A three state invariant

M. Fannes, D. Vanpeteghem

April 1, 2022

Instituut voor Theoretische Fysica
K.U.Leuven
Celestijnenlaan 200D, B-3001 Heverlee, Belgium

Abstract

For triples of probability measures, pure quantum states and mixed quantum states we obtain the exact constraints on the fidelities of pairs in the sequence. We show that it is impossible to decide between a quantum model, either pure or mixed, and a classical model on the basis of the fidelities alone. Next, we introduce a quantum three state invariant called phase and show that any sequence of pure quantum states is uniquely reconstructible given the fidelities and phases.

1 Preliminary

The transition probability or overlap between states is one of the fundamental ingredients of quantum mechanics. It lies at the basis of its probabilistic interpretation. Two states with an overlap close to one are almost equal. This motivates the term fidelity which will be used as a synonym of transition probability.

*E-mail: mark.fannes@fys.kuleuven.ac.be
†E-mail: dimitri.vanpeteghem@fys.kuleuven.ac.be
‡Research Assistant of the Fund for Scientific Research, Flanders (Belgium) (F.W.O., Vlaanderen)
Also in the context of classical probability there is a quite common notion of distance between probability measures, the Hellinger distance based on overlaps of densities. This distance is given by \( d_{H}^2(\mu; \lambda) = 1 - A(\mu; \lambda) \), where \( A \) is called the affinity between \( \lambda \) and \( \mu \). Affinity is the classical counterpart of transition probability.

We shall be concerned here with the notion of fidelity in three different settings: probability measures, pure quantum states and mixed quantum states. As there are natural inclusions between these three sets extending the affinity between classical measures to fidelity for mixed quantum states, we gradually widen our scope when passing from probability measures to mixed quantum states.

Notions of closedness of states belonging to a sequence generated by a dynamics or by a coding procedure are obviously important to decide either on the regular or the chaotic nature of the sequence [3] or on compressibility issues, see [7, 6]. In previous work, we used the spectrum of the Gram matrix of the sequence for this purpose, see [2, 4]. This spectrum is however a complicated function depending on the full sequence.

The point of this paper is twofold. In Section 2, we analyse sequences of three states. This is the simplest non-trivial situation. We obtain the precise constraints on the fidelities of pairs of states in the sequence for measures and for pure and mixed quantum states. They turn out to coincide. In other words, on the basis of an admissible triple of fidelities it is impossible to decide whether one deals with probability measures or with pure or mixed quantum states.

Next, we introduce in Section 3 a quantum three state invariant called phase and we show that, for pure quantum states, any arbitrary sequence can be uniquely reconstructed on the basis of the fidelities of pairs and phases of triples in the sequence.

We recall the basic definitions.

The fidelity between two probability measures \( \lambda = (\lambda_1, \lambda_2, \ldots, \lambda_N) \) and \( \mu = (\mu_1, \mu_2, \ldots, \mu_N) \) on an event space with \( N \) elements is given by

\[
F(\lambda; \mu) := \left( \sum_{j=1}^{N} \sqrt{\lambda_j \mu_j} \right)^2 .
\]

We may extend fidelity to general probability measures by using the Radon-Nikodym derivative.
For quantum systems, we call expectation functionals on the observables states. E.g., in standard quantum mechanics a normalised vector $\varphi$ in the Hilbert space $\mathcal{H}$ of the system yields a pure state

$$P_\varphi(X) := \langle \varphi, X \varphi \rangle,$$

$X$ an Hermitian operator on $\mathcal{H}$.

Writing

$$P_\varphi(X) = \operatorname{Tr}(\varphi \langle \varphi | X \rangle)$$

we see that $P_\varphi$ is uniquely determined by the one-dimensional projector on the subspace $\mathbb{C} \varphi$ and we shall therefore identify $|\varphi \rangle \langle \varphi |$ with $P_\varphi$. A (normal) mixed state on $\mathcal{H}$ is then a general density matrix $\rho$.

The fidelity between $P_\varphi$ and $P_\psi$ is the usual quantum mechanical transition probability between $\varphi$ and $\psi$

$$F(P_\varphi; P_\psi) := |\langle \varphi, \psi \rangle|^2 = \operatorname{Tr}(P_\varphi P_\psi). \quad (2)$$

For mixed states, Uhlmann extended the notion by using the purification procedure, i.e. by obtaining a mixed states as a marginal of a pure state on a composite system, see [8]. This leads to

$$F(\rho; \sigma) := \left( \operatorname{Tr} \sqrt{\rho^{\frac{1}{2}} \sigma \rho^{\frac{1}{2}}} \right)^2 = \left( \operatorname{Tr} \sqrt{\sigma^{\frac{1}{2}} \rho \sigma^{\frac{1}{2}}} \right)^2. \quad (3)$$

An isometric transformation $U$ induces the transformation $\rho \mapsto U \rho U^* = \rho \circ \operatorname{Ad}(U^*)$ on density matrices. The spectrum of $\rho$, taking degeneracies into account, remains invariant up to multiplicities of zero. This is also the case for the fidelity

$$F(\rho; \sigma) = F(U \rho U^*; U \sigma U^*) = F(\rho \circ \operatorname{Ad}(U^*); \sigma \circ \operatorname{Ad}(U^*)).$$

Again, fidelity between states can be extended to general quantum probability spaces, see [1, 8]. It is straightforward to check that the three definitions (1)–(3) of fidelity are compatible.

A simple example is given by states on the matrices of dimension 2. In this case there is an affine isomorphism between the density matrices of dimension 2 and the unit ball in $\mathbb{R}^3$ explicitly given by the Bloch transformation

$$\rho_x := \frac{1}{2} \left( \mathbb{1} + x \cdot \sigma \right), \quad x \in \mathbb{R}^3, \quad \|x\| \leq 1.$$

Here $\sigma$ are the usual Pauli matrices. The two dimensional case is rather misleading as the topological and convex boundaries of the state space coincide,
they are namely the unit sphere in $\mathbb{R}^3$. For the $d$-dimensional matrices, the state space has $d^2 - 1$ real dimensions, its topological boundary $d^2 - 2$ while the pure state space has dimension $2(d - 1)$. So, the topological boundary has many flat pieces. The Uhlmann fidelity can be readily computed for the two dimensional case and one obtains

$$F(\rho_x; \rho_y) = \frac{1}{2} \left( 1 + x \cdot y + \sqrt{1 - \|x\|^2} \sqrt{1 - \|y\|^2} \right).$$

In particular, for pure states, i.e. $\|x\| = \|y\| = 1$, the fidelity is the square of the cosine of half the angular distance between $x$ and $y$.

2 Fidelities of triples

In this section, we consider a triple of states or measures and compute the fidelities pairwise. We then look for the constraints between the three fidelities $F_{12}$, $F_{13}$ and $F_{23}$. Plotting $(F_{12}^{1/2}, F_{13}^{1/2}, F_{23}^{1/2})$ in $\mathbb{R}^3$ we obtain subsets of $(\mathbb{R}^+)^3$ when the states run either through the measures, the pure or the quantum mixed states. These sets are obviously ordered by inclusion. Moreover they are closed, convex and compact. The convexity follows from the direct sum construction. E.g. for the Uhlmann fidelity

$$\text{Tr} \sqrt{\left( \frac{1}{2} (\rho_1 \oplus \rho_2) \right)^{1/2} (\sigma_1 \oplus \sigma_2) \left( \frac{1}{2} (\rho_1 \oplus \rho_2) \right)^{1/2}}$$

$$= \frac{1}{2} \left( \text{Tr} \sqrt{\rho_1^{1/2} \sigma_1^{1/2}} + \text{Tr} \sqrt{\rho_2^{1/2} \sigma_2^{1/2}} \right).$$

Lemma 1. Let $\varphi_1$, $\varphi_2$ and $\varphi_3$ be three normalised vectors in a Hilbert space $\mathcal{H}$ and let $F_{jk} := F(P_{\varphi_j}; P_{\varphi_k})$, then

$$F_{12} + F_{13} + F_{23} \leq 1 + 2\sqrt{F_{12}F_{13}F_{23}}. \quad (4)$$

Proof. The three dimensional matrix

$$G = \begin{pmatrix}
1 & \langle \varphi_1, \varphi_2 \rangle & \langle \varphi_1, \varphi_3 \rangle \\
\langle \varphi_2, \varphi_1 \rangle & 1 & \langle \varphi_2, \varphi_3 \rangle \\
\langle \varphi_3, \varphi_1 \rangle & \langle \varphi_3, \varphi_2 \rangle & 1
\end{pmatrix}$$

is positive semi-definite. In particular, $\det(G) \geq 0$ or

$$0 \leq 1 + 2 \text{Re} \left( \langle \varphi_1, \varphi_2 \rangle \langle \varphi_2, \varphi_3 \rangle \langle \varphi_3, \varphi_1 \rangle - |\langle \varphi_1, \varphi_2 \rangle|^2 - |\langle \varphi_1, \varphi_3 \rangle|^2 - |\langle \varphi_2, \varphi_3 \rangle|^2 \right).$$
Hence
\[ F_{12} + F_{13} + F_{23} = |\langle \varphi_1, \varphi_2 \rangle|^2 + |\langle \varphi_1, \varphi_3 \rangle|^2 + |\langle \varphi_2, \varphi_3 \rangle|^2 \]
\[ \leq 1 + 2 \Re \left( \langle \varphi_1, \varphi_2 \rangle \langle \varphi_2, \varphi_3 \rangle \langle \varphi_3, \varphi_1 \rangle \right) \]
\[ \leq 1 + 2 |\langle \varphi_1, \varphi_2 \rangle||\langle \varphi_2, \varphi_3 \rangle||\langle \varphi_3, \varphi_1 \rangle| \]
\[ = 1 + 2 \sqrt{F_{12}F_{13}F_{23}}, \]
which proves (4).

Let us denote by \( C_3 \) the compact convex subset of \( \mathbb{R}^3 \)
\[ \{ \mathbf{x} = (x_1, x_2, x_3) \mid 0 \leq x_j \leq 1 \text{ for } j = 1, 2, 3 \text{ and } x_1^2 + x_2^2 + x_3^2 \leq 1 + 2x_1x_2x_3 \}. \]
The convex boundary of \( C_3 \) is
\[ \partial_c(C_3) = \{(0, 0, 0), (0, 0, 1), (0, 1, 0), (0, 0, 0), (1, 0, 0), (0, 1, 1)\} \]
\[ \cup \{ \mathbf{x} \mid 0 \leq x_j < 1 \text{ for } j = 1, 2, 3 \text{ and } x_1^2 + x_2^2 + x_3^2 = 1 + 2x_1x_2x_3 \}. \]

**Lemma 2.** \( C_3 = \{(F_{12}^3, F_{13}^3, F_{23}^3)\} \) where the fidelities are computed for probability measures on a space with six points.

**Proof.** The extreme point \((0, 0, 0)\) can be realised with three degenerate measures on a space of three points, \((1, 0, 0)\), \((0, 1, 0)\) and \((0, 0, 1)\) on one with two points and \((1, 1, 1)\) with a single point. Using convexity and the shape of \( C_3 \), it is then sufficient to show that any extreme point of the surface \( \{ \mathbf{x} \mid 0 \leq x_j < 1 \text{ for } j = 1, 2, 3 \text{ and } x_1^2 + x_2^2 + x_3^2 = 1 + 2x_1x_2x_3 \} \) can be obtained by transition probabilities between measures on a space with two points.

Suppose that \( x_1 \leq x_2 \leq x_3 \) and put \( \lambda_1 := (1, 0) \), \( \lambda_2 := (x_1^2, 1 - x_1^2) \) and \( \lambda_3 := (x_2^2, 1 - x_2^2) \). We then have that
\[ F(\lambda_1 ; \lambda_2) = x_1^2, \quad F(\lambda_1 ; \lambda_3) = x_2^2, \quad \text{and} \]
\[ F(\lambda_2 ; \lambda_3) = (x_1x_2 + \sqrt{(1 - x_1^2)(1 - x_2^2)})^2. \]
Solving the equation \( x_1^2 + x_2^2 + x_3^2 = 1 + 2x_1x_2x_3 \) for \( x_3 \) and taking into account that \( 0 \leq x_1 \leq x_2 \leq x_3 \leq 1 \) we find that \( F(\lambda_2 ; \lambda_3) = x_3^2 \). \( \square \)
Lemma 2 shows that any triple of transition probabilities that can be obtained by transition probabilities between pure quantum states can also be reached by classical measures. Our next aim is to show the rather surprising fact that we still remain in the set $C_3$ when we consider Uhlmann fidelities between three arbitrary mixed quantum states.

**Proposition 1.** Let $\rho_1, \rho_2$ and $\rho_3$ be three density matrices on a Hilbert space $\mathcal{H}$ and let $F_{jk} := F(\rho_j; \rho_k)$, then

$$F_{12} + F_{13} + F_{23} \leq 1 + 2\sqrt{F_{12}F_{13}F_{23}}.$$

*Proof.* We may assume that the $\rho_j$ have full support. The general case is obtained by continuity. Denoting $F(\rho_1; \rho_2)^{\frac{1}{2}}$ by $a$, we certainly have that $0 < a \leq 1$. Therefore

$$0 < F(\rho_1; \rho_3) + F(\rho_2; \rho_3) - 2a\sqrt{F(\rho_1; \rho_3)F(\rho_2; \rho_3)}$$

and we wish to obtain the upper bound $1 - a^2$. Using the polar decomposition and the assumption on the support of the $\rho_j$, there exist unitaries $U$ and $V$ such that

$$\rho_1^{\frac{1}{2}} \rho_3^{\frac{1}{2}} = U |\rho_1^{\frac{1}{2}} \rho_3^{\frac{1}{2}}| \quad \text{and} \quad \rho_2^{\frac{1}{2}} \rho_3^{\frac{1}{2}} = V |\rho_2^{\frac{1}{2}} \rho_3^{\frac{1}{2}}|.$$ 

In these formulas $|X|$ denotes the absolute value of an operator $X$, i.e. $|X| := (X^*X)^{\frac{1}{2}}$. We now express the fidelities as follows

$$F_{12}^{\frac{1}{2}}(\rho_1; \rho_3) = \text{Tr} \sqrt{\rho_3^{\frac{1}{2}} \rho_1^{\frac{1}{2}} \rho_3^{\frac{1}{2}}} = \text{Tr} |\rho_1^{\frac{1}{2}} \rho_3^{\frac{1}{2}}| = \text{Tr} U^{*} \rho_1^{\frac{1}{2}} \rho_3^{\frac{1}{2}}.$$ 

Using the Hilbert-Schmidt scalar product between Hilbert-Schmidt operators, $\langle X, Y \rangle_{HS} := \text{Tr} X^*Y$, the fidelities become

$$F_{12}^{\frac{1}{2}}(\rho_1; \rho_3) = \langle f, h \rangle_{HS} \quad \text{and} \quad F_{23}^{\frac{1}{2}}(\rho_2; \rho_3) = \langle g, h \rangle_{HS}$$

with

$$f := \rho_1^{\frac{1}{2}} U, \quad g := \rho_2^{\frac{1}{2}} V \quad \text{and} \quad h := \rho_3^{\frac{1}{2}}.$$ 

We can then verify the following properties

$$\langle f, h \rangle_{HS} = |\langle f, h \rangle_{HS}|, \quad \langle g, h \rangle_{HS} = |\langle g, h \rangle_{HS}|,$$

$$||f||_{HS} = ||g||_{HS} = ||h||_{HS} = 1, \quad \text{and}$$

$$|\langle f, g \rangle| = |\text{Tr} U^{*} \rho_1^{\frac{1}{2}} \rho_2^{\frac{1}{2}} V| \leq \sup_{W \text{ unitary}} |\text{Tr} \rho_1^{\frac{1}{2}} \rho_2^{\frac{1}{2}} W| = F_{12}^{\frac{1}{2}}(\rho_1; \rho_2) = a.$$ 

The statement of the proposition now follows from Lemma 3. \qed
Lemma 3. Let \( f \) and \( g \) be normalised vectors in a Hilbert space \( \mathcal{H} \) and let \( a \) be such that \(|\langle f, g \rangle| \leq a \leq 1\), then
\[
\sup_{h, \|h\| \leq 1} \left( |\langle f, h \rangle|^2 + |\langle g, h \rangle|^2 - 2a|\langle f, h \rangle||\langle g, h \rangle| \right) = (1-a)(1+|\langle f, g \rangle|) \leq (1-a^2).
\]

Proof. As the supremum is always non-negative, we may impose the additional restriction \( h \in \text{span}\{f, g\} \). If \( h \) does not belong to this subspace, decompose it into \( h_1 \oplus h_2 \) with \( h_1 \in \text{span}\{f, g\} \). Next replace \( h \) by \( h_1/\|h_1\| \).

Evaluating the functional with this new \( h \) will return a value at least as large as that with the original \( h \).

So let \( h = \alpha f + \beta g \) with \( \alpha, \beta \in \mathbb{C} \) such that
\[
\|h\|^2 = |\alpha|^2 + |\beta|^2 + 2\Re(\overline{\alpha}\beta\langle f, g \rangle) = 1. \tag{5}
\]

Using this normalisation condition we compute
\[
|\langle f, h \rangle|^2 = |\alpha + \beta\langle f, g \rangle|^2 = 1 - |\beta|^2(1 - |\langle f, g \rangle|^2)
\]
and
\[
|\langle g, h \rangle|^2 = |\overline{\alpha}\langle f, g \rangle + \beta|^2 = 1 - |\alpha|^2(1 - |\langle f, g \rangle|^2).
\]

Hence, the functional of \( h \) we have to maximise does not depend on the phase of \( \overline{\alpha}\beta\langle f, g \rangle \). The normalisation condition (5) can be satisfied if and only if
\[
\left| |\alpha|^2 + |\beta|^2 - 1 \right| \leq 2|\alpha||\beta||\langle f, g \rangle|.
\]

Putting \( \lambda := |\alpha| \), \( \mu := |\beta| \) and \( t := |\langle f, g \rangle| \) we have to compute
\[
I := \sup_{\lambda, \mu} \left( 2 - (\lambda^2 + \mu^2)(1-t^2) - 2a\sqrt{1 - \lambda^2(1-t^2)}\sqrt{1 - \mu^2(1-t^2)} \right)
\]
subject to the constraints
\[
0 \leq \lambda, \quad 0 \leq \mu, \quad \text{and} \quad |\lambda^2 + \mu^2 - 1| \leq 2\lambda\mu t
\]
with \( t \) satisfying \( 0 \leq t \leq a \leq 1 \). The supremum is attained choosing \( \lambda = \mu \), with \( \lambda \) such that
\[
\frac{1}{2(1+t)} \leq \lambda^2 \leq \frac{1}{2(1-t)}.
\]
We obtain for \( I \) the value
\[
I = 2(1-a)\left(1 - \frac{1-t^2}{2(1+t)} \right) = (1-a)(1+t) \leq (1-a^2).
\]
\qed
3 Phase, a three state invariant

For three pure states $\omega_j := P_{\phi_j}$ with $\phi_j \in \mathcal{F}$ and $\|\phi_j\| = 1$, $j = 1, 2, 3$ we introduce the complex number $e^{i\Phi(\omega_1; \omega_2; \omega_3)}$ by the relation

$$
\langle \phi_1, \phi_2 \rangle \langle \phi_2, \phi_3 \rangle \langle \phi_3, \phi_1 \rangle = e^{i\Phi(\omega_1; \omega_2; \omega_3)} F^{\frac{1}{2}}(\omega_1; \omega_2) F^{\frac{1}{2}}(\omega_2; \omega_3) F^{\frac{1}{2}}(\omega_3; \omega_1).
$$

This definition implicitly assumes that all fidelities are strictly positive. It is easy to see that there is no continuous extension to the case of zero fidelities. Obviously $\Phi$ is invariant under isometric transformations and

$$
\Phi(\omega_1; \omega_2; \omega_3) = \Phi(\omega_2; \omega_3; \omega_1) \quad \text{and} \quad \Phi(\omega_1; \omega_2; \omega_3) = -\Phi(\omega_2; \omega_1; \omega_3).
$$

The relevance of other invariants than the fidelity was e.g. underlying the study of the spectrum of the Gram matrix of a sequence of states as in [2]. An other instance was considered in [5] where compressibility was shown to depend monotonically on the elementary symmetric invariants of the Gram matrix. Here we shall argue the need for such an invariant to reconstruct sequences of pure states, up to unitary invariance of course.

Let us first consider the example of a two level system. Let $x$ be a unit vector in $\mathbb{R}^3$ that defines through the Bloch transformation a pure state on the $2 \times 2$ matrices. Let us fix in the canonical basis of $\mathbb{C}^2$ a vector $\phi_x$ that generates the state. Using standard spherical coordinates $x = (\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta)$ we choose

$$
\phi_x := \left( \frac{\cos \theta}{2}, \frac{\sin \phi}{2} \right), \quad \theta \in (0, \pi), \quad \phi \in (0, 2\pi).
$$

Fix now three unit vectors $x, y$ and $z$ in $\mathbb{R}^3$. A straightforward computation shows that

$$
\cos(\Phi(\rho_x; \rho_y; \rho_z)) = \frac{\cos^2(\theta_{xy}) + \cos^2(\theta_{xz}) + \cos^2(\theta_{yz}) - 1}{2 \cos(\theta_{xy}) \cos(\theta_{xz}) \cos(\theta_{yz})}.
$$

Here, $\theta_{xy}$ denotes the angular distance between $x$ and $y$. We need of course also $\sin(\Phi(\rho_x; \rho_y; \rho_z))$ in order to determine $\Phi$ uniquely. The angle $\Phi$ turns out to be zero if and only if there is a permutation $(\alpha, \beta, \gamma)$ of $(x, y, z)$ such that $\theta_{\alpha} = \theta_{\beta} - \theta_{\gamma}$, i.e. if $x, y$ and $z$ are collinear.

Consider next the following rather trivial problem. The fidelity between two degenerate classical probabilities is either one or zero according to whether
the points in which the measures live coincide or not. Suppose that we are given for a sequence \( \delta = \{\delta_1, \delta_2, \ldots, \delta_n\} \) of Dirac measures the pairwise fidelities \( F_{jk} := F(\delta_j; \delta_k) \). We can obviously reconstruct the sequence \( \delta \), up to renaming points and reshuffling. It suffices to determine the multiplicity of each \( \delta_j \) in the sequence by counting the number of \( k \)'s such that \( F_{jk} = 1 \).

The analogous quantum problem is less trivial.

**Proposition 2.** For \( n = 1, 2, \ldots \) there is generically, up to isometric transformations and reshuffling, a unique sequence \( \omega = (\omega_1, \omega_2, \ldots, \omega_n) \) of pure states on a Hilbert space \( H \) with given fidelities \( F_{jk} := F(\omega_j; \omega_k) \) (\( j < k \)) and phases \( \Phi_{jkl} := \Phi(\omega_j; \omega_k; \omega_l) \) (\( j < k < l \)).

**Proof.** Writing \( \omega_j = P_{\varphi_j} \), we shall reconstruct the \( \varphi_j \) in a canonical way. More precisely

\[
\varphi_j = \sum_{\ell=1}^{j} c_{j\ell} e_{\ell}
\]

where \( \{e_1, e_2, \ldots\} \) is the standard basis in \( \ell^2(\mathbb{N}_0) \), up to multiplication of \( e_{\ell} \) by a complex number \( z_{\ell} \) of modulus one. As \( \varphi_j \) is only determined up to a phase and using the freedom to choose the phases \( z_{\ell} \) of the standard basis, we may assume that \( c_{j1} > 0 \) and \( c_{jj} > 0 \). It remains to determine the \( c_{jk} \) with \( 1 < k < j \). This can be done recursively. We start with \( c_{11} = 1 \). For \( j = 2 \)

\[
c_{21} = F_{12}^{\frac{1}{2}} \quad \text{and} \quad c_{22} = (1 - F_{12})^{\frac{1}{2}}.
\]

For \( j = 3 \), \( c_{31} = F_{13}^{\frac{1}{2}} \). In order to determine the complex coefficient \( c_{32} \), we use the data \( F_{13} \) and \( \Phi_{123} \)

\[
e^{-i\Phi_{123}} \langle \varphi_1, \varphi_2 \rangle \langle \varphi_2, \varphi_3 \rangle \langle \varphi_3, \varphi_1 \rangle = F_{12}^{\frac{1}{2}} F_{13}^{\frac{1}{2}} F_{23}^{\frac{1}{2}}.
\]

This equation determines \( \langle \varphi_2, \varphi_3 \rangle \) and from there on \( c_{32} \) as

\[
\langle \varphi_2, \varphi_3 \rangle = c_{21} c_{31} + c_{22} c_{32}.
\]

Given the coefficients \( c_{k\ell} \) with \( 1 \leq k < j \) and \( 1 \leq \ell \leq k \), we determine
uniquely the $c_{j\ell}$ with $1 \leq \ell \leq j$ by the equations

\begin{itemize}
  \item $c_{j1} = F^\frac{1}{2}_{1j}$
  \item $e^{-i\Phi_{12j}} \langle \varphi_1, \varphi_2 \rangle \langle \varphi_j, \varphi_1 \rangle = F^\frac{1}{2}_{12j} F^\frac{1}{2}_{1j} F^\frac{1}{2}_{2j}$
  \item $e^{-i\Phi_{13j}} \langle \varphi_1, \varphi_3 \rangle \langle \varphi_j, \varphi_1 \rangle = F^\frac{1}{2}_{13j} F^\frac{1}{2}_{1j} F^\frac{1}{2}_{3j}$
  \item \ldots
  \item $c_{jj} = \left(1 - |c_{j1}|^2 - \cdots - |c_{jj-1}|^2 \right)^{\frac{1}{2}}$
\end{itemize}

It is already clear from the three state case that only specifying the fidelities of pairs in a sequence of pure states is insufficient to reconstruct the sequence. A simple parameter count shows that we need $(n-1)^2$ real parameters for a sequence of length $n$. The fidelities provide $n(n-1)/2$ parameters and we therefore need $(n-1)(n-2)/2$ more. The whole set of phases provides $n(n-1)(n-2)/6$ which is far too much for large $n$. The argument of the proof is however based on the specification of phases $\Phi_{1kj}$ with $1 < k < j$ which is the minimal number needed.

To conclude, we propose an extension of the phase to the mixed state case based on the purification of states. To keep things as simple as possible we shall only deal with density matrices $\rho$ on $\mathcal{H}$ with non-degenerate spectrum and trivial kernel. The general case can be dealt with taking the support of the density matrix into account. We briefly remind here the purification construction, also known as GNS construction. A complex conjugation on $\mathcal{H}$ is a complex antilinear transformation $\varphi \mapsto \overline{\varphi}$ such that

$\overline{\varphi} = \varphi \quad \text{and} \quad \langle \overline{\varphi}, \overline{\psi} \rangle = \langle \psi, \varphi \rangle$.

To any operator $A$ on $\mathcal{H}$ we may associate a conjugate operator $\overline{A}$ by the relation $\overline{A}\varphi := \overline{A\varphi}$. It is straightforward to check that $\overline{A}$ is a complex linear operator on $\mathcal{H}$ and that

$\overline{\alpha A + B} = \overline{\alpha} \overline{A} + \overline{B}, \quad \overline{AB} = \overline{A} \overline{B}, \quad \text{and} \quad \overline{A^*} = (\overline{A})^*$.

Let $\{f_1, f_2, \ldots\}$ be an orthonormal basis of $\mathcal{H}$ diagonalising $\rho$: $\rho f_j = r_j f_j$. As standard purification of $\rho$, we consider the vector

$$\Omega_\rho := \sum_j r_j^{\frac{1}{2}} f_j \otimes \overline{f_j} \quad \text{in} \quad \mathcal{H} \otimes \mathcal{H}. \quad (6)$$
Then $\rho$ is the marginal of the pure state $X \mapsto \langle \Omega_\rho, X \Omega_\rho \rangle$. The expansion of $\Omega_\rho$ in (6) is the Schmidt decomposition of $\Omega_\rho$. There are many pure states in the tensor system that have $\rho$ as a marginal. They are all of the form $1 \otimes U \Omega_\rho$ with $U$ a unitary operator on $\mathcal{H}$. We shall use this freedom of choice to extend the notion of phase from pure states to mixed ones, namely $\Phi(\rho_1; \rho_2; \rho_3)$ is such that

$$\left| e^{i \Phi(\rho_1; \rho_2; \rho_3)} - 1 \right| = \inf_{U_1, U_2, U_3} \left| e^{i \Phi(1 \otimes U_1 \Omega_1, 1 \otimes U_2 \Omega_2, 1 \otimes U_3 \Omega_3)} - 1 \right|.$$  (7)

Here the infimum is taken over all unitaries on $\mathcal{H}$.

We can rephrase the variational problem (7). Let $\{g_1, g_2, \ldots\}$ be the orthogonal basis of eigenvectors of a density matrix $\sigma$ with corresponding eigenvalues $s_j$ and let $V$ be another unitary on $\mathcal{H}$, then

$$\langle 1 \otimes U \Omega_\rho, 1 \otimes V \Omega_\sigma \rangle = \sum_{jk} r_j s_j^2 f_j \otimes U f_j, g_k \otimes V g_k$$

$$= \sum_{jk} r_j s_j^2 \langle f_j, g_k \rangle \langle V g_k, U f_j \rangle$$

$$= \text{Tr} \rho \frac{1}{2} \sigma \frac{1}{2} V^* U.$$

A study of the phase for mixed states will be the subject of a forthcoming paper.

**Acknowledgements** It is a pleasure to acknowledge stimulating and interesting discussions with R. Alicki, M. Horodecki, R. Horodecki and P. Spincemaille. This work was partially supported by F.W.O., Vlaanderen grant G.0109.01.

**References**

[1] H. Araki and G.A. Raggio: A remark on transition probability, *Lett. Math. Phys.* 6, 237–240 (1982)

[2] M. De Cock, M. Fannes and P. Spincemaille: On quantum dynamics and statistics of vectors, *J. Phys. A* 32, 6547–6571 (1999)

[3] M. Fannes and P. Spincemaille: Multiple return times in the quantum baker map, *Phys. Lett. A* 294, 74–78 (2002)
[4] M. Fannes and P. Spincemaille: The mutual affinity of random measures, *Periodica Mathematica Hungarica*, **47**, 51–71 (2003)

[5] G. Mitchison and R. Jozsa: Towards a geometrical interpretation of quantum information compression e-Print: quant-ph/0309177

[6] D. Petz and M. Mosonyi: Stationary quantum source coding, *J. Math. Phys.* **42**, 4857–4864 (2001)

[7] B. Schumacher: Quantum coding, *Phys. Rev. A* **51**, 2738–2747 (1995)

[8] A. Uhlmann: The transition probability in the state space of a ∗-algebra, *Rep. Math. Phys.* **9**, 273–279 (1976)