

Optimal Purification of Single Qubits

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(Received 28 December 1998)

We introduce a new decomposition of the multiqubit states of the form $\rho^{\otimes N}$ and employ it to construct the optimal single qubit purification procedure. The same decomposition allows us to study optimal quantum cloning and state estimation of mixed states. [S0031-9007(99)09247-9]

PACS numbers: 03.67.-a, 03.65.Bz

Quantum data processing [1], such as quantum cryptography, teleportation, or computation, rely on an ample supply of qubits in nearly pure quantum states. However, maintaining unknown and uncorrupted entanglement or superpositions in the presence of the coupling to the environment is usually difficult and a great deal of recent research has been focused on issues such as entanglement purification [2]. In particular, several entanglement purification protocols have been devised but so far none of them has been proved to be optimal, i.e., it is not clear what is the maximal fraction of purified entangled particles for a given initial state and a prescribed degree of purification. This paper addresses a less complicated, but nevertheless interesting, question of purifying unknown quantum superpositions of qubits. It provides a definite and constructive answer regarding the optimality of the single-qubit purification procedures. The solution of the problem involves a particular decomposition of density operators of multiqubit systems. This decomposition seems to be a useful tool on its own as it also gives some insight into the related problems of the optimal cloning [3] and the optimal state estimation [4] of mixed states. It can be generalized to dimensions $d > 2$ by extending the mathematical formalism to include irreducible representations of $SU(d)$.

Suppose we are given N identical qubits, each in an unknown state described by a density operator

$$\rho = \frac{1}{2}(\mathbf{1} + \lambda \vec{n} \cdot \vec{\sigma}) = c_1 |1_{\vec{n}}\rangle\langle 1_{\vec{n}}| + c_0 |0_{\vec{n}}\rangle\langle 0_{\vec{n}}|, \quad (1)$$

where $\lambda \vec{n}$ is the Bloch vector, $|\vec{n}| = 1$, $c_1 - c_0 = \lambda > 0$, $c_1 + c_0 = 1$, and $|0_{\vec{n}}\rangle, |1_{\vec{n}}\rangle$ are the two eigenstates of ρ . The goal is to obtain the maximum number of qubits in a state "as close as possible" to the unknown state $|1_{\vec{n}}\rangle$, i.e., to *purify the state* ρ . Before we define the purification procedure in more precise mathematical terms, let us rewrite ρ as a convex sum

$$\rho = \lambda \frac{1}{2}(\mathbf{1} + \vec{n} \cdot \vec{\sigma}) + (1 - \lambda) \frac{1}{2} \mathbf{1}, \quad (2)$$

where the first term on the right-hand side represents the purified state $\frac{1}{2}(\mathbf{1} + \vec{n} \cdot \vec{\sigma}) = |1_{\vec{n}}\rangle\langle 1_{\vec{n}}|$ and the second one the maximally mixed state $\frac{1}{2} \mathbf{1}$. Thus, given N identically and independently prepared qubits, one can

distill from the set at most λN of perfectly purified qubits. In the following, we show that this limit is achievable when $N \rightarrow \infty$ and we describe the optimal purification procedure for any finite N .

In general, a purification procedure \mathcal{P} consists of a set of operations and measurements on the N qubits and perhaps on additional ancillas. Depending on the outcomes of the measurements some of the qubits will be discarded and we will end up with $M \leq N$ qubits whose reduced density operators are closer to the ideal state $|1_{\vec{n}}\rangle$. Thus \mathcal{P} is described by a set of linear completely positive maps \mathcal{P}_M such that $\mathcal{P}_M(\rho^{\otimes N}) = \rho_M$ where ρ_M is an unnormalized density operator describing M qubits. The probability of obtaining M qubits is $P_M = \text{tr}(\rho_M)$ and their corresponding fidelities $F_M^k = \langle 1_{\vec{n}} | \rho_k | 1_{\vec{n}} \rangle$, where ρ_k is the normalized reduced density operator of qubits $k = 1, 2, \dots, M$. These probabilities and fidelities depend both on the direction \vec{n} and the length λ of the Bloch vector of the original qubits, and thus we write them as $P_M(\lambda, \vec{n})$ and $F_M^k(\lambda, \vec{n})$. Given that we are not interested in the fidelity of a particular qubit, nor in a particular direction of the Bloch vector but rather in their average values, we define

$$P_M(\lambda) = \int d\vec{n} P_M(\lambda, \vec{n}), \quad (3a)$$

$$F_M(\lambda) = \frac{1}{P_M(\lambda)} \int d\vec{n} P_M(\lambda, \vec{n}) \frac{1}{M} \sum_{k=1}^M F_M^k(\lambda, \vec{n}), \quad (3b)$$

where the integral refers to the complete solid angle. Thus, any given \mathcal{P} is characterized by these two quantities namely, the probability of obtaining M valid qubits and their corresponding fidelity. This fact implies that there is no unique way of defining optimality. For example, a procedure might give with small probability a large number of qubits of high fidelity, whereas another one might give with a large probability a smaller number of qubits of higher fidelity. Nevertheless, it turns out that there is a procedure \mathcal{P} which has the following unique properties: (1) given any other purification procedure \mathcal{P}' characterized by P'_M and F'_M , it is always possible to obtain these values by first applying \mathcal{P} and then some prescribed operations and measurements; (2) after

applying \mathcal{P} , it is impossible to increase the fidelity of the outgoing qubits even at the cost of decreasing the number of qubits. The first property is a consequence of the fact that \mathcal{P} is, in a certain sense, reversible. It implies that after applying it, we can still obtain the optimal results whatever we mean by optimal. The second property implies that after applying \mathcal{P} , it is impossible to purify further. As a consequence, our procedure is optimal for any reasonable definition of optimality (in which the fidelity is not allowed to decrease).

Let us introduce now an important concept that will be used later on to prove optimality of our protocol. We say that a procedure \mathcal{P}^s is *symmetric* if: (i) the reduced density operators of the M qubits are identical; (ii) the maps \mathcal{P}_M^s are covariant [5], that is,

$$\mathcal{P}_M^s[(U\rho U^\dagger)^{\otimes N}] = U^{\otimes M} \mathcal{P}_M^s(\rho^{\otimes N}) (U^\dagger)^{\otimes M} \quad (4)$$

for all $U \in \text{SU}(2)$. These conditions imply that the probability of obtaining M qubits is independent of \vec{n} and that the fidelities of all the qubits are the same, which simplifies the calculations. Moreover, they are the only ones that have to be analyzed since for any arbitrary purification protocol \mathcal{P} one can construct a symmetric one which gives exactly the same values of $P_M(\lambda)$ and $F_M(\lambda)$. To do that, we proceed as follows: (1) we apply the same random unitary U operator to the N qubits; (2) we apply the procedure \mathcal{P} ; (3) we apply the operator U^\dagger to the M resulting qubits; (4) we permute the M qubits randomly.

We shall start with a set of $N = 2J$ qubits (the $2J + 1$ case can be solved in an analogous way) and decompose their state $\rho^{\otimes N}$ into the sum of density operators $\rho_{j,\alpha}$ which are supported on orthogonal subspaces $S_{j,\alpha_j} = \text{span}\{|j, m, \alpha_j\rangle; m = -j, -j + 1, \dots, j\}$, where $j = 0, 1, \dots, J$, $\alpha_j = 1, 2, \dots, d_j$, and

$$d_j = \binom{2J}{J-j} - \binom{2J}{J-j-1} \quad (j \neq J), \quad (5)$$

$d_J = 1$. States $|j, m, \alpha\rangle$ are constructed from an arbitrary basis $\{|0\rangle, |1\rangle\}$ of a single qubit in such a way that: (i) for a fixed j and α , vectors $|j, m, \alpha\rangle$ form a basis for the $(2j + 1)$ -dimensional irreducible representation of $\text{SU}(2)$; (ii) for a fixed j and m , vectors $|j, m, \alpha\rangle$ form a basis for the d_j -dimensional representation of S_N (symmetric group) corresponding to the Young diagram $(2j, 2J - 2j)$. In particular, we choose

$$|j, m, 1\rangle = |j, m\rangle \otimes |\Psi_-\rangle^{\otimes J-j}, \quad (6)$$

where $|j, m\rangle$ is the symmetric state of $2j$ qubits with $j - m$ qubits in the state $|0\rangle$ and the rest in $|1\rangle$, and $|\Psi_-\rangle$ is the singlet state of two qubits. The rest of the states are constructed by using permutation operators, $\Pi_i \in S_N$,

$$|j, m, \alpha\rangle = \sum_i h_i \Pi_i |j, m, 1\rangle, \quad (7)$$

and the coefficients h_i are chosen so that the corresponding states are orthonormal. Although we have defined the basis $|j, m, \alpha\rangle$ in terms of the states $|i\rangle$ ($i = 0, 1$),

we could have used any other basis $|i_{\vec{n}}\rangle = U_{\vec{n}}|i\rangle$ where $U_{\vec{n}} \in \text{SU}(2)$ to define $|j, m, \alpha\rangle_{\vec{n}}$. One can check that

$$\begin{aligned} |j, m, \alpha\rangle_{\vec{n}} &= U_{\vec{n}}^{\otimes N} |j, m, \alpha\rangle \\ &= \sum_{m'} D_{m',m}^j(\vec{n}) |j, m', \alpha\rangle, \end{aligned} \quad (8)$$

where $D_{m',m}^j(\vec{n})$ are the corresponding matrix elements. Using (8) one immediately sees that the subspaces $S_{j,\alpha}$ are the same if we take any basis $|j, m, \alpha\rangle_{\vec{n}}$ to construct them. We also define a set of unitary operators $U_{j,\alpha}$ which transform $S_{j,\alpha}$ into $S_{j,1}$ while leaving the other subspaces untouched. We take $U_{j,\alpha}|j, m, \alpha\rangle = |j, m, 1\rangle$ and $U_{j,\alpha}|j, m, 1\rangle = |j, m, \alpha\rangle$. Again, using (8) one can easily check that these definitions are valid for all \vec{n} , i.e. $U_{j,\alpha}|j, m, 1\rangle_{\vec{n}} = |j, m, \alpha\rangle_{\vec{n}}$.

The decomposition itself reads

$$\rho^{\otimes N} = \sum_{j=0}^J p_j \frac{1}{d_j} \sum_{\alpha=1}^{d_j} \rho_{j,\alpha}, \quad (9)$$

where

$$p_j = d_j [c_0 c_1]^{J-j} \frac{c_1^{2j+1} - c_0^{2j+1}}{c_1 - c_0}, \quad (10a)$$

$$\rho_{j,\alpha} = U_{j,\alpha} \rho_{j,1} U_{j,\alpha}^\dagger \quad \text{for } \alpha \neq 1, \quad (10b)$$

$$\rho_{j,1} = \rho_j \otimes (|\Psi_-\rangle\langle\Psi_-|)^{\otimes J-j}, \quad (10c)$$

$$\begin{aligned} \rho_j &= \frac{c_1 - c_0}{c_1^{2j+1} - c_0^{2j+1}} \sum_{m=-j}^j \\ &\quad \times c_0^{j-m} c_1^{j+m} |j, m\rangle_{\vec{n}} \langle j, m|. \end{aligned} \quad (10d)$$

This last density operator can be conveniently written as a convex sum of density operators corresponding to identical pure states of $2j$ qubits:

$$\begin{aligned} \rho_j &= \frac{c_1 - c_0}{c_1^{2j+1} - c_0^{2j+1}} (2j + 1) \\ &\quad \times \int \frac{d\Omega}{4\pi} n(\theta)^{2j} (|\Psi(\theta, \phi)\rangle\langle\Psi(\theta, \phi)|)^{\otimes 2j}, \end{aligned} \quad (11)$$

where $n(\theta) = c_1 \cos^2(\theta/2) + c_0 \sin^2(\theta/2)$ and

$$|\Psi(\theta, \phi)\rangle = \sqrt{c_1} \frac{\cos(\theta/2)}{\sqrt{n(\theta)}} |1\rangle_{\vec{n}} + \sqrt{c_0} \frac{\sin(\theta/2)}{\sqrt{n(\theta)}} e^{i\phi} |0\rangle_{\vec{n}}. \quad (12)$$

Any state of the form $\rho^{\otimes N}$ can be decomposed into the $\rho_{j,\alpha}$ components as in Eq. (9); this can be seen by writing $\rho^{\otimes N} = \sum_{k=0}^N c_0^k c_1^{N-k} \hat{P}_k$, where \hat{P}_k is a projector on the subspace with exactly k qubits in state $|0\rangle_{\vec{n}}$. Expressing these projectors in terms of the basis vectors $|j, m, \alpha\rangle_{\vec{n}}$ immediately gives Eq. (9).

Let us now use decomposition (9) to introduce our purification procedure. Given the state $\rho^{\otimes N}$ we perform a measurement defined by the projections on the subspaces $S_{j,\alpha}$. This provides us with one of the states $\rho_{j,\alpha}$. If $\alpha \neq 1$ we apply the unitary transformation $U_{j,\alpha}^\dagger \rho_{j,\alpha} U_{j,\alpha}$

to obtain $\rho_{j,1}$. The resulting density operator, $\rho_{j,1} = \rho_j \otimes (|\Psi_{-}\rangle\langle\Psi_{-}|)^{\otimes J-j}$ gives a clear separation between the first $2j$ qubits in state ρ_j and the remaining qubits paired into $J - j$ singlets. Since the singlet state carries no information about ρ , we can discard the last $2(J - j)$ qubits. This procedure gives, with probability p_j , $2j$ qubits in state ρ_j . The reduced density operators of the resulting qubits coincide and have the fidelity

$$f_j = \frac{1}{2j} \left[\frac{(2j+1)c_1^{2j+1}}{c_1^{2j+1} - c_0^{2j+1}} - \frac{c_1}{c_1 - c_0} \right]. \quad (13)$$

This procedure gives [cf. Eq. (3)] $P_M = p_{j=M/2}$ and $F_M = f_{j=M/2}$ if M is even and $P_M = 0$ otherwise.

In order to illustrate our considerations with an example, let us take the simplest case of $N = 2$ qubits. The density operator $\rho^{\otimes 2}$ can be decomposed into two terms supported, respectively, on the singlet (antisymmetric, $S_{0,1}$) and the triplet (symmetric, $S_{1,1}$) subspace,

$$\begin{aligned} \rho^{\otimes 2} &= \sum_{j=0}^1 p_j \rho_{j,1} \\ &= c_0 c_1 |\Psi_{-}\rangle\langle\Psi_{-}| + (c_0^2 |0\rangle\langle 0| \\ &\quad + c_0 c_1 |\Psi_{+}\rangle\langle\Psi_{+}| + c_1^2 |1\rangle\langle 1|). \end{aligned} \quad (14)$$

Our purification procedure consists of projecting onto the symmetric or antisymmetric subspaces. After successful projection on the symmetric subspace, we keep both qubits; otherwise, we discard both qubits since the singlet state does not depend on \vec{n} , and therefore the qubits do not carry any information about the original state. This procedure is symmetric and gives $P_2(\lambda) = 1 - c_0 c_1 = (3 + \lambda^2)/4 = 1 - P_0(\lambda)$ and $F_2(\lambda) = c_1(1 - c_0/2)/(1 - c_0 c_1) > c_1$. Thus, with probability $P_2(\lambda)$ we obtain a higher fidelity than the original one.

In general, the average distillability factor (or yield) and the mean fidelity of our procedure are given, respectively, by

$$D_N(\lambda) \equiv \sum_{j=0}^J p_j \frac{2j}{2J} \approx \lambda + \frac{1}{N} \frac{1 - \lambda}{\lambda} + O(1/N^2), \quad (15a)$$

$$\bar{F}_N(\lambda) \equiv \sum_{j=0}^J p_j f_j \approx 1 - \frac{1}{2N} \frac{1 - \lambda}{\lambda^2} + O(1/N^2). \quad (15b)$$

In the limit $N \gg 1$, the mean fidelity tends to one whereas the yield tends to λ , the length of the Bloch vector. In fact, one can check that in this limit the distribution p_j becomes narrower and narrower (that is, the width divided by the mean value tends to zero). This means that if N is sufficiently large we will basically obtain $N\lambda$ qubits in the unknown pure state $|1\rangle_{\vec{n}}$.

In order to show that we have an optimal procedure we will first show that given any other purification procedure \mathcal{P}' it is always possible to obtain the same values P'_M and F'_M once we have applied our procedure \mathcal{P} . Suppose

we have applied \mathcal{P} to the N qubits, obtained the outcome corresponding to a particular subspace $S_{j,\alpha}$, applied the corresponding operator $U_{j,\alpha}^\dagger$, and discarded the last $2(J - j)$ qubits. In order to obtain the results of the procedure \mathcal{P}' we just have to add $J - j$ pairs of qubits in singlet states, apply the operation $U_{j,\alpha}$ to the whole set, and then apply the procedure \mathcal{P}' . It is straightforward to show that this whole procedure gives the same values of P'_M and F'_M . The intuitive idea behind all this is very simple: according to (9) the density operator $\rho^{\otimes N}$ can always be regarded as describing the situation in which we have prepared with probability p_j/d_j the state $\rho_{j,\alpha}$. Thus, our measurement only identifies the state which has been prepared without disturbing it, whereas the operation $U_{j,\alpha}$ is unitary. Therefore, this procedure is effectively reversible.

Now, we complete the proof of optimality by showing that after having applied \mathcal{P} , it is impossible to increase the averaged fidelity of the outgoing qubits. The idea is to show that any purification procedure which produces 1 qubit out of $2j$ qubits in state ρ_j has at most a fidelity $F_1(\lambda) = f_j$ given by (13). This automatically implies that there exists no procedure that produces M qubits (for any M) with fidelity higher than f_j for if it existed, we could construct a procedure that gives 1 qubit of fidelity larger than f_j by simply discarding the remaining $M - 1$ qubits, which contradicts our previous statement. Therefore, we restrict ourselves to symmetric procedures that produce one qubit out of $2j$ qubits in a state ρ_j . Let us consider a general linear and completely positive map \mathcal{P}_1 . It follows from the covariance condition (4) that for any single qubit in state $|\Psi\rangle$ we have

$$\mathcal{P}_1[(|\Psi\rangle\langle\Psi|)^{\otimes 2j}] = x|\Psi\rangle\langle\Psi| + y|\Psi^\perp\rangle\langle\Psi^\perp|, \quad (16)$$

where $x, y \geq 0$, $x + y \leq 1$, and $\langle\Psi^\perp|\Psi\rangle = 0$ (this can be easily proved by showing that the result must commute with any rotation around the axis defined by the Bloch vector corresponding to $|\Psi\rangle$). Using Eq. (11) and the fact that \mathcal{P}_1 is linear we can obtain $\mathcal{P}_1(\rho_j)$ and express the fidelity of $\mathcal{P}_1(\rho_j)/\text{tr}[\mathcal{P}_1(\rho_j)]$ in terms of x and y . The maximum value occurs for $(x, y) = (1, 0)$ and gives exactly f_j , which completes the proof.

Interestingly enough, the methods introduced above can be used to study the optimal cloning [3,5,6] of mixed states. In this case the goal is to start with N qubits, all in the state ρ given in Eq. (1), and produce exactly $M \geq N$ qubits each in a state as close as possible to $|1\rangle_{\vec{n}}$ [7]. More specifically, defining the average fidelity as in (3b), we define the optimal cloning procedure C as the one which gives a maximal value of F_M . Again, one can easily show that symmetric procedures C^s are optimal by using the same four steps as before. Moreover, since to all practical purposes the purification procedure defined above is reversible, we can study independently the optimal cloning of $2j$ qubits in the state ρ_j and at the

end average with the corresponding probabilities p_j . Let us then consider a symmetrical procedure that produces M qubits out of $2j$ qubits and that is described by a linear trace preserving positive map C_j . The corresponding fidelity will be $\langle 1_{\vec{n}} | \text{tr}_{M-1}[C_j(\rho_j)] | 1_{\vec{n}} \rangle$, where tr_{M-1} denotes the trace over any $M-1$ particles. Using the property (4) we have

$$\text{tr}_{M-1}[C_j(|\Psi\rangle\langle\Psi|^{\otimes 2j})] = x|\Psi\rangle\langle\Psi| + (1-x)|\Psi^\perp\rangle\langle\Psi^\perp|, \quad (17)$$

where

$$x \leq F_{2j,M}^{\text{pur}} \equiv \frac{M(2j+1) + 2j}{M(2j+2)}, \quad (18)$$

since otherwise C_j would give for pure states better clones than the optimal cloning procedure [3]. Using the decomposition (11), linearity, and (17) we obtain that the optimal value occurs for the largest value of x , i.e., for $x = F_{2j,M}^{\text{pur}}$. Thus, the fidelity of the optimal cloning procedure for mixed states is

$$F_{N,M}^{\text{mix}} = \sum_{j=0}^J p_j [F_{2j,M}^{\text{pur}} f_j + (1 - F_{2j,M}^{\text{pur}})(1 - f_j)], \quad (19)$$

where p_j , f_j , and $F_{2j,M}^{\text{pur}}$ are given in (10a), (13), and (18), respectively. Defining $\lambda_{N,M}^{\text{mix}} = 2F_{N,M}^{\text{mix}} - 1$ we obtain $\lambda_{N,M}^{\text{mix}} = \lambda_{N,\infty}^{\text{mix}}(M+2)/M$, where

$$\lambda_{N,\infty}^{\text{mix}} = \sum_{j=0}^J p_j (2f_j - 1) \frac{j}{j+1} \equiv 2F_{N,\infty}^{\text{mix}} - 1, \quad (20)$$

with $F_{N,\infty}^{\text{mix}}$ being the maximal fidelity in the $N \rightarrow \infty$ cloning of mixed states. Actually, using the same arguments as in [6] one can show that this fidelity is the maximal fidelity with which one can estimate the state $|1_{\vec{n}}\rangle$ starting from N copies of the state ρ . This way of estimating copies of mixed states might be interesting in the following context: Alice is sending N qubits in an unknown pure state to Bob via the depolarizing channel and Bob's goal is to determine the state that Alice is sending. In Fig. 1 we have plotted $\lambda_{N,\infty}^{\text{mix}}$ as a function of N for various values of the length of the Bloch vector.

In conclusion, we have introduced in this paper a new decomposition of the multiqubit states of the form $\rho^{\otimes N}$. This decomposition was instrumental in constructing the optimal single qubit purification procedure (and proving that it is indeed optimal) and in extending the remit of acceptable input states for the optimal quantum cloners.

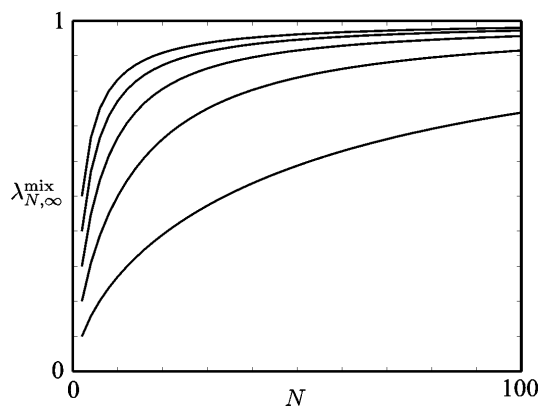


FIG. 1. Maximum achievable length of the Bloch vector $\lambda_{N,\infty}^{\text{mix}}$ in the cloning $N \rightarrow \infty$ as function of the initial number of copies of the state ρ . The values of the initial lengths of the Bloch vector are, from bottom to top, $\lambda = 0.2, 0.4, 0.6, 0.8, 1$.

The decomposition, apart from having applications in restoring quantum superpositions via the single qubit purification, seems to be a useful mathematical tool on its own.

We thank R. Werner for discussions. Work supported by the Austrian Science Foundation (SFB F15), TMR network ERB-FMRX-CT96-0087, Institute for Quantum Information GmbH, Hewlett-Packard, The Royal Society London, and Elsag-Bailey. After completing this work we learned that Vidal *et al.* (unpublished) have used a similar decomposition in the context of optimal measurements.

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