Optimal purification of a generic \( n \)-qudit state

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We propose a quantum algorithm for the purification of a generic mixed state \( \rho \) of a \( n \)-qudit system by using an ancillary \( n \)-qudit system. The algorithm is optimal in that (i) the number of ancillary qudits cannot be reduced, (ii) the number of parameters which determine the purification state \( |\Psi\rangle \) exactly equals the number of degrees of freedom of \( \rho \), and (iii) \( |\Psi\rangle \) is easily determined from the density matrix \( \rho \). Moreover, we introduce a quantum circuit in which the quantum gates are unitary transformations acting on a \( 2^n \)-qudit system. These transformations are determined by parameters that can be tuned to generate, once the ancillary qudits are disregarded, any given mixed \( n \)-qudit state.

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I. INTRODUCTION

Purification is one of the basic tools in quantum information science [1, 2]: Given a mixed quantum system \( S \) described by a density matrix \( \rho \) it is possible to introduce another ancillary system \( A \), such that the state \( |\Psi\rangle \) of the composite system \( S + A \) is a pure state and \( \rho \) is recovered after partial tracing over \( A \): \( \rho = \text{Tr}_A(|\Psi\rangle\langle\Psi|) \). The ancillary system may be a physical environment that must be taken into account when doing experiments on the system \( S \), but not necessarily so. It may be a fictitious environment that allows us to prove interesting results about the system under investigation.

Purification is a tool of great value in quantum information science, with countless applications, for instance in the study of the distance between quantum states [2], of the geometry of quantum states [3] and of the quantum capacity of noisy quantum channels [4]. Besides its theoretical relevance, purification is interesting for experimental implementations of quantum information protocols requiring mixed state. While the direct generation of a mixture \( \rho \) of quantum states necessarily involves statistical errors, this problem can be avoided if the purification state \( |\Psi\rangle \) is generated. Of course, the price to pay is that one has to work with the enlarged system \( S + A \), including the ancillary system \( A \).

Due to the partial trace structure the purification state \( |\Psi\rangle \) of a density matrix \( \rho \) cannot be uniquely defined, as any unitary transformation \( U_A \otimes 1_S \) acting non-trivially on the ancillary system only maps the state \( |\Psi\rangle \) into a new state \( |\Psi'\rangle = (U_A \otimes 1_S)|\Psi\rangle \) which is again a purification of \( \rho \). In this paper, we propose a quantum protocol that selects a specific purification \( |\Psi\rangle \). Such purification turns out to be very convenient since the state \( |\Psi\rangle \) depends on a number of parameters exactly equal to the number of degrees of freedom of a generic mixed state \( \rho \) and is easily determined as a function of \( \rho \). Furthermore, we design a quantum circuit given by a sequence of quantum gates acting on both the system and the ancillary qudits. The parameters which determine such quantum gates can be tuned to generate, once the ancillary qudits are disregarded, any mixed state \( \rho \) of system \( S \). Finally, our protocol works for any system of \( n \) qudits and requires \( n \) ancillary qudits. We show that the number of ancillary qudits is optimal, that is, it cannot be reduced if we wish to design a quantum circuit capable of generating any \( n \)-qudit mixed state.

Our paper is organized as follows. To set the notations, we first briefly review the concept of purification (Sec. II). Then we propose our purification scheme, moving from simple to more and more complex cases. We start with the purification of a single qubit mixed state (Sec. III), then we proceed with the qutrit (Sec. IV) and the two-qubit (Sec. V) cases and finally we illustrate the generic \( n \)-qudit case (Sec. VI). Appendix A provides a short account of the diagrams of states, namely of a tool very useful for the purposes of the present paper.

II. PURIFICATION

Given a quantum system \( S \) described by the density matrix \( \rho \), it is possible to introduce another ancillary system \( A \), such that the state \( |\Psi\rangle \) of the composite system is pure and

\[
\rho = \text{Tr}_A(|\Psi\rangle\langle\Psi|). \tag{1}
\]

This procedure, known as purification, allows us to associate a pure state \( |\Psi\rangle \) with a density matrix \( \rho \). A generic pure state of the global system \( S + A \) is given by

\[
|\Psi\rangle = \sum_{\alpha=0}^{M-1} \sum_{i=0}^{N-1} C_{\alpha i} |\alpha\rangle |i\rangle, \tag{2}
\]

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with \( \{|\alpha\rangle\} \) and \( \{|\tilde{i}\rangle\} \) basis sets for the Hilbert spaces \( \mathcal{H}_A \) and \( \mathcal{H}_S \), of dimensions \( M \) and \( N \), associated with the subsystems \( A \) and \( S \). Given a generic density matrix for system \( S \),

\[
\rho = \sum_{i,j=0}^{N-1} \rho_{ij} |i\rangle \langle j|,
\]

(3)

we say that the state \( |\Psi\rangle \) defined by Eq. (2) is a purification of \( \rho \) if

\[
\rho = \text{Tr}_A(|\Psi\rangle \langle \Psi|) = \sum_{\alpha=0}^{M-1} \sum_{i,j=0}^{N-1} C_{\alpha i} C_{\alpha j}^* |i\rangle \langle j|.
\]

(4)

The equality between (3) and (4) implies

\[
\rho_{ij} = \sum_{\alpha=0}^{M-1} C_{\alpha i} C_{\alpha j}^*.
\]

(5)

It is clear that (5) always admits a solution, provided the Hilbert space of system \( A \) is large enough. More precisely, it is sufficient to consider a system \( A \) whose Hilbert space dimension is the same as that of system \( S \). Indeed, if we express the reduced density matrix using its diagonal representation,

\[
\rho = \sum_i p_i |i\rangle \langle i|,
\]

(6)

a purification for the density matrix (6) is given by

\[
|\Psi\rangle = \sum_i \sqrt{p_i} |i'\rangle \langle i|,
\]

(7)

with \( \{|i'\rangle\} \) orthonormal basis for \( \mathcal{H}_A \). This purification procedure requires the diagonalization of the density matrix \( \rho \) and therefore is in general only numerically feasible.

In what follows, we propose a different purification scheme, which is optimal in that, for the purification of a generic \( n \)-qudit state, the number \( m = n \) of qudits of the ancillary system \( A \) cannot be reduced. While this is the case also for the well-known purification (7) based on the spectral decomposition (6), we anticipate that our method readily provides a purification state \( |\Psi\rangle \) that depends on a number of parameters exactly equal to the number of degrees of freedom of a generic \( \rho \). Note that, even when the number of ancillary qudits is optimal \((m = n \text{ so that } M = N)\), the number \( 2N^2 - 2 \) of real coefficients \( C_{\alpha i} \) determining the purification state (2) is in general much larger than the number \( N^2 - 1 \) of real free parameters that must be set to determine a generic density matrix of size \( N \). Different choices of the coefficients \( C_{\alpha i} \) are therefore possible. Our choice provides a purification state \( |\Psi\rangle \) depending on a number \( N^2 - 1 \) of real parameters exactly equal to the number of real freedoms of a generic mixed states \( \rho \). Furthermore, the coefficient \( C_{\alpha i} \) in (2) can be easily determined from conditions (5), in spite of the fact that these equations are nonlinear. Finally, we will see in the next sections that our scheme suggest a very convenient quantum circuit for the preparation of a generic density matrix \( \rho \). To illustrate the working of our purification method, we discuss cases of increasing complexity, from a single qubit state to a generic \( n \)-qudit state.

### III. QUBIT

#### A. Mixed-state purification

We consider \( M = N = 2 \) and set

\[
\begin{cases}
C_{00} \in \mathbb{R}_+, \\
C_{10} \in \mathbb{R}_+, C_{11} = 0.
\end{cases}
\]

(8)

We first determine \( C_{01} \) from (5):

\[
|C_{11}| = |C_{01}|^2 + |C_{11}|^2 = |C_{01}|^2,
\]

(9)

where the last equality follows from the second line of (8). Since we have also chosen \( C_{01} \) to be real and nonnegative, we simply obtain

\[
C_{01} = \sqrt{|C_{01}|}.
\]

(10)

Then we can determine \( C_{00} \) from the condition

\[
\rho_{01} = C_{00}C_{01}^* + C_{10}C_{11}^* = C_{00}C_{01},
\]

(11)

since \( C_{01} \) is already known from (9). Finally, knowing \( C_{00} \), we can derive \( C_{10} \) from the condition

\[
\rho_{00} = |C_{00}|^2 + |C_{10}|^2.
\]

(12)

Taking into account that \( C_{10} \in \mathbb{R}_+ \), we have

\[
C_{10} = \sqrt{|\rho_{00}| - |C_{00}|^2}.
\]

(13)

Note that, in the special case in which \( \rho_{11} = 0 \) we can remove any ambiguity in the definition of the purification state \( |\Psi\rangle \) by setting \( C_{00} = 0 \). In this case, \( \rho = |0\rangle \langle 0| \) is already a pure state and its “purification” is \( |\Psi\rangle = |10\rangle \). Alternatively, one can reshuffle the basis state according to \( |0\rangle \leftrightarrow |1\rangle \). For a generic state \( \rho_{11} \neq 0 \) and the state \( |\Psi\rangle \) reads, in the \( \{|\alpha\rangle = |00\rangle, |01\rangle, |10\rangle, |11\rangle\} \) basis, as follows:

\[
|\Psi\rangle = \begin{bmatrix}
C_{00} \\
C_{01} \\
C_{10} \\
C_{11}
\end{bmatrix}
= \begin{bmatrix}
\frac{\rho_{01}}{\sqrt{|C_{01}|}} \\
\frac{\sqrt{|C_{01}|}}{\rho_{11}} \\
\sqrt{\rho_{00} - |C_{00}|^2} \\
0
\end{bmatrix}.
\]

(14)
The qubits run from top to bottom from the least significant (LSB) to the most significant (MSB).

**B. Mixed-state generation**

In this subsection, we provide a quantum circuit generating the state $|\Psi\rangle$ of (14), namely the purification of a generic single-qubit density matrix $\rho$. After disregarding the ancillary qubit (this corresponds to performing the partial trace of the density matrix $|\Psi\rangle\langle\Psi|$ over the ancillary qubit), we obtain the mixed state $\rho$. Therefore, we end up with an experimentally viable procedure for the generation of a generic mixed single-qubit state by means of a two-qubit state subjected to controlled unitary transformations.

The quantum circuit generating the state $|\Psi\rangle$ is shown in Fig. 1. A square box with a greek letter inside (here, $\alpha$ or $\theta$) stands for a rotation operator. Its matrix representation in the $\{|0\rangle, |1\rangle\}$ reads as follows:

$$R(\alpha) = \begin{bmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{bmatrix}. \quad (15)$$

The full circle with $-\phi$ above is the phase-shift gate, defined by the diagonal matrix

$$\text{PHASE}(-\phi) = \text{diag}(1, e^{-i\phi}). \quad (16)$$

As an overall phase factor is arbitrary, the action of this gate is equivalently represented by the matrix $\text{diag}(e^{i\phi}, 1)$. In the controlled-gates, the empty circle on the control qubit means that the gate acts non trivially (differently from identity) on the target qubit if and only if the state of the control qubit is $|0\rangle$.

On the other hand, any single-qubit density matrix can be generated by means of the quantum circuit in Fig. 1. Given the input state $|\Psi_i\rangle = |00\rangle$, the output state is

$$|\Psi_f\rangle = \begin{bmatrix} \cos \alpha \cos \theta e^{i\phi} \\ \cos \alpha \sin \theta \\ \sin \alpha \\ 0 \end{bmatrix}. \quad (17)$$

This state is equal to the purification state (14), provided we set

$$\begin{cases} \sin \alpha = C_{10}, \\ \cos \alpha \sin \theta = C_{01}, \\ \cos \alpha \cos \theta e^{i\phi} = C_{00}. \end{cases} \quad (18)$$

From the first equation we determine $\alpha$, then from the second $\theta$ and finally from the third $\phi$, as a function of the coefficients $C_{ij}$, which in turn are determined by our purification protocol from the density matrix elements $\rho_{ij}$. Note that, since by construction $C_{01}, C_{10} \geq 0$, we can take $\alpha, \theta \in [0, \pi]$, finally, the phase $\phi \in [0, 2\pi]$.

For a straightforward extension of the results presented in this section from the purification of a single qubit to more complex systems it is convenient to express the quantum circuit in Fig. 1 in terms of diagrams of states [5], of which a very brief account is given in Appendix A. The diagram of states corresponding to the purification circuit of Fig. 1 is shown in Fig. 2. Note that, given the input state $|00\rangle$, the output state (17) is immediately written following the information flow along the thick lines of the diagram of states. We stress that other optimal purifications, where the purification state is determined by $N^2 - 1 = 3$ real parameters, are possible. Our choice corresponds to setting $C_{11} = 0$ and $C_{01}, C_{10}$ real. We will see that the diagrams of states immediately lead to optimal purifications also for arbitrarily complex systems.

**C. “Invasion” of the Bloch ball**

Using the quantum circuit in Fig. 1 we can write a generic single-qubit state as

$$\rho = \sum_{k=1}^{2} p_k |\psi_k\rangle \langle \psi_k|, \quad (19)$$

with $p_1 = \cos^2 \alpha$, $p_2 = \sin^2 \alpha$, $|\psi_1\rangle$ generic single-qubit pure state and $|\psi_2\rangle = |0\rangle$. The matrix representation of $\rho$ in the $\{|0\rangle, |1\rangle\}$ basis is given by

$$\rho = \cos^2 \alpha \begin{bmatrix} \cos^2 \theta & \cos \theta \sin \theta e^{-i\phi} \\ \cos \theta \sin \theta e^{i\phi} & \sin^2 \theta \end{bmatrix} + \sin^2 \alpha \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 + Z & X - iY \\ X + iY & 1 - Z \end{bmatrix}. \quad (20)$$

FIG. 1: Quantum circuit for the purification of a single qubit. The qubits run from top to bottom from the least significant (LSB) to the most significant (MSB).

FIG. 2: Diagram of states for the purification of a single qubit. Starting from the input state $|00\rangle$, information flows on the thick lines. We explicitly indicate at the right hand side that the coefficients $C_{01}$ and $C_{10}$ are real, while $C_{11} = 0$. 

- **LSB**: Least Significant Bit
- **MSB**: Most Significant Bit
IV. QUTRIT

We consider \( M = N = 3 \) and set
\[
\begin{aligned}
C_{02} \in \mathbb{R}_+, \\
C_{11} \in \mathbb{R}_+, \ C_{12} = 0, \\
C_{20} \in \mathbb{R}_+, \ C_{21} = C_{22} = 0.
\end{aligned}
\] (21)

We first obtain \( C_{02} \) from
\[
\rho_{22} = |C_{02}|^2 + |C_{12}|^2 + |C_{22}|^2 = |C_{02}|^2.
\] (22)

Once \( C_{02} \geq 0 \) is determined as \( C_{02} = \sqrt{\rho_{22}} \), we obtain \( C_{01} \) and \( C_{00} \) from
\[
\rho_{12} = C_{01} C_{02}^* + C_{11} C_{12}^* + C_{21} C_{22}^* = C_{01} C_{02},
\] (23)
\[
\rho_{02} = C_{00} C_{02}^* + C_{01} C_{12}^* + C_{20} C_{22}^* = C_{00} C_{02}.
\] (24)

Then we obtain \( C_{11} \) from
\[
\rho_{11} = |C_{01}|^2 + |C_{11}|^2 + |C_{21}|^2 = |C_{01}|^2 + C_{11}^2,
\] (25)

and, finally, \( C_{10} \) and \( C_{20} \) from
\[
\rho_{01} = C_{00} C_{01}^* + C_{10} C_{11}^* + C_{20} C_{21}^* = C_{00} C_{01} + C_{10} C_{11},
\] (26)
\[
\rho_{00} = |C_{00}|^2 + |C_{10}|^2 + C_{20}^2.
\] (27)

We stress that conditions (21) lead to a purification state determined by \( N^2 - 1 = 8 \) free real parameters, exactly corresponding to the number of real freedoms needed to set a generic density matrix for a qutrit. Conditions (21) are readily derived if the purification of a generic qutrit state is implemented by means of the diagram of states shown in Fig. 4. In this figure, a box with two geek letters written on top of it (for instance, \( \alpha_1 \) and \( \alpha_2 \)) represents a unitary transformation whose matrix representation has, in the \( \{|0\rangle, |1\rangle, |2\rangle\} \) basis, the first column given by
\[
\begin{bmatrix}
\cos \alpha_1 \
\cos \alpha_2 \\
\cos \alpha_1 \sin \alpha_2 \\
\sin \alpha_1
\end{bmatrix}
\] (28)

Such transformation maps the input state \( |0\rangle \) into
\[
\cos \alpha_1 \cos \alpha_2 |0\rangle + \cos \alpha_1 \sin \alpha_2 |1\rangle + \sin \alpha_1 |2\rangle.
\] (29)

Finally, the box with the letter \( \theta_3 \) on top of it represents the rotation \( R(\theta_3) \) acting on the two-dimensional subspace spanned by the state \(|0\rangle \) and \(|1\rangle \), with \( R \) defined by (15).

Given the input state \(|0\rangle\), the output purification state \(|\Psi\rangle = \sum_{\alpha,i} C_{\alpha i} |\alpha i\rangle \) can be immediately written by following the thick lines of the diagram of states in Fig. 4.
qutrit. To simplify the plot, only the thick lines corresponding to the information flow are shown inside the boxes. The angles $\alpha_i, \theta_j \in [0, \frac{\pi}{2}]$, while the phases $\phi_k \in [0, 2\pi)$.

We obtain

$$
\begin{align*}
C_{00} &= \cos \alpha_1 \cos \alpha_2 \cos \theta_1 \cos \theta_2 e^{i\phi_1}, \\
C_{01} &= \cos \alpha_1 \cos \alpha_2 \cos \theta_1 \sin \theta_2 e^{i\phi_2}, \\
C_{02} &= \cos \alpha_1 \cos \alpha_2 \sin \theta_1, \\
C_{10} &= \cos \alpha_1 \sin \alpha_2 \cos \theta_3 e^{i\phi_3}, \\
C_{11} &= \cos \alpha_1 \sin \alpha_2 \sin \theta_3, \\
C_{12} &= 0, \\
C_{20} &= \sin \alpha_1, \\
C_{21} &= 0, \\
C_{22} &= 0.
\end{align*}
$$

These relations can be easily inverted to obtain the parameters $\{\alpha_j, \theta_j, \phi_j\}$ as a function of the coefficients $C_{ij}$ and, therefore, of the elements of the density matrix $\rho$. Therefore, the quantum circuit represented by the diagram of states of Fig. 4 can be used to generate any given qutrit state $\rho$, once the ancillary qutrit is disregarded. Finally, we point out that the number of real parameters $\{\alpha_j, \theta_j, \phi_j\}$ that determine the state $|\Psi\rangle$ is equal to 8, that is, exactly to the number of parameters needed to determine a (generally mixed) single-qutrit state $\rho$.

It is clear from the purification drawn in Fig. 4 that we can write a generic single-qutrit state as

$$
\rho = \sum_{k=1}^{3} p_k |\psi_k\rangle \langle \psi_k|,
$$

with $p_1 = \cos^2 \alpha_1 \cos^2 \alpha_2$, $p_2 = \cos^2 \alpha_1 \sin^2 \alpha_2$, $p_3 = \sin^2 \alpha_1$, $|\psi_1\rangle$ generic single-qutrit pure state, $|\psi_2\rangle$ pure state residing in the two-dimensional subspace spanned by $|0\rangle$ and $|1\rangle$, and $|\psi_3\rangle = |0\rangle$. The picture developed in Sec. III C about the “invasion” of the single-qubit Bloch ball by means of suitably scaled and translated pure-qubit Bloch spheres may be generalized to the single-qutrit case. The role of the Bloch sphere is here played by the surface of single-qutrit pure states and the volume of all single-qutrit states is “invaded” when the parameters $p_k$ are varied, with the constraint $\sum_k p_k = 1$.

**V. TWO QUBITS**

We consider $M = N = 4$ and set

$$
\begin{align*}
C_{03} &\in \mathbb{R}_+, \\
C_{12} &\in \mathbb{R}_+, \\
C_{13} &= 0, \\
C_{21} &= C_{22} = C_{23} = 0, \\
C_{30} &\in \mathbb{R}_+, \\
C_{31} &= C_{32} = C_{33} = 0.
\end{align*}
$$

We first obtain $C_{03}$ from

$$
|\rho_{03}|^2 = |C_{00}|^2 + |C_{10}|^2 + |C_{11}|^2 + |C_{12}|^2 = |C_{03}|^2,
$$

then $C_{02}, C_{01},$ and $C_{00}$ from

$$
\begin{align*}
\rho_{23} &= C_{02}^* C_{03} + C_{12}^* C_{13} + C_{22}^* C_{23} + C_{32}^* C_{33} = C_{02} C_{03}, \\
\rho_{13} &= C_{01}^* C_{03}^* + C_{11}^* C_{13} + C_{21}^* C_{23} + C_{31}^* C_{33} = C_{01} C_{03}, \\
\rho_{03} &= C_{00}^* C_{03} + C_{10}^* C_{13} + C_{20}^* C_{23} + C_{30}^* C_{33} = C_{00} C_{03},
\end{align*}
$$

then $C_{12}$ from

$$
\rho_{22} = |C_{02}|^2 + |C_{12}|^2 + |C_{22}|^2 + |C_{32}|^2 = |C_{02}|^2 + |C_{12}|^2,
$$

then $C_{11}$ and $C_{10}$ from

$$
\begin{align*}
\rho_{12} &= C_{01}^* C_{02} + C_{11}^* C_{12} + C_{21}^* C_{22} + C_{31}^* C_{32} \\
&= C_{01} C_{02} + C_{11} C_{12},
\end{align*}
$$

then $C_{21}$ from

$$
\begin{align*}
\rho_{11} &= |C_{01}|^2 + |C_{11}|^2 + |C_{21}|^2 + |C_{31}|^2 \\
&= |C_{01}|^2 + |C_{11}|^2 + |C_{21}|^2,
\end{align*}
$$

then $C_{20}$ from

$$
\begin{align*}
\rho_{01} &= C_{00}^* C_{01} + C_{10}^* C_{11} + C_{20}^* C_{21} + C_{30}^* C_{31} \\
&= C_{00} C_{01} + C_{10} C_{11} + C_{20} C_{21},
\end{align*}
$$

and, finally, $C_{30}$ from

$$
\rho_{00} = |C_{00}|^2 + |C_{10}|^2 + |C_{20}|^2 + |C_{30}|^2.
$$

As for the previous examples, we point out that the number $N^2 - 1 = 15$ of free parameters determining the purification state $|\Psi\rangle$ cannot be reduced given a generic
two-qubit mixed state $\rho$. Moreover, conditions (32) are determined from the diagram of states for the purification of a generic two-qubit state shown in Fig. 5. Following the information flow from the input states $|0000\rangle$ we can immediately write down the output purification state $|\Psi\rangle = \sum_{\alpha_i} C_{\alpha i} |\alpha_i\rangle$. We obtain

$$
\begin{align*}
C_{0000} &= \cos \alpha_1 \cos \alpha_2 \cos \theta_1 \cos \theta_2 e^{i\phi_1}, \\
C_{0001} &= \cos \alpha_1 \cos \alpha_2 \cos \theta_1 \sin \theta_2 e^{i\phi_2}, \\
C_{0010} &= \cos \alpha_1 \cos \alpha_2 \sin \theta_1 \cos \theta_2 e^{i\phi_3}, \\
C_{0011} &= \cos \alpha_1 \cos \alpha_2 \sin \theta_1 \sin \theta_2, \\
C_{0100} &= \cos \alpha_1 \sin \alpha_2 \cos \theta_2 \cos \theta_3 e^{i\phi_4}, \\
C_{0101} &= \cos \alpha_1 \sin \alpha_2 \cos \theta_2 \sin \theta_3 e^{i\phi_5}, \\
C_{0110} &= \cos \alpha_1 \sin \alpha_2 \sin \theta_2, \\
C_{0111} &= 0, \\
C_{1000} &= \sin \alpha_1 \cos \alpha_3 \cos \theta_6 e^{i\phi_6}, \\
C_{1001} &= \sin \alpha_1 \cos \alpha_3 \sin \theta_6, \\
C_{1010} &= 0, \\
C_{1011} &= 0, \\
C_{1100} &= \sin \alpha_1 \sin \alpha_3, \\
C_{1101} &= 0, \\
C_{1110} &= 0, \\
C_{1111} &= 0.
\end{align*}
$$

As in the previous cases, we can invert these equations and determine the parameters $\{\alpha_j, \theta_k, \phi_l\}$ in terms of the coefficients $C_{\alpha i}$ and, therefore, of the elements of the density matrix $\rho$.

We can see from Fig. 5 that a generic two-qubit state can be written as

$$
\rho = \sum_{k=1}^{4} p_k |\psi_k\rangle\langle\psi_k|,
$$

with $p_1 = \cos^2 \alpha_1 \cos^2 \alpha_2$, $p_2 = \cos^2 \alpha_1 \sin^2 \alpha_2$, $p_3 = \sin^2 \alpha_1 \cos^2 \alpha_3$, and $p_4 = \sin^2 \alpha_1 \sin^2 \alpha_3$. The “invasion” picture developed in Sec. III C can be extended also to the present case, with the volume of all two-qubit states “invaded” when the parameters $p_k$ are varied, under the constraint $\sum_k p_k = 1$. Note that the number of real parameters $\{\alpha_i, \theta_k, \phi_l\}$ used to determine the state $|\Psi\rangle$ is 15, that is, exactly the number of parameters required to determine a generic two-qubit state.

VI. $n$ QUDITS

We consider $M = N = d^n$ and set

$$
\begin{align*}
C_{0,0,-1} &\in \mathbb{R}^+, \\
C_{1,0,-2} &\in \mathbb{R}^+, C_{1,0,-1} = 0, \\
C_{2,0,-3} &\in \mathbb{R}^+, C_{2,0,-2} = C_{2,0,-1} = 0, \\
&\vdots \\
C_{N,0,-1} &\in \mathbb{R}^+, C_{N,0,-1} = C_{N,0,-2} = \ldots = C_{N,0,-N-1} = 0.
\end{align*}
$$

The general procedure for determining the coefficient $C_{\alpha i}$ is clear from the previous examples.

- We first determine $C_{0,0,-1}$ from $\rho_{-1,-1}$,
- then $C_{0j}$ from $\rho_{j,-1}$, with $j = N - 2, ..., 0$,
- then $C_{1j}$ from $\rho_{j,-2}$,
- then $C_{ij}$ from $\rho_{j,-2}$, with $j = N - 3, ..., 0, \ldots$,
- and, finally, $C_{N,-1,0}$ from $\rho_{00}$.

This purification is optimal as the number of qudits of the ancillary system cannot be reduced. The number of real free parameters that must be set to determine a density matrix of size $d^n$ is $d^{2n} - 1$ (the $-1$ term comes from the normalization condition $\text{Tr}(\rho) = 1$). Therefore, an ancillary system of $n - 1$ qudits is not sufficient to purify $\rho$, as a pure state $|\Psi\rangle$ in the Hilbert space of $n + (n - 1) = 2n - 1$ qudits has $2d^{2n-1} - 2$ freedoms (the $-2$ term is due to the normalization condition for $|\Psi\rangle$ and to the fact that a global phase factor in $|\Psi\rangle$ is arbitrary). This number is not sufficient as $2d^{2n-1} - 2 < d^{2n-1}$ for any $d \geq 2, n \geq 1$. On the other hand, as illustrated Fig. 6, the number of free real parameters in our purification method is exactly $d^{2n} - 1$. From the schematic drawing in Fig. 5 we can also see that the $n$-qudit state can be written as

$$
\rho = \sum_{k=1}^{d^n} p_k |\psi_k\rangle\langle\psi_k|,
$$
we obtain a total number of $d$ numbers plus the lines, one for each state of the computational basis. We can spaces of decreasing dimension, from $d$ of the density matrix protocol can be seen as the Cholesky decomposition [6] quantum hardware at disposal. The implementation of the protocol will depend on the specific system of size $N$ purification protocol. That is to say, the same purifica-

with the pure states from $|\psi_1\rangle$ to $|\psi_{dn}\rangle$ residing in sub-
spaces of decreasing dimension, from $d^n$ to 1.

We note that the tensor product structure of many-
qudit quantum systems does not play any role in our purification protocol. That is to say, the same purifica-
tion scheme applies to a system of $n$ qudits or to a single system of size $N = d^n$. Of course, the practical im-
plementation of the protocol will depend on the specific quantum hardware at disposal.

From the mathematical viewpoint, our purification protocol can be seen as the Cholesky decomposition [6] of the density matrix $\rho$. If we consider the coefficients $C_{\alpha i}$, as elements of a $d^n \times d^n$ matrix $C$, then its transpose $D \equiv C^T$ is a upper triangular matrix and Eq. (5) reads

$$\rho = C^T C^{*} = D D^{T^{*}} = D D^{\dagger},$$

namely it is the Cholesky decomposition of the density matrix $\rho$. Such decomposition is unique when $\rho$ is positive, while the ambiguities arising when $\rho$ is singular may be removed by suitable prescriptions or reshuffling as previously discussed for the single-qubit case.

It is interesting to remark that the Cholesky decomposition has already been used in the context of quantum information science in parametrizing the density operator in order to guarantee positivity [7]. The purpose of Ref. [7] was to present a universal technique for quantum-

state estimation.

### VII. FINAL REMARKS

In summary, we have proposed an algorithm for the purification of a generic $n$-qudit state. This algorithm

is optimal, in that the number $n$ of ancillary qudits used for the purification cannot be further reduced. Moreover, our algorithm can also be seen as a quantum protocol for the generation of a generic $n$-qudit state by means of suit-
able unitary operations applied both to the system and to the ancillary qudits, with the ancillary qudits eventually disregarded. While also the well-known purification (7) based on the spectral decomposition (6) uses $n$ ancillary qudits, our method is optimal in that it readily provides a purification state that depends on a number of param-
eters exactly equal to the number of degrees of freedom of the generic $n$-qudit state that we wish to purify.

It is well known that the purification $|\Psi\rangle$ of a generic mixed state $\rho$ cannot be uniquely determined, as the partial trace over the ancillary qudits is invariant under any unitary transformation $U_A \otimes I_S$ acting non trivially on the ancillary qudits only. Indeed, we have

$$\rho = Tr_A (|\Psi\rangle \langle \Psi|) = Tr_A (|\Psi'\rangle \langle \Psi'|),$$

with

$$|\Psi'\rangle = (U_A \otimes I_S)|\Psi\rangle.$$ It is sufficient to add the unitary transformation $U_A \otimes I_S$ at the end of our purification protocol to obtain any $2n$-
qudit purification $|\Psi'\rangle$ of a $n$-qudit state $\rho$. On the other hand, we can say that our protocol selects a very conven-
ient purification as the coefficients of the wave function $|\Psi\rangle$ in the computational basis are easily determined from the density matrix $\rho$ and the quantum circuit generating $\rho$ can be immediately drawn.

### APPENDIX A: DIAGRAMS OF STATES

Diagrams of states [5] graphically represent how quantum information is elaborated during the execution of a quantum circuit. In the usual way of drawing a quantum circuit [1, 2] each horizontal line represents a qubit. In contrast, in diagrams of states we draw a horizontal line for each state of the computational basis. Therefore, diagrams of states are less synthetick but may help us to clearly visualize quantum information flow in a quantum circuit.

For the purposes of the present paper, it will be suffi-
cient to show the diagrams of states for elementary single-
qubit quantum gates. The phase-shift gate PHASE($\phi$), defined by Eq. (16), and the rotation gate $R(\theta)$, defined by Eq. (15), are shown in Fig. 7 and Fig. 8, respec-
tively. Finally, the generation of a generic single-qubit state $\cos \theta |0\rangle + \sin \theta e^{i\phi} |1\rangle$ starting from the input state $|0\rangle$ is shown in Fig. 9. The information flows on the thick lines, from left to right, while thinner lines correspond to absence of information. Note that, following the thick lines, the final state can here be immediately written.
FIG. 7: Quantum circuit (left) and diagram of states (right) for the phase-shift gate.

FIG. 8: Quantum circuit (left) and diagram of states (right) for the $R(\theta)$ gate.

FIG. 9: Quantum circuit (left) and diagram of states (right) for the generation of a generic single-qubit state. To simplify the plot, only the thick lines corresponding to the information flow are shown inside the boxes.

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[8] Similar procedures can be applied to higher dimensional cases whenever diagonal elements of the density matrix $\rho$ are equal to zero. For the sake of simplicity, we will not discuss any longer in our paper such special cases.