{Tr } \omega A = \text{Tr } \omega' A', \quad \text{Tr } \rho B = \text{Tr } \rho' B',$$

whenever

$$\{A', B'\} = \{A, B\}_X, \quad \{\omega', \rho'\} = \{\omega, \rho\}^X.$$

Therefore,

$$G_k(\omega, \rho) = G_k(\omega', \rho') \text{ if } \{\omega', \rho'\} = \{\omega, \rho\}^X. \quad (a)$$

Proof of Theorem 2: As we have just seen, both sides of (13) do not change along a Γ -orbit of X -transforms (15).

Step 1 in the proof is to show $F_k \leq G_k$. To this end we first take a pair $\{\omega, \rho\}$ with an invertible ρ . We transform the given pair according to (15) by $X = \sqrt{\rho}$. The new pair is $\{\omega', \mathbf{1}\}$ with $\omega' = \sqrt{\rho}\omega\sqrt{\rho}$. By (a) and Lemma 2 it suffices to prove $F_k \leq G_k$ for the new pair, i.e. we estimate $G_k(\omega', \mathbf{1})$ from below.

We choose a pair $\{A, B\}$ from PAIRS_m arbitrarily. Let ϕ_1, ϕ_2, \dots be an eigenbasis of A and a_1, a_2, \dots the corresponding eigenvalues. By sandwiching $ABA = A$ between these eigenvectors of A one gets

$$\langle \phi_i, B\phi_k \rangle = a_i^{-1} \delta_{ik} \text{ for } i, k \geq m.$$

Now we can write

$$\mathrm{Tr} A\omega' + \mathrm{Tr} B = \sum_1^m a_i \langle \phi_i, \omega' \phi_i \rangle + \sum_1^m a_i^{-1} + \sum_{j>m} \langle \phi_j, B\phi_j \rangle.$$

With positive reals a and x it holds $ax + a^{-1} \geq 2\sqrt{x}$. Using this inequality to estimate the first two sums from below and neglecting the last term, we arrive at

$$\mathrm{Tr} A\omega' + \mathrm{Tr} B \geq 2 \sum_1^m \sqrt{\langle \phi_i, \omega' \phi_i \rangle}.$$

The square root is concave. Hence, see [10], Eq. 1-46,

$$\sum_1^m \sqrt{\langle \phi_i, \omega' \phi_i \rangle} \geq \sum_1^m \langle \phi_i, \sqrt{\omega'} \phi_i \rangle \geq F_k(\omega, \rho)$$

The last inequality sign is an estimation of the m smallest eigenvalues (due to Fan and Horn) and respects $F_k(\omega', \mathbf{1}) = F_k(\omega, \rho)$. It results in

$$\frac{1}{2} \inf(\mathrm{Tr} A\omega + \mathrm{Tr} B\rho) \geq F_k(\omega, \rho) \quad (20)$$

at first for the pairs $\{\omega', \mathbf{1}\}$ and then, by Γ -invariance, for all pairs $\{\omega, \rho\}$ with invertible ρ . However, both sides of (20) are continuous in ω and ρ . Thus step one terminates in the validity of (20) for all ω and all ρ . The inequality is equivalent to $G_k \geq F_k$.

In step 2 we show $G_k \leq F_k$ at first for invertible ρ . As above we reduce the problem by Γ -invariance to that of a pair consisting of ω' and $\mathbf{1}$. We now choose ϕ_1, \dots, ϕ_m to be eigenvectors of ω' belonging to the m smallest eigenvectors of ω' . The latter are $\lambda_{k+1}^2, \dots, \lambda_{k+m}^2$ by Lemma 2. Define

$$A' = \sum_1^m a_i |\phi_i\rangle\langle\phi_i|, \quad B' = \sum_1^m a_i^{-1} |\phi_i\rangle\langle\phi_i|,$$

and consider

$$\mathrm{Tr} A' \omega' + \mathrm{Tr} B' = \sum_{j=1}^m a_j \lambda_{j+k}^2 + \sum_{j=1}^m a_j^{-1}.$$

If $\lambda_{j+k} > 0$ we choose $a_j = \lambda_{j+k}^{-1}$. Otherwise we set $a_j = c^{-1} > 0$ arbitrarily. If n of the m eigenvalues λ_{j+k} are zero, then our convention implies

$$\mathrm{Tr} A' \omega' + \mathrm{Tr} B' = 2 \sum_{j=1}^m \lambda_{j+k} + nc = 2F_k(\omega', \mathbf{1}) + nc,$$

and hence $G_k \leq F_k + nc$. Since c can be made arbitrarily small we arrive at the required inequality $G_k \leq F_k$. Now, relying on Γ -invariance (16) and (a), the inequality is shown true for all pairs of invertible density operators.

Combining steps one and two we see: $F_k(\omega, \rho) = G_k(\omega, \rho)$ if both arguments are invertible. Hence F_k is concave for these pairs. But F_k is a continuous function of ω and ρ by (8). Therefore, F_k is jointly concave and Theorem 1 is valid.

But one knows that a concave function is semi-continuous from below, see [7], Theorem 10.2, where semi-continuity from above is stated for convex functions. Because F_k is continuous and concave it dominates every function which is concave and coincides for convexly inner points with F_k . This means $F_k \geq G_k$ always. Now step one of the proof provides $F_k = G_k$. \square

4. Equivalence and partial order

It is tempting to collect pairs of positive (density) operators into equivalence classes according to their partial fidelities. For the purpose of the present paper we call two pairs *equivalent*, and we write

$$\{\omega, \rho\} \sim \{\omega', \rho'\}, \quad (21)$$

iff their k -fidelities are equal, $F_k(\omega, \rho) = F_k(\omega', \rho')$ for $k = 0, 1, \dots, d-1$. The relation \sim is an equivalence relation. Notice that $\{\omega, \rho\} \sim \{\rho, \omega\}$. Generally, an equivalence class contains a lot of Γ -orbits. But there is an important exception:

LEMMA 3. *If both operators, ω and ρ , are invertible, the equivalence class of $\{\omega, \rho\}$ consists exactly of all pairs $\{\omega, \rho\}^X$, $X \in \Gamma$.* \square

Proof: The assumption is valid if and only if 0 does not belong to the eigenvalues (7). This takes place if the smallest one is different from zero, hence iff $F_{d-1} \neq 0$. Thus, if the assumption of the lemma is valid for one member of an equivalence class, then it is true for all members. Let $\{\omega_1, \rho_1\}$ be in the equivalence class of $\{\omega, \rho\}$. Transforming the latter by $X = \sqrt{\rho}$ and the former by $X_1 = \sqrt{\rho_1}$ by the recipe (15) results accordingly in Γ -equivalent pairs $\{\omega', \mathbf{1}\}$ and $\{\omega'_1, \mathbf{1}\}$. Being in the same equivalence class, ω' and ω'_1 have to have equal eigenvalues and they are even unitarily equivalent. Thus all the pairs considered belong to the same Γ -orbit. \square

Let us write $\{\omega', \rho'\} \leq \{\omega, \rho\}$ if both, $\omega - \omega'$ and $\rho - \rho'$, are positive operators. A simple example is as follows: Write $\omega = \omega' + \omega_0$, $\rho = \rho' + \rho_0$, and assume orthogonality between ω' and ρ_0 and between ρ' and ω_0 , i.e. $\omega_0\rho' = 0$, $\rho_0\omega' = 0$. Then $\{\omega, \rho\}$ and $\{\omega', \rho'\}$ belong to the same equivalence class. To see what we can learn from $\{\omega', \rho'\} \leq \{\omega, \rho\}$ generally, we proceed in two steps, $\{\omega', \rho'\} \leq \{\omega, \rho'\}$ and $\{\omega, \rho'\} \leq \{\omega, \rho\}$. Consider the second one. It implies $\sqrt{\omega}\rho'\sqrt{\omega} \leq \sqrt{\omega}\rho\sqrt{\omega}$ and, because taking the square root does not destroy the inequality,

$$(\sqrt{\omega}\rho'\sqrt{\omega})^{1/2} \leq (\sqrt{\omega}\rho\sqrt{\omega})^{1/2}.$$

The sums of its m smallest eigenvalues, which are the partial fidelities, obey the same inequality. Further, if the traces of both positive operators happen to be equal, the operators themselves have to be equal one to another. Repeating the arguments for the first step and combining both, we arrive at the lemma.

LEMMA 4. *If*

$$\{\omega, \rho\} \geq \{\omega', \rho'\} \quad (22)$$

then

$$F_k(\omega, \rho) \geq F_k(\omega', \rho'), \quad k = 0, 1, \dots, d-1. \quad (23)$$

If in addition to (22) $F(\omega, \rho) = F(\omega', \rho')$ is true, then all partial fidelities must be equal in pairs, and the two pairs belong to the same equivalence class: $\{\omega, \rho\} \sim \{\omega', \rho'\}$. \square

Given ω, ρ , Alberti [8] has shown, even in the C*-category, that there is one and only one pair $\{\omega_0, \rho_0\}$ which has the same transition probability (and, therefore, the same fidelity), and which is minimal with respect to \geq . This *minimal pair* satisfies

$$\{\omega_0, \rho_0\} \leq \{\omega', \rho'\}$$

whenever

$$\{\omega', \rho'\} \leq \{\omega, \rho\} \quad \text{and} \quad F(\omega', \rho') = F(\omega, \rho)$$

is valid.

We see that every equivalence class contains a minimal pair and, therefore, a Γ -orbit of minimal pairs. It is tempting to believe that there is only one minimal Γ -orbit in every equivalence class of pairs. But I do not know whether this conjecture is true.

Now one may go a step further, anticipating the ideas of majorization [9], or those of partially ordering orbits belonging to certain classes of transformations [10]. To do so, let us call $\{\omega_1, \rho_1\}$ *F-dominated* by $\{\omega_2, \rho_2\}$ iff

$$F_k(\omega_1, \rho_1) \leq F_k(\omega_2, \rho_2), \quad k = 0, 1, 2, \dots \quad (24)$$

From Theorem 1 we get the following corollary

COROLLARY. If $\{\omega_2, \rho_2\}$ is contained in the convex hull of the \sim -equivalence class of $\{\omega_1, \rho_1\}$ then (24) takes place. \square

We thus get a new partial ordering (or majorization tool) for pairs of positive (density) operators which seems worthwhile to investigate. There is a link, indeed a morphism, to singular number majorization. Denote by $\text{sing}(B)$ the decreasingly ordered singular numbers of the operator B , that is

$$\text{sing}(B) = \text{spec}(\sqrt{B^*B}) = \text{spec}(\sqrt{BB^*}) = \text{sing}(B^*),$$

and by $\text{sing}[B]$ the set of all operators C with $\text{sing}(C) = \text{sing}(B)$, the *singular number class* of B . In particular,

$$\text{spec}((\sqrt{\omega}\rho\sqrt{\omega})^{1/2}) = \text{sing}(\sqrt{\rho}\sqrt{\omega}).$$

There are many useful rules governing the partial order of the singular number classes (see [9], 9.E and [10], 2.4 (Theorem 2-8), 2.5). With them one easily proves lemma.

LEMMA 5. *The following items are mutually equivalent:*

- a) $\{\omega_1, \rho_1\}$ is F -dominated by $\{\omega_2, \rho_2\}$,
- b) $\sqrt{\omega_2}\sqrt{\rho_2}$ is contained in the convex hull of $\text{sing}[\sqrt{\omega_1}\sqrt{\rho_1}]$,
- c) there are finitely many operators A_i, B_i , all with operator norms not exceeding 1, such that

$$\sqrt{\omega_2}\sqrt{\rho_2} = \sum A_i \sqrt{\omega_1} \sqrt{\rho_1} B_i.$$

5. More about PAIRS

It is our aim to get some insight into the structure of PAIRS. Let $\{A, B\} \in \text{PAIRS}_m$ with $0 < m \leq d = \dim \mathcal{H}$. k is defined by $k + m = d$. Let us write A, B as block matrices with respect to an eigenvector basis of A as in the proof of Theorem 2. Then, with a positive $m \times m$ matrix A_{11} ,

$$A = \begin{pmatrix} A_{11} & 0 \\ 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}. \quad (25)$$

Here B_{11} is $m \times m$, B_{12} is $m \times k$, and B_{22} is $k \times k$. The equation $ABA = A$ results in $B_{11} = A_{11}^{-1}$. Having this in mind, one gets from $BAB = B$,

$$B_{11} = A_{11}^{-1}, \quad B_{22} = B_{21}A_{11}B_{12}, \quad B_{12}^* = B_{21}. \quad (26)$$

Notice that B_{12} can be chosen arbitrarily: Given the first member, A , of the pair, B depends freely on km complex parameters.

There is a further representation of the pairs in PAIRS_m . Call $2m$ vectors, $\psi_1, \psi_2, \dots, \psi_m, \varphi_1, \varphi_2, \dots, \varphi_m$, a *bi-orthogonal system of length m* if

$$\langle \psi_i, \varphi_j \rangle = \delta_{ij}, \quad i, j = 1, 2, \dots, m. \quad (\text{A})$$

Together with m positive numbers, a_1, a_2, \dots, a_m , we obtain from (A) a pair of operators

$$A = \sum a_i |\psi_i\rangle\langle\psi_i|, \quad B = \sum a_i^{-1} |\varphi_i\rangle\langle\varphi_i|, \quad (\text{B})$$

for which $ABA = A$ and $BAB = B$ can be checked. Let us prove that *every pair from PAIRS_m can be gained by this procedure.*

Let $\{A, B\} \in \text{PAIRS}_m$. Because AB is diagonalizable with eigenvalues 0 and 1, there is $X \in \Gamma$ such that $XABX^{-1}$ is a hermitian projection operator. Hence the operators

$$A_1 = XAX^*, \quad B_1 = (X^{-1})^*BX^{-1}$$

commute. Therefore there is a representation

$$A_1 = \sum a_i |\phi_i\rangle\langle\phi_i|, \quad B_1 = \sum a_i^{-1} |\phi_i\rangle\langle\phi_i|$$

with m orthonormal vectors ϕ_1, \dots, ϕ_m . But

$$\psi_i = X^{-1}\phi_i, \quad \varphi_i = X^*\phi_i$$

is bi-orthogonal with length m . Transforming A_1 and B_1 back to A and B gives the desired representation of the pair.

The bi-orthonormal system (A) of (B) can be chosen *balanced*,

$$\langle\psi_i, \psi_i\rangle = \langle\varphi_i, \varphi_i\rangle, \quad i = 1, \dots, m. \quad (\text{C})$$

Indeed, the necessary changes in the norms can be compensated by adjusting the a_i . Now we insert (B) into the right-hand side of (13) and observe that

$$\text{Tr } A\omega + \text{Tr } B\rho = \sum_1^m (a_j \langle\psi_j|\omega|\psi_j\rangle + a_j^{-1} \langle\varphi_j|\rho|\varphi_j\rangle).$$

By varying the free parameters a_j we arrive at the theorem.

THEOREM 3. *Let $m + k = \dim \mathcal{H}$. Then*

$$F_k(\omega, \rho) = \inf \sum_{i=1}^m \sqrt{\langle\psi_i, \omega\psi_i\rangle\langle\varphi_i, \rho\varphi_i\rangle}, \quad (27)$$

where the infimum runs through all balanced bi-orthogonal systems of length m . \square

Finally, assume that the infimum in (13) is attained by $\{A, B\} \in \text{PAIRS}_m$,

$$F_k(\omega, \rho) = \frac{1}{2} (\text{Tr } A\omega + \text{Tr } B\rho), \quad m + k = \dim \mathcal{H}. \quad (28)$$

If we vary the minimizing pair, the first variation must vanish,

$$\left(\frac{d}{ds} \right)_{s=0} c(s) = 0, \quad c(s) = (\text{Tr } A_s\omega + \text{Tr } B_s\rho),$$

where, with $X_s = \exp sY$ and any operator Y ,

$$A_s = X_s^* A X_s, \quad B_s = X_s^{-1} B (X_s^*)^{-1}.$$

We take the first derivative and obtain

$$\left(\frac{d}{ds} \right)_{s=0} A_s = Y^* A + A Y, \quad \left(\frac{d}{ds} \right)_{s=0} B_s = -Y B - B Y^*.$$

After inserting in $\dot{c}(0) = 0$ and a rearrangement it results in

$$\mathrm{Tr} Y(A\rho - \omega B)^* + \mathrm{Tr} Y^*(A\rho - \omega B) = 0.$$

As Y could be chosen arbitrarily, we arrive at

$$A\rho = \omega B \tag{29}$$

as a necessary condition for the validity of (28).

Is there any $\{A, B\} \in \mathrm{PAIRS}_m$ fulfilling (28) and minimizing (13)? If we can Γ -transform ω, ρ to the form τ, τ , then the answer is positive. Indeed, we then can choose a projection operator P_m onto the m smallest eigenvalues of τ and we get

$$F_k(\tau, \tau) = \mathrm{Tr} P_m \tau, \quad \{P_m, P_m\} \in \mathrm{PAIRS}_m,$$

i.e. the problem is solved in that case. Now, if ω and ρ are both invertible, there is a unique positive X such that

$$X\omega X = X^{-1}\rho X^{-1} := \tau, \quad X > 0, \tag{30}$$

The choice (30) ensures (28) with $A = X P_m X$, $B = X^{-1} P_m X^{-1}$. To get X one has to solve $X^2 \omega X^2 = \rho$. There is a unique positive solution X which is the square root of the geometric mean [11] between ρ and ω^{-1} ,

$$X^2 = \omega^{-1/2} (\omega^{1/2} \rho \omega^{1/2})^{1/2} \omega^{-1/2}$$

as one can convince oneself by inserting into $X^2 \omega X^2 = \rho$.

Acknowledgement

I like to thank P. M. Alberti for several good advices and B. Crell, C. Fuchs, H. Narnhofer, and W. Thirring for stimulating discussions. I am thankful for support to the Erwin Schrödinger Institute for Mathematical Physics, Vienna, and, during the Workshop on Complexity, Computation and the Physics of Information, to the Isaac Newton Institute for Mathematical Sciences, Cambridge, and to the European Science Foundation.

REFERENCES

- [1] A. Uhlmann, *Rep. Math. Phys.* **9** (1976), 273; R. Jozsa, *J. Mod. Opt.* **41** (1994), 2315; Ch. A. Fuchs and C. M. Caves: *Open Sys. & Inf. Dyn.* **3** (1995), 345.
- [2] P. M. Alberti and A. Uhlmann: Transition probabilities on C^* - and W^* -algebras. In: H. Baumgärtel, G. Laßner, A. Pietsch, and A. Uhlmann, (eds.), *Proceedings of the Second International Conference on Operator Algebras, Ideals, and their Applications in Theoretical Physics, Leipzig 1983*, pp. 5–11, Leipzig, 1984. BSB B. G. Teubner Verlagsgesellschaft, Teubner-Texte zur Mathematik, Bd. 67.
- [3] P. M. Alberti and A. Uhlmann: On Bures-Distance and $*$ -Algebraic Transition Probability between Inner Derived Positive Linear Forms over W^* -Algebras. *Acta Applicandae Mathematicae* **60** (2000), 1.
- [4] H. Araki and G. A. Raggio: *Lett. Math. Phys.* **6** (1982), 237.
- [5] P. M. Alberti: *Lett. Math. Phys.* **7** (1983), 25.
- [6] P. M. Alberti, private communication.
- [7] R. T. Rockafellar: *Convex Analysis*, Princeton University Press, Princeton 1970.
- [8] P. M. Alberti: *Wiss. Z. KMU Leipzig MNR* **39** (1990), 579; P. M. Alberti, *Z. Anal. Math.* **11** (1992), 293; V. Heinemann, Thesis, Leipzig 1991.
- [9] A. W. Marshall and I. Olkin: *Inequalities: Theory of Majorization and Its Applications*, Mathematics in Science and Engineering **143**, Academic Press, New York 1979.
- [10] P. M. Alberti and A. Uhlmann: *Stochasticity and Partial Order*. VEB Deutscher Verlag der Wissenschaften, Berlin 1981; (M. Hazewinkel, ed.), *Mathematics and its Applications* **9**, D. Reidel Publ. Company, Dordrecht 1982.
- [11] W. Pusz and L. Woronowicz: *Rep. Math. Phys.* **8** (1975), 159.