Note on Purifications of a Qubit

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Abstract

This note provides an explicit parametrization of all purifications of a mixed state in dimension 2 and all joint purifications, if any, of two mixed states in the same dimension. The former is parametrized by $SO(3, R)$, while the latter is parametrized by $SO(2, R)$, except when the state being purified is already pure. Using this, we show how to calculate certain measures of quantum information and as a byproduct we show how to solve one variation of the classical Procustes problem. This manuscript was originally scheduled to appear on the arXiv on October 8th, 2002, but it did not due to alleged illegibility of the pdf version of the manuscript.
1 Introduction

The notion of purification of a mixed state plays an important role in several contexts. It provides insight into the question of decoherence. It is important in quantum information theory from several points of view. For instance, many quantitative measures such as the maximal singlet fraction may be explicitly defined in terms of purifications.

The purpose of this note is to provide an explicit parametrization of all possible purifications of a mixed state in two dimensions, and joint purifications (if any) of two mixed states in a two dimensional Hilbert space. In terms of this explicit parametrization, this note recovers many of the quantitative measures mentioned above. In particular, it shows that the calculation of such measures reduces to optimization problems on the real orthogonal groups, $SO(2, R)$ and $SO(3, R)$.

The balance of this note is organized as follows. In the next section a precise definition of what we mean by purification and joint purification is provided. The same section derives the parametrizations referred to before. The III section shows how to reduce calculations of measures in quantum information to optimization problems, and gives some instances of when this can be done in closed form. As a byproduct, some insight into solving certain variations of the classical Procrustes problem is obtained. Section IV offers some conclusions. In an attempt to extend this mixed states of higher dimensions, we provide a Bloch sphere like characterization of three dimensional mixed and pure states in the appendix. The final section offers some conclusions.

2 Parametrization of Purifications

First, a mixed $2 \times 2$ state is psd, trace 1 matrix, $\rho$. A purification of $\rho$ is a psd, trace 1, projection, $P_\rho$, operating in $C^2 \otimes C^2$, such that the partial trace over the second $C^2$ factor of $P_\rho$ yields $\rho$. Likewise, given a pair, $\rho_1, \rho_2$ of mixed states in $C^2$, every pure state $P_{\rho_1, \rho_2}$ in $C^2 \otimes C^2$ whose partial trace over the first (resp. second) $C^2$ factor is $\rho_2$ (resp. $\rho_1$) is said to be a joint purification of the pair $\rho_1, \rho_2$.

Mixed states in $C^2$ may be represented in many fashions. However, one suitable choice
for the purpose at hand is the following

$$\rho = \frac{1}{2}(I_2 + \sum_{i=1}^{3} \beta_i \sigma_i)$$

where $\beta_i \in R, i = 1, \ldots, 3$ and $i = 1, 2, 3$ stands for $i = x, y, z$ respectively. It is well known that $\| \beta \| \leq 1$, with equality precisely for those $\rho$ which correspond to pure states.

For the same reasons, a mixed state in $C^2 \otimes C^2$ are best represented in the following fashion

$$\rho = \frac{1}{2}(I_4 + \sum_{i=1}^{3} \beta_i \sigma_i \otimes I_2 + \sum_{i=1}^{3} \gamma_i I_2 \otimes \sigma_i + \sum_{i=1}^{3} \sum_{k=1}^{3} \delta_{ik} \sigma_i \otimes \sigma_k)$$

(2.1)

for real $\beta_i, \gamma_i, \delta_{ik}$. This representation is quite popular in the literature. However, to the best of our knowledge, it is never refined further to obtain a Bloch sphere like picture. This is needed for our purposes. The following characterization of mixed states and pure states follows from a direct calculation of squares of a Hermitian matrix (psd matrices are squares of Hermitian matrices and pure states are psd matrices which equal their squares). To avoid circumlocution, we call the vector of $\beta_i$’s as $\beta$, the vector of $\gamma_i$’s as $\gamma$ and the matrix of $\delta_{ik}$’s, $\delta$.

**Proposition 2.1** Every mixed state in $C^2 \otimes C^2$ is of the form in Equation (2.1), with $\beta = \frac{1}{2} (\kappa \beta_0 + \delta_0 \gamma_0)$, $\gamma = \frac{1}{2} (\kappa \gamma_0 + \delta_0 \beta_0)^T$, $\delta = \frac{1}{2} (\kappa \delta_0 - (adj \\delta_0)^T - \beta_0 \gamma_0^T)$, for any $\beta_0, \gamma_0 \in R^3$, $\delta_0 \in gl(3, R)$, $\kappa \in R$ satisfying $\| \beta_0 \|^2 + \| \gamma_0 \|^2 + \text{Tr}(\delta_0^T \delta_0) \leq 4$ and $\kappa$ is the positive square root of the difference of the RHS and the LHS of this inequality. Every pure state is of the form in Equation (2.1), with $\beta = \delta \gamma$, $\gamma = \delta^T \beta$, $\delta = -(adj \delta)^T + \beta \gamma$, $\| \beta \|^2 + \| \gamma \|^2 + \text{Tr}(\delta^T \delta) = 3$.

**Proof:** The proof is a straightforward calculation. We will just record one important calculation going into the verification of this proposition, which will be needed for other purposes in this work. If $\rho_1, \rho_2$ are two mixed states represented via the form in Equation (2.1), then the trace of their product is

$$\text{Tr} (\rho_1 \rho_2) = \frac{1}{4} (1 + <\beta_1, \beta_2> + <\gamma_1, \gamma_2> + \text{Tr}(\delta_2^T \delta_1))$$

(2.2)

Next, note that the partial traces of such a $\rho$ (pure or impure) are precisely the $2 \times 2$ matrices $\frac{1}{2}(I_2 + \sum_{i=1}^{3} \beta_i \sigma_i), \frac{1}{2}(I_2 + \sum_{i=1}^{3} \gamma_i \sigma_i)$. This, of course, directly implies that for any mixed state the lengths of $\beta$ and $\gamma$ is at most one. Further, a simple calculation, left to the reader, shows i) $\det(\delta) = \parallel \beta \parallel^2 - 1$ for a pure state; ii) $\parallel \beta \parallel = \parallel \gamma \parallel$ for a pure state.
Returning to pure states, it follows from $\delta = -[\text{adj} \ (\delta)]^T + \beta \gamma^T$, $\gamma = \delta^T \beta$ and $\text{det}(\delta) = ||\beta||^2 - 1$, that

$$\delta \delta^T = (1- ||\beta||^2)I_3 + \beta \beta^T$$

(2.3)

The following result says that this condition is essentially sufficient to determine purifications of the state, $\frac{1}{2}(I_2 + \sum_{i=1}^3 \beta_i \sigma_i)$. This result also provides a complete parametrization of such purifications.

**Theorem 2.1** Let $\frac{1}{2}(I_2 + \sum_{i=1}^3 \beta_i \sigma_i)$ be a $2 \times 2$ mixed state. Then all possible purifications, $P_\rho$ may be parametrized as matrices of the form in Equation (2.4), with $\beta$ the given the $\beta$, $\gamma = \delta^T \beta$, $\delta$ any solution of the system of equations:

$$\delta \delta^T = (1- ||\beta||^2)I_3 + \beta \beta^T$$

$$\text{det} (\delta) = ||\beta||^2 - 1$$

(2.4)

This system of equations is always solvable. Further, the general solution to this system (and thus the general purification, $P_\rho$) is provided by $\delta = \tilde{\delta}S, S \in SO(3, R)$, with $\tilde{\delta}$ one particular solution of this system, Equation (2.4). Further, the set of purifications of $\rho$ is parametrized by $SO(3, R)$ when $||\beta|| < 1$ and by the unit sphere, $S \in R^3$ when $||\beta|| = 1$.

**Proof:** First, it is clear that any purification has to satisfy the the system Equation (2.4).

Proving the converse statement requires first proving that the respective system does have a solution, for any given $\beta$ within the closed unit sphere in $R^3$, and then that with the choice of $\beta$, $\gamma$ and $\delta$ in the statement of the theorem, $P_\rho$ is indeed pure. In other words, this choice of $\beta, \gamma, \delta$ indeed satisfies the defining relations for pure states, viz., $||\beta||^2 + ||\gamma||^2 + \text{Tr}(\delta^T \delta) = 3$,

$\beta = \delta \gamma; \gamma = \delta^T \beta$ and finally, $\delta = -[\text{adj} \ (\delta)]^T + \beta \gamma^T$.

Case I: $||\beta|| = 0$. In this case $\beta$ is 0. So the system Equation (2.4) reduces to

$$DD^T = I_3, \text{det} (D) = -1$$

Clearly any matrix in $O(3, R)$ with determinant, $-1$, is a solution. In this case, $\gamma = D^T \beta = 0$, and $D \gamma = D0 = 0 = \beta$. So of the defining relations for pure states, only the first and the fourth need checking. The first reduces to verifying $\text{Tr} \ [DD^T] = 3$ (since $\beta = \gamma = 0$), which
obviously holds. The final equation now becomes \( D = -(\text{adj} (D))^T \), which also holds since \( \det (D) = -1 \).

If \( \tilde{D} \in O(3) \) is one solution to Equation (2.4), then so is \( \tilde{D}C, C \in SO(3, R) \). Conversely, if \( D \) is a second solution, then \( C = \tilde{D}^{-1}D \) exists and satisfies

\[
CC^T = \tilde{D}^{-1}D D^T \tilde{D}^{-1} = (\tilde{D}^T \tilde{D})^{-1} = I_3
\]

Obviously \( \det (C) = 1 \). So \( C \in SO(3, R) \).

Case II: \( 0 < \| \beta \| < 1 \): First, the matrix \( (1 - \| \beta \|^2)I_3 + \beta \beta^T \) is positive definite. Indeed

\[
v^T v = v^T v - \beta^T \beta v + (\beta, v)^2 \]

is positive, for \( v \neq 0 \), since \( \| \beta \| < 1 \). So there is always a matrix \( \delta \) satisfying \( \delta \delta^T = (1 - \| \beta \|^2)I_3 + \beta \beta^T \).

Let us compute the determinant of such a \( \delta \). We get

\[
(\det(\delta))^2 = (1 - \| \beta \|^2)^2
\]

Indeed, the eigenvectors of \( (1 - \| \beta \|^2)I_3 + \beta \beta^T \) are \( \beta \) corresponding to eigenvalue 1 and any two vectors orthogonal to \( \beta \) (in \( R^3 \)) corresponding to the repeated eigenvalue \( 1 - \| \beta \|^2 \).

From this the previous equation follows trivially. So, \( \det(\delta) \), for a given solution \( \delta \) of the first equation in the system Equation (2.4), is either the positive or negative square root of \( (1 - \| \beta \|^2)^2 \). To ensure the negative square root, we multiply the given solution \( \delta \) by \( -I_3 \) if needed. This also solves the first equation in Equation (2.4) and has the desired determinant.

Defining \( \gamma = \delta^T \beta \), it is easy to verify \( \beta = \delta \gamma \) and \( \delta = -(\text{adj} (\delta))^T + \beta \gamma^T \). Indeed, \( \delta \gamma = \delta \delta^T \beta = (1 - \| \beta \|^2) \beta + \beta \beta^T \beta = \beta \), yielding the desired conclusion. To verify, \( \| \beta \|^2 + \| \gamma \|^2 + \text{Tr}(\delta \delta^T) = 3 \), we note first that upon taking trace on both sides of the first line in the system (2.4) yields, \( \text{Tr} (\delta \delta^T) = 3 - 2 \| \beta \|^2 \). Since \( \text{Tr} (\delta^T \delta) = \text{Tr} (\delta \delta^T) \), it suffices to show that \( \| \delta \delta^T \beta \|^2 = \| \beta \|^2 \). But \( \| \delta \delta^T \beta \|^2 = \delta^T \delta \delta^T \beta = \delta^T [(1 - \| \beta \|^2)I_3 + \beta \beta^T] \beta = \| \beta \|^2 \).

Finally, to show \( \delta = -[\text{adj} (\delta)]^T + \beta \gamma^T \), we will verify the transposed version. Since, \( \delta \) is invertible, we may premultiply both sides of the first line in the system Equation (2.4) by \( \delta^{-1} \). This, bearing in mind the second line of the system (2.4), yields

\[
\delta^T = -[\text{adj} (\delta)] + \delta^{-1} \beta \gamma^T = -[\text{adj} (\delta)] + \gamma \beta^T
\]

since it was just shown that \( \delta \gamma = \beta \) holds.

To show that the \( \delta \) of all purifications is given by \( \delta C, C \in SO(3, R) \), with \( \delta \) one particular solution of the system (2.4), note first that \( \delta = \delta C \) trivially satisfies (2.4). Conversely, if both
δ and \( \tilde{\delta} \) satisfy Equation (2.4), the polar decomposition theorem plus the fact that both \( \delta \) and \( \tilde{\delta} \) have the same determinant implies that there is a \( C \in SO(3, R) \) such that \( \delta = \tilde{\delta} C \) (for an argument which eschews the polar decomposition theorem see the remark following the proof).

Case III: \( || \beta || = 1 \) - In this case the system (2.3) reduces to

\[
DD^T = \beta \beta^T, \det(D) = 0
\] (2.5)

Since per the first equation \( DD^T \) is rank one, the second equation is superfluous. Once again there is at least one solution to Equation (2.5), viz \( \tilde{\delta} = \beta \beta^T \), for the given \( \beta \).

Next, to verify that any solution to Equation (2.5), together with the given \( \beta \) yields a purification, we first observe that \( \delta \gamma = \delta \delta^T \beta = \beta \), since \( || \beta || = 1 \). Just as in Case II, \( || \gamma || = || \beta || = 1 \). This together with the obvious property that \( \text{Tr} (\delta^T \delta) = || \beta ||^2 = 1 \) yields \( || \beta ||^2 + || \gamma ||^2 + \text{Tr} (\delta^T \delta) = 3 \). To verify, the remaining condition, first note that the matrix \( \delta \) is also a rank one matrix. Indeed, the rank of \( \delta \) is the same as that of \( \delta \delta^T \) (this is valid for any square matrix). So \( \delta \) may be written in the form \( \delta = vu^T \) for some vectors \( u, v \in R^3 \). So,

\[
\text{Tr} (\delta \delta^T) = \text{Tr} (vu^T uu^T) = ||u||^2 ||v||^2 = \text{Tr} (\beta \beta^T) = || \beta ||^2 = 1
\]

Hence, it holds that \( ||u|| \cdot ||v|| = 1 \). So, dividing \( v, u \) by their lengths, if needed, it follows that \( v, u \) may be chosen to be of length one. Now,

\[
\delta \delta^T = vu^T = \beta \beta^T
\]

So either \( v = \beta \) or \( v = -\beta \). Absorbing the negative sign if needed into \( u \), we see \( \delta = \beta u^T \) for a length one vector \( u \). Since \( u \) and \( \beta \) have length 1, and the group \( SO(3, R) \) acts transitively on the sphere in \( R^3 \), it follows that there is some \( C^T \in SO(3, R) \) such that \( u = C^T \beta \). So comparing \( \tilde{\delta} = \beta \beta^T \) with \( \delta = \beta u^T \), we see \( \delta = \tilde{\delta} C \). Since \( C \in SO(3, R) \), this verifies the claim.

Finally, the assertion about the parametrization follows, since, when \( || \beta || < 1 \), two purifications with distinct \( \delta \) matrices are also distinct. When \( || \beta || = 1 \), however, two purifications are distinct only if \( C \beta \not= \beta \). This means the redundancy in the parametrization consists of the isotropy subgroup of \( SO(3, R) \)'s action at the point \( \beta \), which implies the stated condition on the parametrization in this situation.
Remark 2.1 Alternative argument for part of Case II: In the following a different proof, which avoids the polar decomposition theorem, in Case II of the previous proof is given. This calculation may be of interest in its own right. Suppose $\delta$ and $\tilde{\delta}$ are two solutions of Equation (2.4), then letting $C = (\tilde{\delta})^{-1}\delta$, it is clear that $\det(C) = 1$. Further,

$$CC^T = (\tilde{\delta})^{-1}[(1 - ||\beta||^2)I_3 + \beta\beta^T](\tilde{\delta}^T)^{-1} = (1 - ||\beta||^2)[\tilde{\delta}^T \delta]^{-1} + \tilde{\gamma}\tilde{\gamma}^T, \text{ where } \tilde{\gamma} = \delta^T \beta$$

A direct calculation shows that $\tilde{\delta}^T \tilde{\delta} = (1 - ||\beta||^2)I_3 + \tilde{\gamma}\tilde{\gamma}^T$. Writing the matrix on the RHS of this last equation as $X + Y$, we see that $X$ and $X + Y$ are both invertible and further $Y$ is of rank one. By a trivial modification of the Sherman-Morrison-Woodbury formula, [3], it follows that $(X + Y)^{-1} = X^{-1} - \frac{1}{1+1/||YX^{-1}||}X^{-1}YX^{-1}$, Applying this to $X = (1 - ||\beta||^2)I_3$, $Y = \tilde{\gamma}\tilde{\gamma}^T$, yields

$$CC^T = (1 - ||\beta||^2)[\frac{1}{1 - ||\beta||^2}I_3 - \frac{1}{1 - ||\beta||^2}\tilde{\gamma}\tilde{\gamma}^T] + \tilde{\gamma}\tilde{\gamma}^T = I_3$$

i.e., $C \in SO(3, R)$.

Joint Purifications: Next, we suppose that two mixed states are given, i.e., $\rho_\beta = \frac{1}{2}(I_2 + \sum_{i=1}^3 \beta_i \sigma_i)$, $\rho_\gamma = \frac{1}{2}(I_2 + \sum_{i=1}^3 \gamma_i \sigma_i)$, with prespecified $\beta, \gamma \in R^3$ are given. When does there exist a pure state $P$ in $C^2 \otimes C^2$, such that the partial trace of $P$ over the second system yields $\rho_\beta$, while that over the first yields $\rho_\gamma$. The aim is to parametrize all such $P$s.

Clearly, a necessary condition is that $||\beta|| = ||\gamma|| \leq 1$. This is also sufficient.

Theorem 2.2 Suppose $\beta, \gamma \in R^3$ satisfy $||\beta|| = ||\gamma|| \leq 1$. Then they can be jointly purified. Further, there is at least one solution, $\delta$, to the system Equation (2.4) which yields, per the prescription of Th 2.1, such a joint purification. Given one such solution, $\tilde{\delta}$, the most general joint purification is given by $\delta C$, with $C \in SO(3, R)$ satisfying $C\gamma = \gamma$. This is a set parametrized by $SO(2, R)$, except when when $\beta = \gamma = 0$, in which case it is parametrized by $SO(3, R)$ or when $||\beta|| = 1$, in which case there is a unique joint purification.

Proof: Clearly, if we can find a solution $\delta$ to the system Equation (2.4), which further satisfies the condition $\delta^T \beta = \gamma$ for the given $\beta, \gamma$, the proof of Th 2.1 shows that the corresponding purification is indeed a joint purification. Suppose, for a specific solution, $\delta_{sp}$, it holds that $\delta_{sp}^T \beta \neq \gamma$. Then, computing

$$||\delta_{sp}\beta||^2 = \beta^T \delta_{sp}^T \delta_{sp}^T \beta = \beta^T \beta \beta^T \beta = \beta^T[1 - ||\beta||^2]\beta + ||\beta||^4 = ||\beta||^2 = ||\gamma||^2$$
The last equation follows from the hypothesis $||\beta||=||\gamma||$. Thus, $\delta^{T}_{sp}\beta$ has the same length as $\gamma$. Now, $SO(3, R)$ acts transitively on spheres of any radius. So, there is a $C^T \in SO(3, R)$ satisfying the condition $C^T\delta^{T}_{sp}\beta = \gamma$, i.e., $\tilde{\delta} = \delta_{sp}C$ provides one joint purification. Now of the purifications provided by $\delta = \tilde{\delta}C, C \in SO(3, R)$, only those purifications which satisfy $C^T\gamma = \gamma$ will yield a joint purification. Further, via the same arguments in Theorem 1, the most general joint purification is necessarily supplied by $C\tilde{\delta}$ with $C \in SO(3, R)$ such that $C\gamma = \gamma$.

The collection of all such $C$’s is, of course, the isotropy group at $\gamma$ of $SO(3, R)$’s action on this sphere. This isotropy group is conjugate to the isotropy at the vector $||\gamma|| (1, 0, 0)$, which is precisely $SO(2, R)$. Geometrically, all such $C$’s are rotations in the plane perpendicular to the vector $\gamma$, while $\gamma$ is the axis of rotation. If $||\beta||<1$, then due to the invertibility of the $\delta$ matrix of purifications, it follows that $SO(2, R)$ paramterizes the collection of joint purifications. If $||\beta||=1$, then $\beta\gamma^T = \beta(C\gamma)^T$, for every $C \in SO(3, R)$ fixing $\gamma$. So there is just one joint purification. Finally, if $\gamma = 0$, then the condition $C\gamma = \gamma$ is no constraint on $C \in SO(3, R)$.

**Remark 2.2** It is, of course, possible to induce on the set of purifications the additional structures in the orthogonal groups (or the sphere when $||\beta||=1$). However, this may not be very useful. For instance, the Riemannian metric on the orthogonal groups may not be consistent with the any of the current notions of distance between pure states. However, in a certain sense, these additional structures will be employed later in this work. More precisely, in the next section, some calculations of quantum information measures will be reduced to optimization on the orthogonal groups. The fact that these problems have a solution follows from the compactness of these groups. Further, they can be reduced to optimization problems over products of closed intervals via Euler angles etc.,

### 3 Calculation of Certain Quantum Information Measures

With explicit parametrizations of purifications of a single mixed state and joint purifications of a pair of mixed states, it is possible to compute, either in closed form or via optimization over well defined quantities, several quantum information measures. Many such measures
are often posed as optimization of scalar quantities over some pure states. Below we will give two examples where this can be done in closed form. The first is the maximal singlet fraction. A formula for this essentially appears in [4], where a full proof is not given. Further, the arguments involved in [4] consist of reducing the $\delta$ matrix of some mixed states into a normal form, which seems unmotivated. The proof below shows why that normal form naturally arises. Thus, the argument provided here may be seen as a complement to that in [4]. Secondly, we will compute the joint purification closest to a given (impure) mixed state with the same partial traces. In general, this leads to a variation of the Procustes problem and this variation will be formulated as the solution of a concrete optimization problem over the interval $[0, 2\pi]$. For the special case when this mixed state is the product state $\rho_\beta \otimes \rho_\gamma$ it turns out that all joint purifications are at the same distance. We then explain this from the perspective of the functional being optimized in this generalized Procustes problem.

**Remark 3.1** While optimization over $SO(3, R)$ or $SO(2, R)$ may be viewed as constrained optimization problems and thus amenable to Lagrange multiplier techniques, the methods used below avoid this. In part due to the nature of the function(al)s being optimized, it seems much better to use appropriate parametrizations of these groups and pass directly to an unconstrained optimization, than add further equations via the Lagrange multiplier method.

**Proposition 3.1** (see [4]) Consider a mixed state, $\rho$ in $C^2 \otimes C^2$ represented in the form given by Equation (2.1). Denote the corresponding $\delta$ matrix by $\delta_\rho$. Then its maximal singlet fraction is given by $\frac{1}{4}(1 + \sum_{i=1}^{3} \sigma_i)$, if $\det(\delta_\rho) < 0$ and by $\frac{1}{4}(1 + \sigma_1 + \sigma_2 - \sigma_3)$ if $\det(\delta_\rho) \geq 0$.

Here, the $\sigma_i$ are the singular values of $\delta_\rho$, with $\sigma_i \geq \sigma_j$, $i$ if $i < j$, $i, j = 1, 2, 3$.

Proof: The maximal singlet fraction $f(\rho)$ is defined via the equation $f(\rho) = \max < \psi | \rho | \psi >$, where the maximization is over all pure states $\psi$ which are maximally entangled. This collection of states is precisely the set of pure states locally equivalent to the Bell state. It is easy to see that this is precisely the collection of pure states, which when represented in form Equation (2.1) have $\beta = \gamma = 0$, $\delta = D, D \in O(3, R), \det(D) = -1$. Now the following is true

$$< \psi | \rho | \psi > = \text{Tr}(\rho \rho_\psi)$$
So finding $f(\rho)$ amounts to maximizing $\text{Tr} \ (\rho \rho_\psi)$ over all $\rho_\psi$ which, when represented via Equation (2.1), verify $\beta = \gamma = 0, \delta = D, D \in O(3, R), \det (D) = -1$.

Now by Equation (2.2), this is the same as maximizing the quantity $\frac{1}{4}(1 + \text{Tr} \ (\delta^T \rho D))$, over $D \in O(3, R), \det (D) = -1$. Equivalently it is the maximization of $\text{Tr} \ [(−\delta^T \rho) V], V \in SO(3, R)$. This is closely related to the key step in the solution of the Procustes problem, 2. Some of the steps require careful modification, since the solution in 2 uses optimization over the unitary group. In particular, the argument in 2 will not directly apply to the case $\det (\delta_\rho) \geq 0$. Therefore, only this situation is addressed here. If $\det (\delta_\rho) \geq 0$, then $\det (−\delta^T_\rho) \leq 0$. Therefore, there exist $S, T \in SO(3, R)$ such that

$$S(−\delta^T_\rho)T = −\text{diag} (\sigma_1, \sigma_2, \sigma_3)$$

Hence we get,

$$\text{Tr} \ [(−\delta^T_\rho) V] = \text{Tr} \ [−S^T \text{diag} (\sigma_1, \sigma_2, \sigma_3)T^T V]$$

which equals

$$\text{Tr} \ [−\text{diag} (\sigma_1, \sigma_2, \sigma_3)T^T VS^T]$$

So this last quantity has to be maximized over $V \in SO(3, R)$. Quite clearly the maximum occurs when $T^T V S^T = \text{diag} (−1, −1, 1)$. Now $T, S, \text{diag} (−1, −1, 1)$ are all in $SO(3, R)$, so such a $V$ in $SO(3, R)$ always exists and is unique. This then gives the stated expression for $f(\rho)$. Note $−I_3$ is not in $SO(3, R)$. So $f(\rho)$ cannot be increased further.

Next we look at the distance of the joint purifications of two mixed states given by Bloch vectors $\beta, \gamma$ to a given impure density matrix, $\rho_{\beta, \gamma}$ in $C^2 \otimes C^2$ whose partial trace is also precisely the states represented by $\beta, \sigma$. The choice of distance is the Hilbert-Schmidt distance $d(\rho, \rho_{\beta, \gamma})^2 = \text{Tr} \ (\rho − \rho_{\beta, \gamma})^2$. Suppose the $\delta$ matrix of of $\rho_{\beta, \gamma}$ is denoted $E$. Then from Equation (2.2) it follows

$$d(\rho, \rho_{\beta, \gamma})^2 = \frac{1}{4}(1 + \text{Tr} \ (\delta − E)(\delta − E)^T)$$

Fixing one choice, $D$ for $\delta$ it follows from Th 2, that the most general such $\delta$ is given by $DC$, with $C$ in $SO(3, R)$ satisfying $C\gamma = \gamma$. So the above quantity becomes $\text{Tr}(DD^T + EE^T − DCE^T − ECTD^T)$. Since $D, E$ are fixed minimizing this quantity is the same as maximizing $\text{Tr}(DCE^T + ECTD^T)$. But, $ECTD^T = (DCE^T)^T$. Hence, using the cyclic invariance of
trace, the problem reduces to maximizing, over all $C \in SO(3,R)$ satisfying $C\gamma = \gamma$, the function

$$F_{D,E}(C) = \text{Tr} \ (E^TDC)$$  \hfill (3.6)

We begin with a simple observation

**Lemma 3.1** Suppose $\rho_{\beta,\gamma}$ is the tensor product of the mixed states corresponding to $\beta$ and $\gamma$, then the function $F_{D,E}(C)$ is constant and equals $|| \beta ||^2$, i.e., every joint purification is equidistant from $\rho_{\beta,\gamma}$.

Proof: Since $E = \beta\gamma^T$, in this case, it follows $F_{D,E}(C) = \text{Tr} \ (E^TDC) = \text{Tr} \ (D\gamma\beta^T)$, since $C\gamma = \gamma$. Further, $D\gamma = \beta$ for pure states. So this reduces to $\text{Tr} \ (\beta\beta^T) = || \beta ||^2$.

We now address the general situation. From this analysis a geometric interpretation for the previous lemma will emerge. Now maximizing $F_{D,E}(C)$ would reduce to the key step in the usual PROCUSTES problem, but for the restriction that $C\gamma = \gamma$. For $\gamma = 0$ this is no restriction, though as in the calculation of the maximal singlet fraction care has to be taken since the optimization is over $SO(3,R)$. Therefore, we will study only the $\gamma \neq 0$ situation.

**Proposition 3.2** The maximum of $F_{D,E}(C)$ is given by the maximum of a differentiable function $f(\theta)$ (defined in Equation (3.7) below) over the interval $[0, 2\pi]$. Thus, this maximum exists and can be found by comparing the values of $f$ at $\theta = 0$ and at the critical points of $f$ in $(0, 2\pi)$.

Proof: By the singular value decomposition

$$E^TD = V\Sigma W^T$$

where $V$ is a real matrix with columns $v_i$ eigenvectors of $E^TD(E^TD)^T$, $W$ is a real matrix whose columns, $w_i$ are the eigenvectors of $(E^TD)^TE^TD$ and $\Sigma$ is a diagonal matrix $\text{diag}(\sigma_1, \sigma_2, \sigma_3)$ where the $\sigma_i$ are the singular values of $E^TD$.

Once again by the cyclic invariance of $\text{Tr}$ it follows

$$F_{D,E}(C) = \text{Tr} \ (\Sigma W^TCV)$$

To find the diagonal entries of $W^TCV$, we expand $v_i, w_i$ in some orthogonal basis, whose first member is member is $\gamma$. Denoting the components of $v_i, w_i$ in the first direction by $p_i, s_i$, etc...
respectively, we find
\[ Cv_i = p_i\gamma + R_\theta x_i, i = 1, \ldots, 3 \]

Here \( p_i = \langle v_i, \gamma \rangle \), while the \( x_i \) are precisely the orthogonal projections of the \( v_i \) onto the plane perpendicular to \( \gamma \) (and thus, \( x_i \) is uniquely determined by the \( v_i \)). In fact, since \( \gamma \) is orthogonal to this plane, \( x_i = v_i - p_i\gamma \). \( R_\theta \) is the rotation through \( \theta \) that the matrix \( C \) performs.

Denoting by \( y_i, i = 1, \ldots, 3 \) the orthogonal projections of the \( w_i \) onto the plane perpendicular to \( \gamma \) and \( s_i = \langle w_i, \gamma \rangle \), we find
\[
F_{D,E}(C) = f(\theta) = \sum_{i=1}^{3} \sigma_i p_i s_i + \langle y_i, \sigma_i R_\theta x_i \rangle, \theta \in [0, 2\pi]
\] (3.7)

So maximizing this function will yield the distance of \( \rho_{\beta,\sigma} \) from the set of joint purifications of the mixed states represented by the Bloch vectors \( \beta, \gamma \).

**Remark 3.2** The situation covered by Lemma can now be explained as follows. \( E = \beta \gamma^T \).

So the singular values of \( E^T D \) are the eigenvalues of \( E^T D D^T E \). This is the rank one matrix \( \| \gamma \|^2 \gamma \gamma^T \). Hence the singular values are \( (\| \gamma \|^2, 0, 0) \). Further, \( v_1 = w_1 = \gamma \). Hence, \( x_1 = 0 \). So \( F_{D,E}(C) \) is independent of \( \theta \), i.e., of \( C \). Finally, since \( \| \gamma \| = \| \beta \| \), the stated value for \( F_{D,E}(C) \) is indeed obtained.

**Remark 3.3** In Proposition 3.1, the optimization over \( SO(3,R) \) did not require more than elementary aspects of the group structure of \( SO(3,R) \). For related optimization problems we found the following parametrization of \( SO(3,R) \) useful. Let the normalized eigenvector of the generic \( D \in SO(3,R) \), belonging to the eigenvalue 1, be written in spherical coordinates in the form \( e_D = (\cos \theta_D \sin \phi_D, \sin \theta_D \sin \phi_D, \cos \phi_D) \). Denote the angle of rotation \( D \) performs (counterclockwise) in the plane orthogonal to this eigenvector be \( \psi_D \). Then the effect of \( D \) on any vector in \( v \in \mathbb{R}^3 \) is \( < v, e_D > e_D + R_{\psi_D}(v - < v, e_D > e_D) \). Since the typical optimization problem arising in contexts similar to the ones in this work involve inner products and norms, this representation of \( SO(3,R) \) seems superior to others (over Euler angles or Givens rotations, for instance). In this representation the optimization reduces to optimizing a function \( F(\phi, \theta, \psi) \) over \([0, \pi] \times [0, 2\pi] \times [0, 2\pi]\).
4 Conclusions

This note yielded a complete parametrization of purifications and joint purifications of $2 \times 2$ density matrices. This enabled a reformulation of the calculation of quantum information measures as optimization problems over the real orthogonal groups. In particular, a solution to one variation of the classical Procustes problem was provided. It would be interesting to extend this to density matrices in higher dimensions. The first ingredient in this a clear description of density matrices and pure states, going beyond the fact that they are expressible as real linear combination of certain matrices and necessarily have trace 1. In other words, a full characterization of this real vector of coefficients in this expression is desirable. This is partially addressed by the appendix.

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6 Appendix

How may one generalize this explicit parametrization of purifications? The first ingredient is a Bloch sphere like picture of density matrices in the appropriate $C^n$. For this there are two standard points of departure beyond the setting here. One is to consider higher tensor products of two dimensional spaces or to consider twofold tensor products of spaces of dimension higher than two. In an attempt to achieve this for the second route, we consider the question of describing, in a Bloch sphere fashion, density matrices of a single system first. This already is quite an arduous job as may be seen below.

First we represent a typical $n \times n$ density matrix in the following form:

$$\rho = \frac{1}{n} (I_n + \sum_{i=1}^{n^2-1} \beta_i \lambda_i)$$  \hspace{1cm} (6.8)

where the matrices $\lambda_i$ satisfy i) $\{i\lambda_k, k = 1, \ldots, n^2 - 1\}$ is an orthogonal basis for $su(n)$; ii) their “Jordan” commutator satisfies, $(\lambda_k \lambda_l + \lambda_l \lambda_k) = \frac{4}{n} I_n + \sum_{i=1}^{n^2-1} d_{kli} \lambda_i$, with the $d_{kli}$ a symmetric tensor. Such bases always exist. In principle, the $d_{kli}$ can be found, though we are aware of their enumeration only for $n = 3, 4$ for one particular choice of such a basis, [5].
$n = 3$ this basis is precisely the set of the Gell-Mann matrices. The reasons for choosing this representation is twofold i) eventually we wish to take partial traces of density matrices in $C^n \otimes C^n$. Therefore, having a basis for density matrices in $C^n$ which is maximally traceless will facilitate this computation. ii) The $\lambda_i$’s properties are well known.

For any $n$, using the symmetric tensor, $d_{ijk}$, define a new vector $x \cup y \in R^{n^2-1}$ starting with two vectors $x, y \in R^{n^2-1}$ via

$$x \cup y = \left( \sum_{j,k=1}^{n^2-1} d_{j,k} x_j y_k, \ldots, \sum_{j,k=1}^{n^2-1} d_{j,k} x_j y_k, \ldots \right)$$

The goal now is to characterize the form of the vector $\beta \in R^{n^2-1}$ which ensures $\rho$ is a density matrix. Since $\rho$ is the square of a Hermitian matrix, $M$, we take a generic such $M$, square it and insist its trace be 1. This leads to the following characterization of mixed states and in particular, pure states.

**Proposition 6.1** Every density matrix can be represented in the form in Equation (6.8) with

$$\beta = \frac{2\kappa}{n} \beta_0 + \frac{\beta_0 \cup \beta_0}{n},$$

where $\beta_0$ is any vector in $R^{n^2-1}$ with $|| \beta_0 ||^2 \leq \frac{n^2}{2}$ and $\kappa = \sqrt{\frac{n^2-2||\beta_0||^2}{n}}$.

Conversely any Hermitian matrix admitting such a representation is necessarily a density matrix. $\rho$ is pure precisely if it can be represented in the form in Equation (6.8) with $\langle \beta, \beta \rangle = \frac{n^2-2}{2}$ and $(n-2) \beta = \beta \cup \beta$.

Note that when $n = 2$, this is precisely the usual Bloch sphere, since the Pauli matrices anti-commute, i.e. $\beta \cup \beta = 0$ if $n$ is 2. For $n = 3$, states are pure if the vector $\beta \in R^8$ is of Euclidean length $\sqrt{3}$ and $\beta = \beta \cup \beta$. One can now use this to write down a Bloch sphere like picture for density matrices in $C^n \otimes C^n$. This characterization involves both the Lie product and the Jordan product. However, since even for single systems, the picture provided above requires further analysis the details will be considered in a future study. Indeed even analyzing the implications of an equation of the type $\beta = \beta \cup \beta$ for density matrices in $C^3$ requires further work. However, given specific Hermitian operators (for one or two particles) one can use this characterization to check if they are indeed density matrices and even if they are pure.

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