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 ρ 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 ρ, and (iii) $|\Psi\rangle$ is easily determined from the density matrix ρ. Moreover, we introduce a quantum circuit in which the quantum gates are unitary transformations acting on a $2n$-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 ρ 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 ρ is recovered after partial tracing over $A: \rho = \mathrm{Tr}_A(|\Psi\rangle\langle\Psi|)$. 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 ρ 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 ρ cannot be uniquely defined, as any unitary transformation $U_A \otimes \mathbb{1}_S$ acting nontrivially on the ancillary system only maps the state $|\Psi\rangle$ into a new state $|\Psi'\rangle = (U_A \otimes \mathbb{1}_S)|\Psi\rangle$, which is again a purification of ρ. 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 ρ and is easily determined as a function of ρ. 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 qubits are disregarded, any mixed state ρ 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). The Appendix 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 ρ, it is possible to introduce another ancillary system A, such that the state $|\Psi\rangle$ of the composite system is pure and

$$\rho = \mathrm{Tr}_A(|\Psi\rangle\langle\Psi|). \tag{1}$$

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

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

with $\{|\alpha\rangle\}$ and $\{|i\rangle\}$ 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,

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$$\rho = \sum_{i,j=0}^{N-1} \rho_{ij} |i\rangle\langle j|, \tag{3}$$

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

$$\rho = \mathrm{Tr}_A(|\Psi\rangle\langle\Psi|) = \sum_{\alpha=0}^{M-1} \sum_{i,j=0}^{N-1} C_{\alpha i} C^\star_{\alpha j} |i\rangle\langle j|. \tag{4}$$

The equality between Eqs. (3) and (4) implies

$$\rho_{ij} = \sum_{\alpha=0}^{M-1} C_{\alpha i} C^\star_{\alpha j}. \tag{5}$$

It is clear that Eq. (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,

$$\rho = \sum_i p_i |i\rangle\langle i|, \tag{6}$$

a purification for density matrix (6) is given by

$$|\Psi\rangle = \sum_i \sqrt{p_i} |i'\rangle|i\rangle, \tag{7}$$

with $\{|i'\rangle\}$ orthonormal basis for $\mathcal{H}_A$. This purification procedure requires the diagonalization of the density matrix ρ 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 well-known purification (7) based on 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 ρ. Note that, even when the number of ancillary qudits is optimal ($m=n$ so that $M=N$), the number $2N^2-2$ of real coefficients $C_{\alpha i}$ determining 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 ρ. Furthermore, the coefficient $C_{\alpha i}$ in Eq. (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 ρ. 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

$$C_{01} \in \mathbb{R}_+,$$

$$C_{10} \in \mathbb{R}_+, \quad C_{11}=0. \tag{8}$$

We first determine C_{01} from Eq. (5)

$$\rho_{11} = |C_{01}|^2 + |C_{11}|^2 = |C_{01}|^2, \tag{9}$$

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

$$C_{01} = \sqrt{\rho_{11}}. \tag{10}$$

Then we can determine C_{00} from the condition

$$\rho_{01} = C_{00}C^\star_{01} + C_{10}C^\star_{11} = C_{00}C_{01}, \tag{11}$$

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

$$\rho_{00} = |C_{00}|^2 + |C_{10}|^2. \tag{12}$$

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

$$C_{10} = \sqrt{\rho_{00} - |C_{00}|^2}. \tag{13}$$

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 $|0\rangle \leftrightarrow |1\rangle$ [8]. For a generic state $\rho_{11}\neq 0$ and the state $|\Psi\rangle$ reads, in the $\{|\alpha i\rangle = |00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ basis, as follows:

$$|\Psi\rangle = \begin{bmatrix} C_{00} \\ C_{01} \\ C_{10} \\ C_{11} \end{bmatrix} = \begin{bmatrix} \dfrac{\rho_{01}}{\sqrt{\rho_{11}}} \\ \sqrt{\rho_{11}} \\ \sqrt{\dfrac{\rho_{00}\rho_{11} - \rho_{10}\rho_{01}}{\rho_{11}}} \\ 0 \end{bmatrix}. \tag{14}$$

B. Mixed-state generation

In this subsection, we provide a quantum circuit generating the state $|\Psi\rangle$ of Eq. (14), namely, the purification of a generic single-qubit density matrix ρ. 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 ρ. 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, α or θ) stands for a rotation operator. Its matrix representation in the $\{|0\rangle, |1\rangle\}$ basis reads as follows:

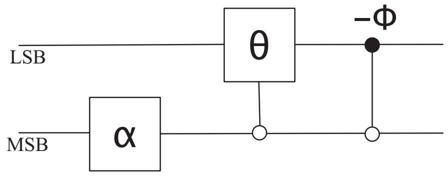

FIG. 1. Quantum circuit for the purification of a single qubit. The qubits run from top to bottom from the least significant (LSB) to the most significant (MSB).

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

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

$$\mathcal{P}(-\phi)=\text{diag}(1,e^{-i\phi}). \tag{16}$$

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 nontrivially (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

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

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

$$\sin\alpha=C_{10},$$

$$\cos\alpha\sin\theta=C_{01},$$

$$\cos\alpha\cos\theta e^{i\phi}=C_{00}. \tag{18}$$

From the first equation we determine α, then from the second θ, and finally from the third ϕ, as a function of the coefficients $C_{\alpha i}$, which in turn are determined by our purification protocol from the density-matrix elements ρ_{ij}. Note that, since by construction $C_{01},C_{10}\geq 0$, we can take $\alpha,\theta\in[0,\frac{\pi}{2}]$. 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 the Appendix. The diagram of states corresponding to the purification circuit of Fig. 1 is shown in Fig. 2. Note that, given the input state $|00\rangle$, 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} and C_{10} real. We will see that the diagrams of states immediately lead to optimal purifications also for arbitrarily complex systems.

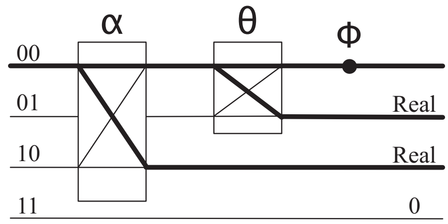

FIG. 2. Diagram of states for the purification of a single qubit. Starting from the input state $|00\rangle$, information flows on the thick lines. We explicitly indicate at the right-hand side that the coefficients C_{01} and C_{10} are real, while $C_{11}=0$.

C. "Invasion" of the Bloch ball

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

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

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

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

The last equality corresponds to the usual Bloch-ball representation of the (generally mixed) single-qubit states. It is clear that once α is fixed, Eq. (20) represents a surface in the (X,Y,Z) space, obtained after contracting the pure-state (unit radius) Bloch sphere of the factor $\cos^2\alpha$ and translating it in the positive Z direction by $\sin^2\alpha$. Plots of this surface for different values of α are shown in Fig. 3. It is clear that all the points of the Bloch ball are recovered when α goes from 0 to $\frac{\pi}{2}$. We can say that there is an "invasion" of the Bloch ball starting from the north pole.

IV. QUTRIT

We consider $M=N=3$ and set

$$C_{02}\in\mathbb{R}_+,$$

$$C_{11}\in\mathbb{R}_+,\quad C_{12}=0,$$

$$C_{20}\in\mathbb{R}_+,\quad C_{21}=C_{22}=0. \tag{21}$$

We first obtain C_{02} from

$$\rho_{22}=|C_{02}|^2+|C_{12}|^2+|C_{22}|^2=|C_{02}|^2. \tag{22}$$

Once $C_{02}\geq 0$ is determined as $C_{02}=\sqrt{\rho_{22}}$, we obtain C_{01} and C_{00} from

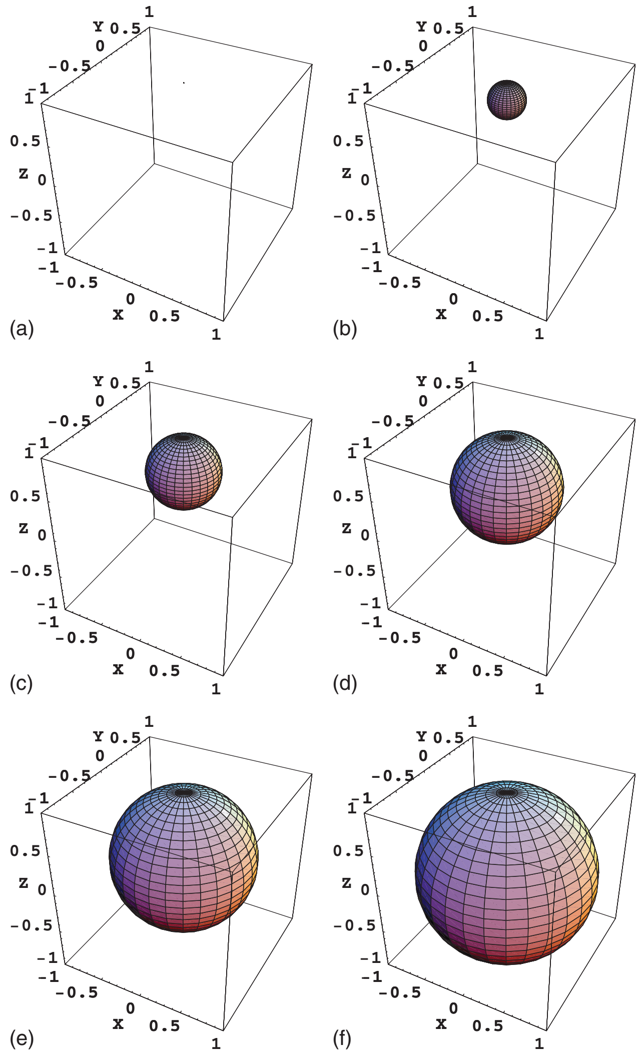

FIG. 3. (Color online) "Invasion" of the Bloch ball: $\cos^2 \alpha = 0$ (top left), $\frac{\pi}{10}$ (top right), $2\frac{\pi}{10}$ (middle left), $3\frac{\pi}{10}$ (middle right), $4\frac{\pi}{10}$ (bottom left), and $\frac{\pi}{2}$ (bottom right).

$$\rho_{12} = C_{01}C_{02}^{\star} + C_{11}C_{12}^{\star} + C_{21}C_{22}^{\star} = C_{01}C_{02}, \tag{23}$$

$$\rho_{02} = C_{00}C_{02}^{\star} + C_{10}C_{12}^{\star} + C_{20}C_{22}^{\star} = C_{00}C_{02}. \tag{24}$$

Then we obtain C_{11} from

$$\rho_{11} = |C_{01}|^2 + |C_{11}|^2 + |C_{21}|^2 = |C_{01}|^2 + C_{11}^2, \tag{25}$$

and, finally, C_{10} and C_{20} from

$$\rho_{01} = C_{00}C_{01}^{\star} + C_{10}C_{11}^{\star} + C_{20}C_{21}^{\star} = C_{00}C_{01}^{\star} + C_{10}C_{11}, \tag{26}$$

$$\rho_{00} = |C_{00}|^2 + |C_{10}|^2 + C_{20}^2. \tag{27}$$

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 Greek letters written on top of it (for instance, α_1 and α_2) represents a unitary transformation whose matrix representation has, in the $\{|0\rangle, |1\rangle, |2\rangle\}$ basis, the first column given by

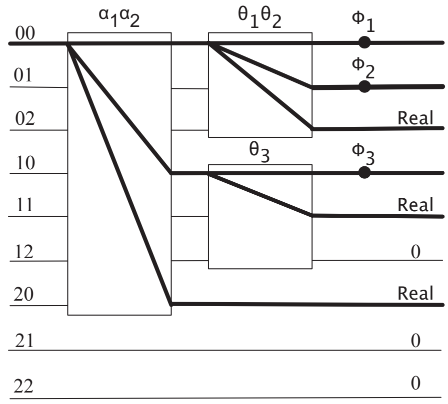

FIG. 4. Diagram of states for the purification of a single qutrit. To simplify the plot, only the thick lines corresponding to the information flow are shown inside the boxes. The angles $\alpha_i, \theta_j \in [0, \frac{\pi}{2}]$, while the phases $\phi_k \in [0, 2\pi)$.

$$\begin{bmatrix} \cos \alpha_1 \cos \alpha_2 \\ \cos \alpha_1 \sin \alpha_2 \\ \sin \alpha_1 \end{bmatrix}. \tag{28}$$

Such transformation maps the input state $|0\rangle$ into

$$\cos \alpha_1 \cos \alpha_2 |0\rangle + \cos \alpha_1 \sin \alpha_2 |1\rangle + \sin \alpha_1 |2\rangle. \tag{29}$$

Finally, the box with the letter θ_3 on top of it represents the rotation $R(\theta_3)$ acting on the two-dimensional subspace spanned by the states $|0\rangle$ and $|1\rangle$, with R defined by Eq. (15).

Given the input state $|00\rangle$, the output purification state $|\Psi\rangle = \Sigma_{\alpha,i} C_{\alpha i} |\alpha i\rangle$ can be immediately written by following the thick lines of the diagram of states in Fig. 4. We obtain

$$C_{00} = \cos \alpha_1 \cos \alpha_2 \cos \theta_1 \cos \theta_2 e^{i\phi_1},$$

$$C_{01} = \cos \alpha_1 \cos \alpha_2 \cos \theta_1 \sin \theta_2 e^{i\phi_2},$$

$$C_{02} = \cos \alpha_1 \cos \alpha_2 \sin \theta_1,$$

$$C_{10} = \cos \alpha_1 \sin \alpha_2 \cos \theta_3 e^{i\phi_3},$$

$$C_{11} = \cos \alpha_1 \sin \alpha_2 \sin \theta_3,$$

$$C_{12} = 0,$$

$$C_{20} = \sin \alpha_1,$$

$$C_{21} = 0,$$

$$C_{22} = 0. \tag{30}$$

These relations can be easily inverted to obtain the parameters $\{\alpha_j, \theta_k, \phi_l\}$ as a function of the coefficients $C_{\alpha i}$ and, therefore, of the elements of the density matrix ρ. Therefore, the quantum circuit represented by the diagram of states of Fig. 4 can be used to generate any given qutrit state ρ, once the ancillary qutrit is disregarded. Finally, we point out that the number of real parameters $\{\alpha_i,\theta_k,\phi_l\}$ 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 ρ.

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

$$\rho=\sum_{k=1}^{3}p_k|\psi_k\rangle\langle\psi_k|, \tag{31}$$

with $p_1=\cos^2\alpha_1\cos^2\alpha_2$, $p_2=\cos^2\alpha_1\sin^2\alpha_2$, $p_3=\sin^2\alpha_1$, $|\psi_1\rangle$ is a single-qutrit pure state, $|\psi_2\rangle$ is a 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 $\Sigma_k p_k=1$.

V. TWO QUBITS

We consider $M=N=4$ and set

$$C_{03}\in\mathbb{R}_+,$$

$$C_{12}\in\mathbb{R}_+,\quad C_{13}=0,$$

$$C_{21}\in\mathbb{R}_+,\quad C_{22}=C_{23}=0,$$

$$C_{30}\in\mathbb{R}_+,\quad C_{31}=C_{32}=C_{33}=0. \tag{32}$$

We first obtain C_{03} from

$$\rho_{33}=|C_{03}|^2+|C_{13}|^2+|C_{23}|^2+|C_{33}|^2=|C_{03}|^2, \tag{33}$$

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

$$\rho_{23}=C_{02}C_{03}^\star+C_{12}C_{13}^\star+C_{22}C_{23}^\star+C_{32}C_{33}^\star=C_{02}C_{03}, \tag{34}$$

$$\rho_{13}=C_{01}C_{03}^\star+C_{11}C_{13}^\star+C_{21}C_{23}^\star+C_{31}C_{33}^\star=C_{01}C_{03}, \tag{35}$$

$$\rho_{03}=C_{00}C_{03}^\star+C_{10}C_{13}^\star+C_{20}C_{23}^\star+C_{30}C_{33}^\star=C_{00}C_{03}. \tag{36}$$

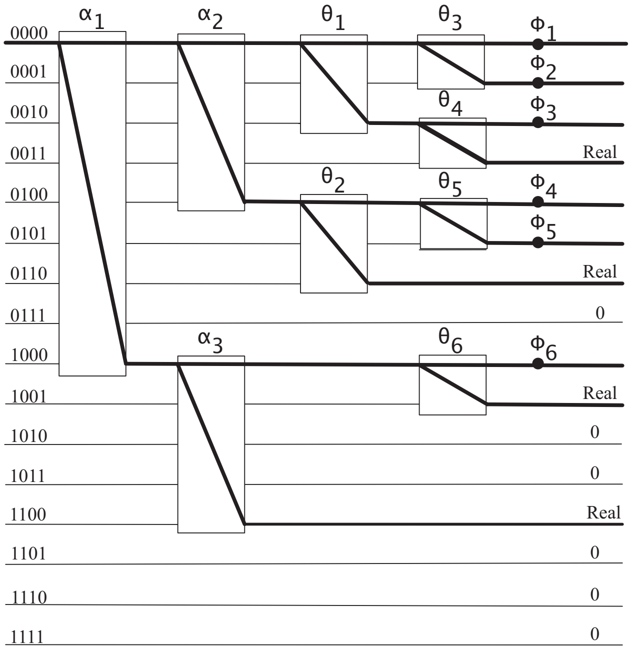

FIG. 5. Diagram of states for the purification of a two-qubit state. To simplify the plot, only the thick lines corresponding to the information flow are shown inside the boxes. The angles $\alpha_i,\theta_j\in[0,\frac{\pi}{2}]$, while the phases $\phi_k\in[0,2\pi)$.

Then we obtain C_{12} from

$$\rho_{22}=|C_{02}|^2+|C_{12}|^2+|C_{22}|^2+|C_{32}|^2=|C_{02}|^2+C_{12}^2, \tag{37}$$

then C_{11} and C_{10} from

$$\rho_{12}=C_{01}C_{02}^\star+C_{11}C_{12}^\star+C_{21}C_{22}^\star+C_{31}C_{32}^\star=C_{01}C_{02}^\star+C_{11}C_{12}, \tag{38}$$

$$\rho_{02}=C_{00}C_{02}^\star+C_{10}C_{12}^\star+C_{20}C_{22}^\star+C_{30}C_{32}^\star=C_{00}C_{02}^\star+C_{10}C_{12}. \tag{39}$$

Also we obtain C_{21} from

$$\rho_{11}=|C_{01}|^2+|C_{11}|^2+|C_{21}|^2+|C_{31}|^2=|C_{01}|^2+|C_{11}|^2+C_{21}^2, \tag{40}$$

then C_{20} from

$$\rho_{01}=C_{00}C_{01}^\star+C_{10}C_{11}^\star+C_{20}C_{21}^\star+C_{30}C_{31}^\star=C_{00}C_{01}^\star+C_{10}C_{11}^\star+C_{20}C_{21}, \tag{41}$$

and, finally, C_{30} from

$$\rho_{00}=|C_{00}|^2+|C_{10}|^2+|C_{20}|^2+C_{30}^2. \tag{42}$$

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 ρ. 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 $|\Psi\rangle=\Sigma_{\alpha,i}C_{\alpha i}|\alpha i\rangle$. We obtain

$$C_{0000}=\cos\,\alpha_1\cos\,\alpha_2\cos\,\theta_1\cos\,\theta_3 e^{i\phi_1},$$

$$C_{0001}=\cos\,\alpha_1\cos\,\alpha_2\cos\,\theta_1\sin\,\theta_3 e^{i\phi_2},$$

$$C_{0010}=\cos\,\alpha_1\cos\,\alpha_2\sin\,\theta_1\cos\,\theta_4 e^{i\phi_3},$$

$$C_{0011}=\cos\,\alpha_1\cos\,\alpha_2\sin\,\theta_1\sin\,\theta_4,$$

$$C_{0100}=\cos\,\alpha_1\sin\,\alpha_2\cos\,\theta_2\cos\,\theta_5 e^{i\phi_4},$$

$$C_{0101}=\cos\,\alpha_1\sin\,\alpha_2\cos\,\theta_2\sin\,\theta_5 e^{i\phi_5},$$

$$C_{0110}=\cos\,\alpha_1\sin\,\alpha_2\sin\,\theta_2,$$

$$C_{0111}=0,$$

$$C_{1000}=\sin\,\alpha_1\cos\,\alpha_3\cos\,\theta_6 e^{i\phi_6},$$

$$C_{1001}=\sin\,\alpha_1\cos\,\alpha_3\sin\,\theta_6,$$

$$C_{1010}=0,$$

$$C_{1011}=0,$$

$$C_{1100}=\sin\,\alpha_1\sin\,\alpha_3,$$

$$C_{1101}=0,$$

$$C_{1110}=0,$$

$$C_{1111}=0. \tag{43}$$

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 ρ.

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

$$\rho=\sum_{k=1}^{4} p_k|\psi_k\rangle\langle\psi_k|, \tag{44}$$

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 $\Sigma_k p_k=1$. 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

$$C_{0,N-1}\in\mathbb{R}_+,$$

$$C_{1,N-2}\in\mathbb{R}_+,\;\; C_{1,N-1}=0,$$

$$C_{2,N-3}\in\mathbb{R}_+,\;\; C_{2,N-2}=C_{2,N-1}=0,$$

$$\vdots$$

$$C_{N-1,0}\in\mathbb{R}_+,\;\; C_{N-1,1}=C_{N-1,2}=\;\ldots\;,$$

$$=C_{N-1,N-1}=0. \tag{45}$$

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

(i) We first determine $C_{0,N-1}$ from $\rho_{N-1,N-1}$,
(ii) then C_{0j} from $\rho_{j,N-1}$, with $j=N-2,\ldots,0$,
(iii) then $C_{1,N-2}$ from $\rho_{N-2,N-2}$,
(iv) then C_{1j} from $\rho_{j,N-2}$, with $j=N-3,\ldots,0,\ldots$,
(v) and, finally, $C_{N-1,0}$ from ρ_{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 $\mathrm{Tr}(\rho)=1$]. Therefore, an ancillary system of $n-1$ qudits is not sufficient to purify ρ, 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

$$\rho=\sum_{k=1}^{d^n} p_k|\psi_k\rangle\langle\psi_k|, \tag{46}$$

with the pure states from $|\psi_1\rangle$ to $|\psi_{d^n}\rangle$ residing in subspaces 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 purification scheme applies to a system of n qudits or to a single system of size $N=d^n$. Of course, the practical implementation 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 ρ. 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

$$\rho=C^T C^{\star}=DD^{T*}=DD^{\dagger}, \tag{47}$$

namely, it is the Cholesky decomposition of the density matrix ρ. Such decomposition is unique when ρ is positive, while the ambiguities arising when ρ is singular may be re-

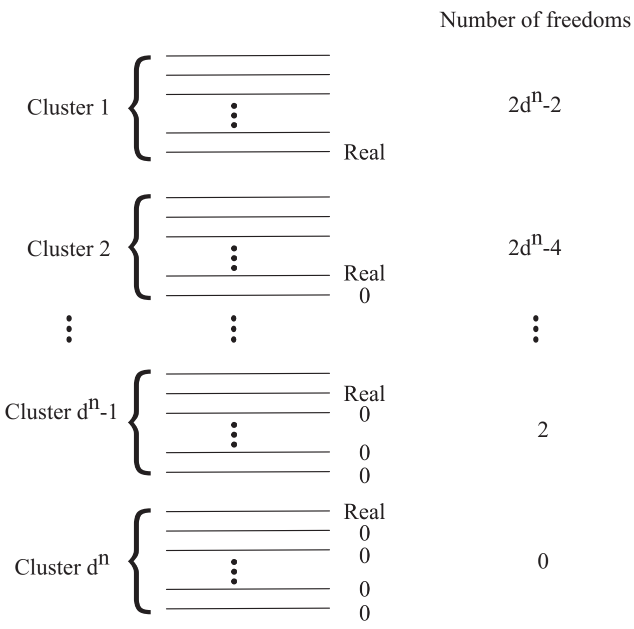

FIG. 6. Sketch of the diagram of states for the purification of a n-qudit state by means of $2n$ qudits. The diagram has d^{2n} lines, one for each state of the computational basis. We can cluster groups of d^n lines. The constraints and the number of real freedoms for each cluster are highlighted. If we add these numbers plus the d^n-1-independent weights in mixture (46), we obtain a total number of $d^{2n}-1$ degrees of freedom.

moved 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 suitable unitary operations applied both to the system and to the ancillary qudits, with the ancillary qudits eventually disregarded. While also well-known purification (7) based on 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 parameters exactly equal to the number of degrees of freedom of the generic n-qubit state that we wish to purify.

It is well known that the purification $|\Psi\rangle$ of a generic mixed state ρ cannot be uniquely determined, as the partial trace over the ancillary qudits is invariant under any unitary transformation $U_A \otimes \mathbb{1}_S$ acting nontrivially on the ancillary qudits only. Indeed, we have

$$\rho = \mathrm{Tr}_A(|\Psi\rangle\langle\Psi|) = \mathrm{Tr}_A(|\Psi'\rangle\langle\Psi'|), \tag{48}$$

with

$$|\Psi'\rangle = (U_A \otimes \mathbb{1}_S)|\Psi\rangle. \tag{49}$$

It is sufficient to add the unitary transformation $U_A \otimes \mathbb{1}_S$ at the end of our purification protocol to obtain any $2n$-qudit purification $|\Psi'\rangle$ of a n-qudit state ρ. On the other hand, we can say that our protocol selects a very convenient purification as the coefficients of the wave function $|\Psi\rangle$ in the computational basis are easily determined from the density matrix ρ and the quantum circuit generating ρ can be immediately drawn.

APPENDIX: 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 synthetic but may help us to clearly visualize quantum information flow in a quantum circuit.

For the purposes of the present paper, it will be sufficient to show the diagrams of states for elementary single-qubit quantum gates. The phase-shift gate $\mathcal{P}(\phi)$, defined by

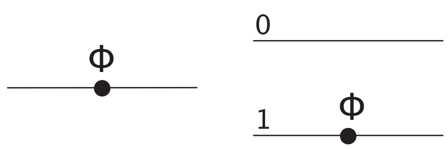

FIG. 7. Quantum circuit (left) and diagram of states (right) for the phase-shift gate.

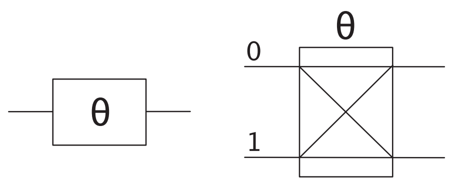

FIG. 8. Quantum circuit (left) and diagram of states (right) for the $R(\theta)$ gate.

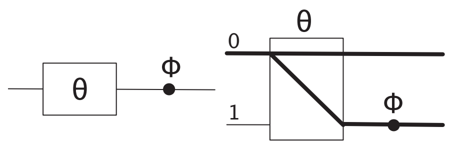

FIG. 9. Quantum circuit (left) and diagram of states (right) for the generation of a generic single-qubit state. To simplify the plot, only the thick lines corresponding to the information flow are shown inside the boxes.

Eq. (16), and the rotation gate $R(\theta)$, defined by Eq. (15), are shown in Fig. 7 and Fig. 8, respectively. 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.

[1] G. Benenti, G. Casati, and G. Strini, *Principles of Quantum Computation and Information, Vol. I: Basic Concepts* (World Scientific, Singapore, 2004); G. Benenti, G. Casati, and G. Strini, *Principles of Quantum Computation and Information, Vol. II: Basic Tools and Special Topics* (World Scientific, Singapore, 2007).

[2] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, 2000).

[3] I. Bengtsson and K. Życzkowski, *Geometry of Quantum States* (Cambridge University Press, Cambridge, 2006).

[4] H. Barnum, M. A. Nielsen, and B. Schumacher, Phys. Rev. A **57**, 4153 (1998).

[5] S. Felloni, A. Leporati, and G. Strini, Int. J. Unconv. Comput. (to be published).

[6] G. H. Golub and C. F. Van Loan, *Matrix Computations*, 3rd ed. (The Johns Hopkins University Press, Baltimore, 1996).

[7] K. Banaszek, G. M. D'Ariano, M. G. A. Paris, and M. F. Sacchi, Phys. Rev. A **61**, 010304(R) (1999).

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