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On an extension problem for density matrices

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We investigate the problem of the existence of a density matrix ρ_{123} on a Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$ with given partial traces $\rho_{12} = \mathrm{Tr}_3\, \rho_{123}$ and $\rho_{23} = \mathrm{Tr}_1\, \rho_{123}$. While we do not solve this problem completely, we offer partial results in the form of some necessary and some sufficient conditions on ρ_{12} and ρ_{23}. The quantum case differs markedly from the classical (commutative) case, where the obvious necessary compatibility condition suffices, namely, $\mathrm{Tr}_1\, \rho_{12} = \mathrm{Tr}_3 \rho_{23}$. *© 2013 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4808218]

I. INTRODUCTION

The problem considered here is closely related to the *quantum marginal problem*, on which there is an extensive literature. However, since the problem we consider involve *overlapping marginals*, results in the literature shed little light on it. We therefore introduce the problem in terms that we find natural, and postpone the discussion of the relation between our results and results on the quantum marginal problem until later in the Introduction.

Let $\mathcal{H}_1$, $\mathcal{H}_2$, $\mathcal{H}_3$ be three finite dimensional Hilbert spaces. Let ρ_{12} be a density matrix on $\mathcal{H}_{12} = \mathcal{H}_1 \otimes \mathcal{H}_2$ and, similarly, let ρ_{23} be a density matrix on $\mathcal{H}_{23} = \mathcal{H}_1 \otimes \mathcal{H}_2$. The question we ask, and which we can only partially resolve, is:

Assuming that there is consistency of the partial traces, namely, $\mathrm{Tr}_1\, \rho_{12} = \rho_2 = \mathrm{Tr}_3\, \rho_{23}$, *what are necessary and sufficient conditions for the existence of a density matrix* ρ_{123} *on* $\mathcal{H}_{123} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$ *such that* $\mathrm{Tr}_1\, \rho_{123} = \rho_{23}$ *and* $\mathrm{Tr}_3\, \rho_{123} = \rho_{12}$?

This question goes back at least to Werner,[17] who proved the existence of consistent pairs for which no extension exists. A simple example is given later in this Introduction.

This is an obvious question to ask in several contexts, e.g., Ref. 9. We note the fact that in classical statistical mechanics the answer is that an extension always exists, and there is a simple formula for it: Given probability densities $\rho_{12}(x, y)$ and $\rho_{23}(y, z)$ with

$$\int \rho_{12}(x, y)\mathrm{d}\mu_1(x) = \int \rho_{23}(y, z)\mathrm{d}\mu_3(z) =: \rho_2(y),$$

we may define

$$\rho_{123}(x, y, z) = \frac{\rho_{12}(x, y)\rho_{23}(y, z)}{\rho_2(y)}. \tag{1.1}$$

If the sample spaces over which x, y, and z range are finite sets, these densities may be identified with diagonal density matrices in a natural way, embedding the discrete classical probability space problem into the quantum mechanical problem.

This extension is not unique, in general, but among all extensions, this one has the maximum entropy, namely, $S_{12} + S_{23} - S_2$. The maximality is a consequence of the Strong Subadditivity of

Entropy (SSA) which says that for any extension

$$S_{12} + S_{23} \geq S_{123} + S_2.$$

The classical SSA inequality is relatively easy to prove (as opposed to its quantum version); see Ref. 11. The principle behind the construction is *conditioning*: Note that for random variables Y and Z with joint density $\rho_{23}(y, z)$, $\rho_{23}(Y, z)/\rho_2(Y)$ is the conditional density for Z given Y.

This construction of extensions by conditioning can be generalized to arbitrarily many factors. Given $\rho_{j,j+1}, j = 1, \ldots, N$, such that

$$\int \rho_{j-1,j}(x_{j-1}, x_j)\mathrm{d}\mu_{j-1}(x_{j-1}) = \int \rho_{j,j+1}(x_j, x_{j+1})\mathrm{d}\mu_{j+1}(x_{j+1}) =: \rho_j(x_j)$$

define

$$\rho_{1,\ldots,N}(x_1, \ldots, x_N) = \rho_{1,2}(x_1, x_2)\prod_{j=2}^{N-1}\frac{\rho_{j,j+1}(x_j, x_{j+1})}{\rho_j(x_j)}.$$

Again this extension is the maximum entropy extension by an interated application of SSA.

However, the construction (1.1), being based on conditional probabilities, does not generalize to the quantum case, where the notion of "conditioning" has no obvious meaningful analog. In general, even for consistent density matrices,

$$\rho_{12}\rho_2^{-1}\rho_{23} \tag{1.2}$$

need not be Hermitian, much less positive definite. While

$$R = \exp[\log\rho_{12} + \log\rho_{23} - \log\rho_2]$$

is Hermitian and positive definite, its partial traces will not equal the desired reduced density matrices, even after renormalization, which would be required since the trace, $\mathrm{Tr}_{123}R$, is never greater than 1, and, generally, is less than 1. This fact follows from the triple Golden-Thompson inequality[10]

$$\mathrm{Tr}_{123}\, R \leq \mathrm{Tr}_2\mathrm{Tr}_{13}\int_0^\infty \rho_{12}\frac{1}{t+\rho_2}\rho_{23}\frac{1}{t+\rho_2}\mathrm{d}t = \mathrm{Tr}_2\int_0^\infty \rho_2\frac{1}{t+\rho_2}\rho_2\frac{1}{t+\rho_2}\mathrm{d}t = \mathrm{Tr}_2\rho_2 = 1.$$

One situation in which the classical formula (1.2) is valid occurs when ρ_{12} and ρ_{23} commute and are consistent. This implies that ρ_2 commutes with ρ_{12} and ρ_{23}. (To see, note that $\rho_2\rho_{23} = \mathrm{Tr}_1(\rho_{12}\rho_{23}) = tr_1(\rho_{23}\rho_{12}) = \rho_{23}\rho_2$, and likewise for $\rho_2\rho_{12} = \rho_{12}\rho_2$.)

We note that if ρ_{12} is pure and $\rho_{12} = \mathrm{Tr}_3\,\rho_{123}$, then $\rho_{123} = \rho_{12}\otimes\rho_3$. Hence ρ_{23} must be a product when there is an extension ρ_{123}. This provides simple examples of compatible pairs with no extension. For example, take ρ_{12} to be pure and ρ_{23} not to be a product, but consistent with ρ_{12}.

In Sec. II, Theorem 2.1 generalizes this observation by identifying a class of non-pure states ρ_{12}, which can only be extended by product states $\rho_{12}\otimes\rho_3$.

Motivated by these examples, and the obvious difference between the classical and quantum cases, we believe that a proper understanding of this problem will lead to a clearer understanding of entanglement and quantum information theory.

A. The quantum marginal problem

The quantum marginal problem, in its simplest form, is the following: Given density matrices ρ_1 and ρ_2, on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, let $\mathcal{C}(\rho_1, \rho_2)$ denote the set of all density matrices ρ_{12} on $\mathcal{H}_1\otimes\mathcal{H}_2$ such that

$$\mathrm{Tr}_1\rho_{12} = \rho_2 \qquad \text{and} \qquad \mathrm{Tr}_2\rho_{12} = \rho_1. \tag{1.3}$$

Here, $\mathcal{C}(\rho_1, \rho_2)$ is the set of *quantum couplings* of ρ_1 and ρ_2.

Note that $\mathcal{C}(\rho_1, \rho_2)$ is never empty; it always contains $\rho_1\otimes\rho_2$. It is also evidently convex and compact, and hence it is the convex hull of its extreme points. Characterizations of the extreme points have been given by Parthasarathy[14] and Rudolph.[16]

Other research has focused on the relations between the spectra of ρ_1, ρ_2, and ρ_{12} that characterize the set of triples of density matrices satisfying (1.3). For results in this direction see the recent papers of Klyachko,[8] and Christandl *et al.*,[4] and references therein.

The general quantum marginal problems concern states on the product of arbitrarily many Hilbert spaces, and the marginals obtained by taking any combination of partial traces – for instance, the partial traces ρ_{12} and ρ_{23} of ρ_{123} as in our problem. Most results pertain to the case of non-overlapping marginals, in contrast to the problem considered here. An exception is the paper by Osborne.[13] He uses the SSA of the von Neumann entropy[12] to prove an upper bound on the number of *orthogonal pure states* ρ_{123} such that $\mathrm{Tr}_1\, \rho_{123} = \rho_{23}$ and $\mathrm{Tr}_3\, \rho_{123} = \rho_{12}$. We shall also employ entropy bounds, but are mainly concerned with the existence, or not, of *mixed-state* extensions ρ_{123} of compatible pairs ρ_{12} and ρ_{23}. For other work on overlapping marginals see the papers of Butterly *et al.*[2] and Hall,[6] who investigate necessary and sufficient conditions for the existence of an extension when one is given *all* of the proper marginals (e.g., for three spaces one has to be given ρ_{12}, ρ_{13}, and ρ_{23}.)

It is natural to use entropy in this investigation, and some early results on the two-space problem are given in terms of entropy. For example, if ρ_{12} is a pure state, then its partial traces ρ_1 and ρ_2 have the same non-zero spectrum.[1] Conversely, if ρ_1 and ρ_2 are two density matrices having the same non-zero spectrum, then there is a pure state ρ_{12} satisfying (1.3). To construct it, assume without loss of generality that $\mathcal{H}_1$ and $\mathcal{H}_2$ have the same dimension. There is a unitary U such that $U\rho_2 U^*$ $= \rho_1$. Define $\Psi := U\sqrt{\rho_2}$, where the matrix on the right is regarded as a vector in $\mathcal{H}_1 \otimes \mathcal{H}_2$. Then $\rho_{12} = |\Psi\rangle\langle\Psi|$ is such a pure state.

If ρ_1 and ρ_2 do not have the same spectrum, then the set $\mathcal{C}(\rho_1, \rho_2)$ cannot contain any pure state. It is natural then to ask for the least entropy element of $\mathcal{C}(\rho_1, \rho_2)$. Since the entropy is concave, the minimum will be attained at an extreme point, and the results of Refs. 14 and 16 are relevant, and lead easily to the minimizer in specific cases. However, a well-known inequality already provides a sharp *a priori* lower bound for this minimum entropy coupling.

The *Araki-Lieb Triangle inequality*[1] says that when (1.3) is satisfied

$$S_{12} \geq |S_1 - S_2|. \tag{1.4}$$

For an interesting discussion of entropy inequalities for a general *classical* marginal problem, see Ref. 5.

II. NECESSARY CONDITIONS FOR THE EXISTENCE OF AN EXTENSION

Strong Subadditivity of Entropy[12] (see also Ref. 11) provides us with two necessary conditions for an extension to exist: Let ρ_{123} be an extension of ρ_{12} and ρ_{23}. Then, discarding the positive term S_{123} in SSA,

$$S_{12} + S_{23} \geq S_2. \tag{2.1}$$

Classically, one has monotonicity of the entropy, meaning $S_{12} \geq S_2$ and $S_{23} \geq S_2$ so that (2.1) hold classically with $2S_2$ on the right side. However, quantum mechanically, equality can hold in (2.1): Let ρ_{12} be a purification of ρ_2, i.e., a pure state $|\Psi\rangle\langle\Psi|$ on $\mathcal{H}_1 \otimes \mathcal{H}_2$ such that $\mathrm{Tr}_2(|\Psi\rangle\langle\Psi|) = \rho_1$. Such purifications always exist. It is well known, and easy to see from the definition, that the set of all possible purifications Ψ of ρ_1 is the set of all operators $\sqrt{\rho_1}U$, regarded as vectors in $\mathcal{H}_1 \otimes \mathcal{H}_2$, where U is a partial isometry from a subspace of $\mathcal{H}_2$ onto the range of ρ_1. Let ρ_{23} be the tensor product of ρ_2 and a pure state. Then $S_{12} = 0$ and $S_{23} = S_2$.

A second form of SSA[12] leads to a sharper necessary condition: Again assume that ρ_{123} is an extension of ρ_{12} and ρ_{23}. Then

$$S_{12} + S_{23} \geq S_1 + S_3. \tag{2.2}$$

As we now explain, whenever (2.2) is satisfied by any consistent pair of density matrices ρ_{12} and ρ_{23} (not necessarily possessing a common extension), then (2.1) is automatically satisfied. To see this, note that by (1.4), $S_2 - S_1 \le S_{12}$ and $S_2 - S_3 \le S_{23}$. Adding these inequalities, we obtain

$$2S_2 \le S_{12} + S_{23} + S_1 + S_3.$$

By (2.2), the right side is no greater than $2(S_{12} + S_{23})$, which yields (2.1).

The density matrices for which there is equality in the triangle inequality have a particular structure: Let m and n be positive integers, and let $\{\lambda_1, \dots, \lambda_m\}$ and $\{\mu_1, \dots, \mu_n\}$ be sets of positive numbers with $\sum_{j=1}^m \lambda_j = \sum_{k=1}^n \mu_k = 1$. Then, as shown in Ref. 3, there exists a density matrix ρ_{12} such that the non-zero eigenvalues of ρ_{12} are $\{\lambda_1, \dots, \lambda_m\}$, the non-zero eigenvalues of ρ_2 are $\{\mu_1, \dots, \mu_n\}$, and the non-zero eigenvalues of ρ_1 are the numbers $\{\lambda_j\mu_k : 1 \le j \le m\,, 1 \le k \le n\}$. For any such ρ_{12}, it is evident that $S_{12} = S_1 - S_2$. Moreover, as shown in Ref. 3, whenever $S_{12} = S_1 - S_2$, the spectra of ρ_{12}, ρ_1, and ρ_2 are related in this way.

The following theorem generalizes the observation that pure states ρ_{12} may only be extended by product states $\rho_{12} \otimes \rho_3$. When ρ_{12} is pure, $0 = S_{12} = S_2 - S_1$.

Theorem 2.1. *Let ρ_{12} be a density matrix such that*

$$S_{12} = S_1 - S_2. \tag{2.3}$$

Then ρ_{12} and ρ_{23} have a common extension if and only if $\rho_{23} = \rho_2 \otimes \rho_3$.

Proof. Using (2.3) in (2.2) we obtain

$$S_1 - S_2 + S_{23} \ge S_3 + S_1,$$

which reduces to $S_{23} \ge S_2 + S_3$. By the subadditivity of the entropy, this means that $S_{23} = S_2 + S_3$, and so $\rho_{23} = \rho_2 \otimes \rho_3$. □

In Sec. IV, we give an example in which (2.2) is satisfied, but there is no common extension.

III. SUFFICIENT CONDITIONS FOR THE EXISTENCE OF AN EXTENSION

We do not have any very general sufficient conditions for compatible pairs to possess a common extension. One general positive statement that can be made is the following.

Theorem 3.1. *Let ρ_{12} and ρ_{23} be a compatible pair of density matrices that posses a common extension ρ_{123} that is positive definite. Let $\|\cdot\|$ denote the trace norm. Then there is an $\epsilon > 0$, depending on the dimensions and the smallest eigenvalue of ρ_{123}, such that if $\widetilde{\rho}_{12}$ and $\widetilde{\rho}_{23}$ is another compatible pair on the same spaces and*

$$\|\rho_{12} - \widetilde{\rho}_{12}\| + \|\rho_{23} - \widetilde{\rho}_{23}\| < \epsilon, \tag{3.1}$$

then $\widetilde{\rho}_{12}$ and $\widetilde{\rho}_{23}$ possess common extension.

Proof. Define

$$\widetilde{\rho}_{123} = \rho_{123} + [\widetilde{\rho}_{12} - \rho_{12}] \otimes \widetilde{\rho}_3 + \widetilde{\rho}_1 \otimes [\widetilde{\rho}_{23} - \rho_{23}] + \widetilde{\rho}_1 \otimes [\rho_2 - \widetilde{\rho}_2] \otimes \widetilde{\rho}_3.$$

It is easily checked that $\mathrm{Tr}_1\widetilde{\rho}_{123} = \widetilde{\rho}_{23}$ and $\mathrm{Tr}_3\widetilde{\rho}_{123} = \widetilde{\rho}_{12}$. Furthermore, $\widetilde{\rho}_{123}$ is self-adjoint, and under the condition (3.1) is positive when ϵ is chosen sufficiently small. □

Remark 3.2. Of course, in this finite dimensional setting, the trace norm could be replaced by any other norm. Also, suppose that ρ_{12} is positive definite, and $\rho_{23} = \rho_2 \otimes \rho_3$ with ρ_3 positive definite. In this case, ρ_{12} and ρ_{23} are compatible and have the positive-definite common extension $\rho_{12} \otimes \rho_3$. The theorem says that any compatible pair that is a small perturbation of ρ_{12} and ρ_{23} has a common extension. However, as Theorem 2.1 shows, the requirement of positive definiteness cannot be dropped.

Let ρ_{12} and ρ_{23} be a consistent pair of density matrices, both of which are separable. Recall that a bipartite density matrix ρ_{12} is *finitely separable* if it is a convex combination of product states; i.e., if

$$\rho_{12} = \sum_{j=1}^{N} \lambda_j \sigma_1^{(j)} \otimes \tau_2^{(j)},$$

where each $\sigma_1^{(j)}$ is a density matrix on $\mathcal{H}_1$, each $\tau_2^{(j)}$ is a density matrix on $\mathcal{H}_2$ and, crucially, each $\lambda_j > 0$. The set of separable density matrices is the closure of the set of finitely separable density matrices.

Separable density matrices are often viewed as being a classical ensemble of product states. As such, separable states are free of *quantum correlations* among observables on $\mathcal{H}_1$ and $\mathcal{H}_2$. Separable bipartite density matrices do, indeed, behave much more like classical joint probability distributions. For example, if ρ_{12} is separable, then (see, e.g., Ref. 3),

$$S_{12} \geq \max\{S_1 \ \ S_2\},$$

and thus when both ρ_{12} and ρ_{23} are separable and compatible, $S_{12} + S_{23} \geq S_1 + S_3$, and thus the condition (2.2), which is necessary for a common extension to exists, is always satisfied.

One might therefore, hope that a common extension ρ_{123} would exist whenever ρ_{12} and ρ_{23} are compatible and both are separable. In Sec. IV, we show that this is not the case: Further conditions must be imposed to ensure the existence of an extension. Here is one case in which a common extension does exist.

Suppose that

$$\rho_{12} = \sum_{j=1}^{n} \lambda_j \, \rho^{(j)} \otimes \sigma^{(j)} \qquad \text{and} \qquad \rho_{23} = \sum_{j=1}^{n} \lambda_j \, \sigma^{(j)} \otimes \tau^{(j)}, \tag{3.2}$$

where the $\rho^{(j)}$, $\sigma^{(j)}$, and $\tau^{(j)}$ are density matrices and the λ_j are positive numbers with $\sum_{j=1}^{n} \lambda_j = 1$. Then

$$\rho_{123} := \sum_{j=1}^{n} \lambda_j \, \rho^{(j)} \otimes \sigma^{(j)} \otimes \tau^{(j)} \tag{3.3}$$

is a common extension.

While this example is based on a strong assumption, namely, that the weights and the factors on $\mathcal{H}_2$ coincide, we shall show in Sec. IV that consistency and separability is not enough.

However, as we now explain, there is a more general version of this construction using coherent states. Good references on coherent states are Refs. 7 and 15.

Let $\mathcal{H}$ be any d dimensional Hilbert space. Define $J = (d - 1)/2$. Then there is an irreducible representation of $SU(2)$ on $\mathcal{H}$. Associated with this representation is a family of pure states $|\Omega\rangle\langle\Omega|$ on $\mathcal{H}$, parameterized by a point Ω in the unit sphere, S^2. Given any self-adjoint operator A on $\mathcal{H}$, there is a function $\widehat{a}(\Omega)$ on S^2 such that

$$A = \int_{S^2} \mathrm{d}\Omega \; \widehat{a}(\Omega) \, |\Omega\rangle\langle\Omega|, \tag{3.4}$$

where the integration is with respect to the uniform probability measure on S^2. The function $\widehat{a}(\Omega)$ is *unique* if we further require that $\widehat{a}(\Omega)$ be a spherical harmonic of degree no higher than $2J$. (See p. 33 and Eq. (4.10) of Ref. 7.) This function $\widehat{a}(\Omega)$ is called the *upper symbol* of the operator A. The upper symbol of A need not be a non-negative function on S^2 even if A is positive definite. However, if $\widehat{a}$ is non-negative, then the operator A defined by (3.4) is positive semidefinite.

Now consider a bipartite density matrix ρ_{12} on $\mathcal{H}_1 \otimes \mathcal{H}_2$ where the dimension of $\mathcal{H}_j = d_j$ for $j = 1, 2$. Suppose that it has a representation

$$\rho_{12} = \int_{S^2} \mathrm{d}\Omega_2 \int_{S^2} \mathrm{d}\Omega_1 \; \widetilde{\rho}_{12}(\Omega_1, \Omega_2) \; (|\Omega_1\rangle\langle\Omega_1| \otimes |\Omega_2\rangle\langle\Omega_2|)$$

with $\widetilde{\rho}_{12}(\Omega_1, \Omega_2)$, a non-negative function on $S^2 \times S^2$ that is a spherical harmonic of degree $d_j - 1$ in Ω_j, $j = 1, 2$.

Then taking the trace over $\mathcal{H}_1$, we find

$$\rho_2 := \mathrm{Tr}_1 \rho_{12} = \int_{S^2} \mathrm{d}\Omega_2 \left[\int_{S^2} \mathrm{d}\Omega_1 \ \widetilde{\rho}_{12}(\Omega_1, \Omega_2) \right] |\Omega_2\rangle\langle\Omega_2|,$$

and evidently $\int_{S^2} \mathrm{d}\Omega_1 \, \widetilde{\rho}_{12}(\Omega_1, \Omega_2)$ has the degree $d_2 - 1$ in Ω_2, which ensures that it is the unique upper symbol of ρ_2 of minimal degree.

Likewise, if ρ_{23} is a density matrix on $\mathcal{H}_2 \otimes \mathcal{H}_3$ with the dimension of $\mathcal{H}_3 = d_j$, and if ρ_{23} is compatible with ρ_{12} and, moreover,

$$\rho_{23} = \int_{S^2} \mathrm{d}\Omega_2 \int_{S^2} \mathrm{d}\Omega_3 \ \widetilde{\rho}_{23}(\Omega_2, \Omega_3) \ (|\Omega_2\rangle\langle\Omega_2| \otimes |\Omega_3\rangle\langle\Omega_3|)$$

with $\widetilde{\rho}_{23}(\Omega_2, \Omega_3)$ being a non-negative function on $S^2 \times S^2$ that is a spherical harmonic of degree $d_j - 1$ in Ω_j, $j = 2, 3$, $\int_{S^2} \mathrm{d}\Omega_3 \, \widetilde{\rho}_{23}(\Omega_2, \Omega_3)$ is the upper symbol of ρ_2, and thus quantum compatibility of ρ_{12} and ρ_{23} implies the classical compatibility of the probability densities $\widetilde{\rho}_{12}(\Omega_1, \Omega_2)$ and $\widetilde{\rho}_{23}(\Omega_2, \Omega_3)$. Hence the classical prescription may be used to define

$$\widetilde{\rho}_{123}(\Omega_1, \Omega_2, \Omega_3) := \frac{\rho_{12}(\Omega_1, \Omega_2)\, \rho_{23}(\Omega_2, \Omega_3)}{\rho_2(\Omega_2)},$$

and it is then the case that

$$\rho_{123} := \int_{S^2} \mathrm{d}\Omega_1 \int_{S^2} \mathrm{d}\Omega_2 \int_{S^2} \mathrm{d}\Omega_3 \ \widetilde{\rho}_{123}(\Omega_1, \Omega_2, \Omega_3) \ (|\Omega_1\rangle\langle\Omega_1| \otimes |\Omega_2\rangle\langle\Omega_2| \otimes |\Omega_3\rangle\langle\Omega_3|)$$

is positive semidefinite, and is a common extension of ρ_{12} and ρ_{23}.

IV. SEPARABLE COMPATIBLE PAIRS WITH NO EXTENSION

In this section, we give examples of compatible pairs ρ_{12} and ρ_{23} that do not have an extension, but nevertheless satisfy the necessary condition (2.2). Moreover, in these examples both ρ_{12} and ρ_{23} will be separable. As we have remarked above, one might expect the extension problem to simplify in the presence of separability. This is not the case, as the following examples show. For simplicity, our examples will be on $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$, but of course may be embedded into higher dimensional spaces.

Lemma 4.1. Let ρ_2 be a non-pure density matrix on $\mathbb{C}^2$; i.e., the rank of ρ_2 is 2. Let $\{\psi_1, \psi_2\}$ be an orthonormal basis of $\mathbb{C}^2$ consisting of eigenvectors of ρ_2. Let $\rho_2\psi_j = \mu_j\psi_j$, $j = 1, 2$. Then there exist two unit vectors ϕ_1 and ϕ_2 in $\mathbb{C}^2$ and positive numbers ν_1 and ν_2 such that

$$\sum_{j=1}^{2} \mu_j |\psi_j\rangle\langle\psi_j| = \rho_2 = \sum_{j=1}^{2} \nu_j |\phi_j\rangle\langle\phi_j|, \tag{4.1}$$

and such that the four vectors ψ_1, ψ_2, ϕ_1, and ϕ_2 are pairwise linearly independent.

Proof. If ρ_2 is $\frac{1}{2}\mathbb{1}$, we may take $\{\psi_1, \psi_2\}$ to be any orthonormal basis of $\mathbb{C}^2$, and then choose $\{\phi_1, \phi_2\}$ to be any other orthonormal basis such that ϕ_1 is not proportional to either ψ_1 or ψ_2. Then the four vectors $\phi_1, \phi_2, \psi_1, \psi_2$ are *pairwise* linearly independent. In this case, we take $\mu_j = \nu_j = \frac{1}{2}$ for $j = 1, 2$.

Next, assume ρ_2 has distinct eigenvalues $\mu_1 > \mu_2$. Let $\{\psi_1, \psi_2\}$ be an orthonormal basis consisting of eigenvectors of ρ_2. Let ϕ_1 be any unit vector that is not proportional to either ψ_1 or ψ_2. Then there is a unique largest number $\nu_1 > 0$, so that $\rho_2 - \nu_1|\phi_1\rangle\langle\phi_1|$ is positive semidefinite. Thus, $\rho_2 - \nu_1|\phi_1\rangle\langle\phi_1|$ is rank one, and hence

$$\rho_2 - \nu_1|\phi_1\rangle\langle\phi_1| = \nu_2|\phi_2\rangle\langle\phi_2|$$

for some unit vector ϕ_2 that is not proportional to ϕ_1 since ρ_2 has rank 2. Likewise, ϕ_2 is not an eigenvector of ρ_2, since by the non-degeneracy, this would force ϕ_1 to be an eigenvector, which it is not. □

Theorem 4.2. *Let ρ_2 be a non-pure density matrix on $\mathbb{C}^2$. Then there exist separable density matrices ρ_{12} and ρ_{23}, extending ρ_2, and such that (2.2) is satisfied (with strict inequality), but such that ρ_{12} and ρ_{23} have no common extension ρ_{123}.*

Proof. Let $\{\psi_1, \psi_2\}$ and $\{\phi_1, \phi_2\}$ be sets of unit vectors such that (1.3) is satisfied, and where $\{\psi_1, \psi_2\}$ is an orthonormal basis of $\mathbb{C}^2$ consisting of eigenvectors of ρ.

Let $\{\chi_1, \chi_2\}$ be any orthonormal basis of $\mathbb{C}^2$, and let $\{\eta_1, \eta_2\}$ be any linearly independent set of unit vectors in $\mathbb{C}^2$. Define

$$\rho_{12} = \sum_{j=1}^{2} \mu_j |\eta_j \otimes \psi_j\rangle\langle \eta_j \otimes \psi_j| \qquad \text{and} \qquad \rho_{23} = \sum_{j=1}^{2} \nu_j |\phi_j \otimes \chi_j\rangle\langle \phi_j \otimes \chi_j|. \tag{4.2}$$

Then evidently $\mathrm{Tr}_1\, \rho_{12} = \mathrm{Tr}_3\, \rho_{23} = \rho_2$. Next, for any vector $(z, w) \in \mathbb{C}^2$, let $(z, w)^\perp = (-\overline{w}, \overline{z})$ so that $(z, w)^\perp$ is orthogonal to (w, z).

Suppose a common extension ρ_{123} does exist. Then $\eta_1^\perp \otimes \psi_1$ is in the nullspace of ρ_{12}, and hence

$$\sum_{j=1}^{2} \langle \eta_1^\perp \otimes \psi_1 \otimes \chi_j, \rho_{123}\, \eta_1^\perp \otimes \psi_1 \otimes \chi_j\rangle = \langle \eta_1^\perp \otimes \psi_1, \rho_{12}\, \eta_1^\perp \otimes \psi_1\rangle = 0.$$

Therefore, since ρ_{123} is positive, both $\eta_1^\perp \otimes \psi_1 \otimes \chi_1$ and $\eta_1^\perp \otimes \psi_1 \otimes \chi_2$ are in the nullspace of ρ_{123}.

Since $\eta_2^\perp \otimes \psi_2$ is in the null space of ρ_{12}, the same argument shows that both $\eta_2^\perp \otimes \psi_2 \otimes \chi_1$ and $\eta_2^\perp \otimes \psi_2 \otimes \chi_2$ are in the nullspace of ρ_{123}. Thus, the four vectors

$$\eta_1^\perp \otimes \psi_1 \otimes \chi_j \qquad \text{and} \qquad \eta_2^\perp \otimes \psi_2 \otimes \chi_j\ , \qquad j = 1, 2$$

belong to the nullspace of ρ_{123}.

Likewise, both $\phi_!^\perp \otimes \chi_1$ and $\phi_2^\perp \otimes \chi_2$ belong to the nullspace of ρ_{23}. Arguing as above, we see that the four vectors

$$\eta_j^\perp \otimes \phi_!^\perp \otimes \chi_1 \qquad \text{and} \qquad \eta_j^\perp \otimes \phi_2^\perp \otimes \chi_2\ , \qquad j = 1, 2$$

belong to the nullspace of ρ_{123}.

Define the unit vectors

$$\Psi_1 = \eta_1^\perp \otimes \psi_1 \otimes \chi_1, \quad \Psi_2 = \eta_1^\perp \otimes \psi_1 \otimes \chi_2, \quad \Psi_3 = \eta_2^\perp \otimes \psi_2 \otimes \chi_1, \ \text{and}\ \Psi_4 = \eta_2^\perp \otimes \psi_2 \otimes \chi_2, \tag{4.3}$$

and the vectors

$$\Phi_1 = \eta_1^\perp \otimes \phi_1^\perp \otimes \chi_1, \quad \Phi_2 = \eta_1^\perp \otimes \phi_2^\perp \otimes \chi_2, \quad \Phi_3 = \eta_2^\perp \otimes \phi_1^\perp \otimes \chi_1, \ \text{and}\ \Phi_4 = \eta_2^\perp \otimes \phi_2^\perp \otimes \chi_2. \tag{4.4}$$

These 8 vectors are in the nullspace of ρ_{123} under the hypotheses imposed so far.

Now let us temporarily impose the additional hypothesis that $\{\eta_1, \eta_2\}$ is orthonormal. Consequently, $\{\eta_1^\perp, \eta_2^\perp\}$ is orthonormal.

We claim that the 8 unit vectors Ψ_j, Φ_j, $j = 1, 2, 3, 4$, are linearly independent. To see this, note that under our additional hypothesis, $\{\Psi_1, \Psi_2, \Psi_3, \Psi_4\}$ and $\{\Phi_1, \Phi_2, \Phi_3, \Phi_4\}$ are orthonormal, and $\langle \Psi_i, \Phi_j\rangle = \delta_{i,j}$. Therefore, if

$$\sum_{j=1}^{4} a_j \Psi_j + \sum_{j=1}^{4} b_j \Phi_j = 0,$$

$$(a_j \Psi_j + b_j \Phi_j) = 0 \qquad \text{for each} \qquad j = 1, 2, 3, 4.$$

However, since the vectors ψ_1 and ϕ_1 are linearly independent, so are the vectors $\psi_1^\perp$ and $\phi_2 = \phi_1^\perp$. Thus Ψ_1 and Φ_1 are linearly independent, and hence $a_1 = b_1 = 0$.

The same sort of argument shows that $a_j = b_j = 0$ for each $j = 1, 2, 3, 4$. Thus the eight vectors Ψ_j, $j = 1, 2, 3, 4$ and Φ_j, $j = 1, 2, 3, 4$ are linearly independent and in the nullspace of ρ_{123}, Since the dimension of $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes C^2$ is 8, this means $\rho_{123} = 0$, which is impossible.

Therefore, the compatible pair of density matrices ρ_{12} and ρ_{23} defined by (4.2) has no common extension.

Next, observe from (4.2) that

$$\rho_1 = \sum_{j=1}^{2} \mu_j |\eta_j\rangle\langle\eta_j|.$$

Since η_1 and η_2 are orthogonal, and since $\eta_1 \otimes \psi_1$ and $\eta_2 \otimes \psi_2$ are orthogonal

$$S_1 = S_{12} = -\sum_{j=1}^{2} \mu_j \log \mu_j .$$

In the same manner we see that

$$S_3 = S_{23} = -\sum_{j=1}^{2} \nu_j \log \nu_j .$$

Thus we have

$$S_{12} + S_{23} = S_1 + S_3.$$

Finally, making a sufficiently small change in $\{\eta_1, \eta_2\}$, we may arrange that this set of unit vectors is no longer orthogonal, but that the 8 unit vectors Ψ_j, Φ_j, $j = 1, 2, 3, 4$ defined in (4.3) and (4.4) are still linearly independent. Then the compatible pair ρ_{12} and ρ_{23} defined by (4.2) has no common extension. It is still true that $S_{23} = S_3$. Also, since $\{\psi_1, \psi_2\}$ is orthonormal, $\{\eta_1 \otimes \psi_1, \eta_2 \otimes \psi_2\}$ is orthonormal, and so $S_{12} = -\sum_{j=1}^{2} \mu_j \log \mu_j$. However, $\rho_1 = \sum_{j=1}^{2} \mu_j |\eta_j\rangle\langle\eta_j|$ and since $\{\eta_1, \eta_2\}$ is not orthogonal,

$$S_1 < -\sum_{j=1}^{2} \mu_j \log \mu_j = S_{12}.$$

Therefore, $S_{12} + S_{23} > S_1 + S_2$. □

Remark 4.3. While the condition that ρ_1 and ρ_2 have the same non-zero spectrum is necessary and sufficient to ensure that there exists a common purification of ρ_1 and ρ_2, the above construction shows that the condition that the nonzero spectrum of ρ_{12} equals that of ρ_3, and that the nonzero spectrum of ρ_{23} equals that of ρ_1, together with compatibility, does not ensure that there exists a common purification of ρ_{12} and ρ_{23}. Indeed, let $\{\eta_1, \eta_2\}$, $\{\psi_1, \psi_2\}$, $\{\phi_1, \phi_2\}$, and $\{\chi_1, \chi_2\}$ be four orthonormal bases of $\mathbb{C}^2$ having no vectors (or their opposites) in common. Then with $\mu_j = \nu_j = 1/2$, $j = 1, 2$, (4.2) defines a compatible pair of density matrices with $\rho_2 = \frac{1}{2}I$. The non-zero spectrum of ρ_{12}, ρ_{23}, ρ_1, and ρ_3 is $\{1/2, 1/2\}$, and yet there is no common extension of ρ_{12} and ρ_{23}, as the proof of Theorem 4.2 shows.

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