Completely positive covariant two-qubit quantum processes and optimal quantum NOT operations for entangled qubit pairs

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The structure is investigated of all completely positive quantum operations that transform pure two-qubit input states of a given degree of entanglement in a covariant way. Special cases thereof are quantum NOT operations which transform entangled pure two-qubit input states of a given degree of entanglement into orthogonal states in an optimal way. Based on our general analysis all covariant optimal two-qubit quantum NOT operations are determined. In particular, it is demonstrated that only in the case of maximally entangled input states can these quantum NOT operations be performed perfectly.

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I. INTRODUCTION

The current interest in processing quantum information [1] has also revived the interest in fundamental limitations of quantum theory $[2]$. It is well known, for example, that an arbitrary quantum state cannot be copied perfectly $[3]$. Similar no-go theorems are also known for other elementary tasks of quantum-information processing $[2]$. One of these tasks, for example, concerns the problem of transforming an arbitrary quantum state into an orthogonal one. It is well accepted that for arbitrary (unknown) pure quantum states such a quantum NOT operation cannot be performed perfectly due to its antilinear character $[4,5]$. In view of such no-go theorems it is natural to investigate to what extent such elementary tasks of quantum-information processing can be performed in an optimal way. In this context quantum operations that treat all possible input states of interest in a covariant way have received considerable attention [5]. Such a covariant behavior guarantees that the quantum process under consideration achieves its goal for all input states of interest with the same quality.

Recently, the problem of optimizing quantum NOT operations with respect to arbitrary one-qubit input states stimulated both theoretical $[4]$ and experimental investigations $[6]$. By now many aspects of optimal quantum NOT operations are well understood at least as far as general one-qubit input states are concerned $[4]$. Nevertheless, much less is known about optimal quantum NOT operations for entangled input states. In particular, if one is interested in constructing quantum NOT operations that are optimal for entangled input states of a particular degree of entanglement only, the general no-go theorem for quantum NOT operations does not apply because the input states form a restricted subset and not a linear subspace of the Hilbert space.

Motivated by these developments in this paper the problem of constructing optimal quantum NOT operations for entangled quantum states is addressed. In order to obtain a detailed first understanding of this still open problem we concentrate our discussion on the simplest possible input states, namely, pure two-qubit states of a given degree of entanglement. The main aim of this paper is twofold. First, the general structure is investigated of completely positive quantum processes that transform all possible pure two-qubit inputs states of a given degree of entanglement in a covariant way. Surprisingly it turns out that all these processes can be represented in a systematic way by convex sums of four special quantum processes, some of which have already been discussed previously in the literature. Second, based on this general analysis the structure is discussed of two-qubit quantum processes that transform an arbitrary pure two-qubit input state of a given degree of entanglement into an orthogonal quantum state in an optimal way. It is shown that in the special case of maximally entangled pure input states such quantum NOT operations can be performed perfectly and the general structure of these perfect quantum NOT operations is presented. These optimal quantum NOT operations may have interesting future applications in the context of other primitives of quantum-information processing, such as remote state preparation [7]. Finally, our work analyzes some of the problems studied for a single qubit $[8]$ in the case of two qubits.

This paper is organized as follows. In Sec. II the most general structure is discussed of completely positive twoqubit quantum processes that treat pure two-qubit input states of a given degree of entanglement in a covariant way. The construction of optimal covariant quantum NOT operations and of perfect NOT operations for maximally entangled input states is discussed in Sec. III. In Sec. IV the general representation of all possible completely positive covariant two-qubit processes is discussed once again. Thereby, it is demonstrated that all these processes are convex sums of four special quantum operations whose physical significance is apparent from the results obtained in Sec. III.

II. COMPLETELY POSITIVE COVARIANT TWO-QUBIT QUANTUM PROCESSES

In this section the general structure is investigated of all completely positive quantum processes that transform pure two-qubit input states of a given degree of entanglement in a covariant way.

Let us start by considering a general quantum operation [1] Π that maps an arbitrary two-qubit mixed input state ρ_{in} onto a mixed two-qubit output state ρ_{out} , i.e.,

$$
\Pi: \quad \rho_{in} \to \rho_{out}. \tag{1}
$$

If this is to treat pure two-qubit input states of a given degree of entanglement in a covariant way it has to satisfy the covariance condition $[9,10]$

$$
\Pi(U_1 \otimes U_2 \rho_{in} U_1^{\dagger} \otimes U_2^{\dagger}) = U_1 \otimes U_2 \Pi(\rho_{in}) U_1^{\dagger} \otimes U_2^{\dagger}.
$$
 (2)

This requirement has to be satisfied for arbitrary unitary onequbit transformations $U_1, U_2 \in SU(2)$ [11]. The restriction of the quantum map (1) to quantum operations reflects the physical requirement that Π should be implementable by a unitary transformation possibly involving also additional quantum systems but under the constraint that initially the two-qubit system of interest and these additional ancillary systems are uncorrelated $[1]$. As will be seen later, the covariance condition (2) implies the requested independence of the quality of performance of this quantum operation on the possible input states $\left[12,13\right]$.

For implementing the covariance condition (2) on the quantum process of (1), it is convenient to decompose the input state ρ_{in} into its angular-momentum irreducible tensor components $T(\frac{1}{2}, \frac{1}{2})_{K,q}$ [14], i.e.,

$$
\rho_{in} = \sum_{K,q;K',q'} \exp\left\{ \left[T \left(\frac{1}{2}, \frac{1}{2} \right)_{K,q}^{\dagger} \otimes T \left(\frac{1}{2}, \frac{1}{2} \right)_{K',q'}^{\dagger} \right] \rho_{in} \right\} + \sum T \left(\frac{1}{2}, \frac{1}{2} \right)_{K,q} \otimes T \left(\frac{1}{2}, \frac{1}{2} \right)_{K',q'} \tag{3}
$$

with

$$
T\left(\frac{1}{2},\frac{1}{2}\right)_{0,0} = \frac{1}{\sqrt{2}}I, \quad T\left(\frac{1}{2},\frac{1}{2}\right)_{1,1} = -(\sigma_x + i\sigma_y)/2,
$$

$$
T\left(\frac{1}{2},\frac{1}{2}\right)_{1,0} = \sqrt{2}\sigma_z/2, \quad T\left(\frac{1}{2},\frac{1}{2}\right)_{1,-1} = (\sigma_x - i\sigma_y)/2,
$$
 (4)

and with $K \in \{0, 1\}$ and $-K, -K+1, \ldots \leq q \leq \ldots, K-1, K$.

Thereby, σ_i with $i=x, y, z$ are the three orthogonal components of the Pauli spin operators with respect to fixed orthogonal *xyz* axes. (For the sake of convenience some basic facts about angular-momentum tensor operators are summarized in Appendix A.) The corresponding most general linear covariant output state has the form $[12,15]$

$$
\rho_{out} = \sum_{K,q;K',q'} \lambda(K,K')
$$

$$
\times \text{Tr}\left\{ \left[T\left(\frac{1}{2},\frac{1}{2}\right)_{K,q}^{\dagger} \otimes T\left(\frac{1}{2},\frac{1}{2}\right)_{K',q'}^{\dagger} \right] \rho_{in} \right\}
$$

$$
\times T\left(\frac{1}{2},\frac{1}{2}\right)_{K,q} \otimes T\left(\frac{1}{2},\frac{1}{2}\right)_{K',q'}.
$$
 (5)

According to Eq. (3) the most general two-qubit input state can be written in the form

$$
\rho_{in}(\vec{P}, \vec{Q}, \mathcal{M}) = \frac{1}{4} \Big(I \otimes I + \sum_{i=x,y,z} P_i \sigma_i \otimes I + \sum_{i=x,y,z} Q_i I \otimes \sigma_i
$$

+
$$
\sum_{i,j=x,y,z} M_{ij} \sigma_i \otimes \sigma_j \Big) \tag{6}
$$

with the aid of the two local vectors of coherence, \vec{P} $= (P_x, P_y, P_z)$ and $\vec{Q} = (Q_x, Q_y, Q_z)$, and with the correlation tensor $\mathcal{M} = (M_{ij})_{i,j=x,y,z}$ [16]. Because we are looking for trace-preserving maps, we obtain the condition $\lambda(0,0) = 1$. Using the notation $V = \lambda(1,0)$, $X = \lambda(0,1)$, $Y = \lambda(1,1)$ the corresponding output state of (5) is given by

$$
\rho_{out} = \frac{1}{4} \Big(I \otimes I + \sum_{i=x,y,z} (VP_i) \sigma_i \otimes I + \sum_{i=x,y,z} (XQ_i)I \otimes \sigma_i
$$

$$
+ \sum_{i,j=x,y,z} (YM_{ij}) \sigma_i \otimes \sigma_j \Big) \equiv \rho_{in} (V\vec{P}, X\vec{Q}, Y\mathcal{M}). \tag{7}
$$

In the special case of a normalized pure input state $|\psi\rangle$ $= \alpha |\uparrow \uparrow\rangle + \beta |\downarrow \downarrow\rangle$ which is quantized in the *z* direction this yields the explicit matrix representation

in the eigenbasis of σ , $\otimes \sigma$. Therefore, an arbitrary triple (X, V, Y) defines the most general covariant map between an input state (6) and an output state (7). Further restrictions are imposed on these parameters by complete positivity $\lceil 8 \rceil$. As shown in detail in Appendix B, complete positivity requires that all components of the triple (X, V, Y) have to be real valued and they have to satisfy the relations

$$
1+3X+3V+9Y \ge 0, \quad 1+3X-V-3Y \ge 0,
$$

$$
1-X+3V-3Y \ge 0, \quad 1-X-V+Y \ge 0,
$$
 (9)

or equivalently

$$
-\frac{1}{3} \le X, V \le 1, \quad \max\left\{-\frac{1+3X+3V}{9}, -1+X+V\right\}
$$

$$
\le Y \le \frac{1+3\min\{X, V\} - \max\{X, V\}}{3}.
$$
 (10)

Thus, provided these relations are satisfied the process defined by the covariant output state (7) is completely positive. A Kraus representation of this deterministic quantum operation is given by

$$
\rho_{out} = \Pi_{V,X,Y}(\rho_{in}(\vec{P}, \vec{Q}, \mathcal{M})) = \sum_{i,j=0,x,y,z} K_{ij}\rho_{in}(\vec{P}, \vec{Q}, \mathcal{M})K_{ij}^{\dagger}
$$

$$
= \rho_{in}(V\vec{P}, X\vec{Q}, Y\mathcal{M})
$$
(11)

with

$$
K_{00} = 1 / 4 (1 + 3X + 3V + 9Y)^{1/2} I \otimes I,
$$

\n
$$
K_{i0} = \frac{1}{4} (1 + 3X - V - 3Y)^{1/2} \sigma_i \otimes I,
$$

\n
$$
K_{0i} = 1 / 4 (1 - X + 3V - 3Y)^{1/2} I \otimes \sigma_i,
$$

$$
K_{ij} = \frac{1}{4}(1 - X - V + Y)^{1/2}\sigma_i \otimes \sigma_j, \quad i, j \in \{x, y, z\}.
$$
 (12)

Trace preservation is implied by the relation

$$
\sum_{i,j=0,x,y,z} K_{ij}^{\dagger} K_{ij} = I.
$$
 (13)

The set of all possible completely positive universal quantum operations characterized by triples (V, X, Y) is represented by the convex tetrahedron *ABCD* of Fig. 1. The physical significance of the extremal points of this tetrahedron is discussed in Sec. IV.

III. OPTIMAL QUANTUM NOT OPERATIONS FOR PURE ENTANGLED QUBIT PAIRS

Starting from the general results of Sec. II we can specify different types of completely positive covariant quantum processes. In the following we determine quantum processes that describe a quantum NOT operation acting on arbitrary pure two-qubit states of a given degree of entanglement in an optimal way.

Let us first of all summarize the basic problems that arise if one wants to construct a quantum NOT operation for arbitrary input states of a complex Hilbert space H . Such a quantum NOT operation has to map an arbitrary pure input state $|\phi\rangle \in \mathcal{H}$ onto another pure orthogonal state $|\phi\rangle^{\perp} \in \mathcal{H}$ in such a way that $\langle \phi | \phi^{\perp} \rangle = 0$ holds. An ideal quantum NOT operation has to be antilinear $[5]$ and hence it is not possible to represent its operation by a complete positive quantum operation. In view of this no-go property of quantum mechanics it is of interest to construct quantum operations which approximate quantum NOT operations in the best possible way only for a restricted class of input states.

One of the simplest examples in this context is the construction of an optimal quantum NOT operation for pure twoqubit states of a given degree of entanglement. For this purpose it is convenient first of all to decompose the relevant four-dimensional Hilbert space H of two qubits into the possible classes of pure two-qubit states

$$
\Omega_{\alpha} = \{ (U_1 \otimes U_2)(\alpha | \uparrow\rangle \otimes |\uparrow\rangle + \beta | \downarrow\rangle \otimes |\downarrow\rangle) | U_1, U_2 \in \text{SU}(2) \}
$$
\n(14)

with the same degree of entanglement. Thereby, the parameter α ($0 \le \alpha \le \frac{1}{\sqrt{2}}, \beta = \sqrt{1-\alpha^2}$) characterizes the degree of entanglement of the pure states in a given class Ω_{α} [10,15]. Note that in the special case $\alpha=0$ the two-qubit state is separable (SEP) whereas in the opposite extreme case $\alpha = 1/\sqrt{2}$ it is maximally entangled (ME). We are interested in constructing linear and completely positive quantum processes U_{α} which map an arbitrary pure input state, say $|\phi\rangle \in \Omega_{\alpha}$, in an

FIG. 1. The parameter space of points (V, X, Y) for which the covariant process $\Pi_{V,X,Y}$ is completely positive forms the tetrahedron *ABCD*.

optimal way onto its orthogonal complement, i.e.,

$$
U_{\alpha}: \quad \rho_{in} = |\phi\rangle\langle\phi| \Rightarrow \rho_{out}. \tag{15}
$$

For the solution of this optimization problem a measure is needed that quantifies how close the output state ρ_{out} is to the orthogonal complement of the input state $|\phi\rangle$. Definitely, the Hilbert space of two qubits H is the direct sum of two Hilbert spaces, namely, the span of the vector $|\phi\rangle$, say \mathcal{H}_{ϕ} , and its three-dimensional orthogonal complement $\mathcal{H}_{\phi}^{\perp}$. Therefore, a convenient measure is given by the minimal distance between the output state ρ_{out} and all mixed states contained in the orthogonal complement of the input, i.e.,

$$
D(\rho_{out}|\phi^{\perp}) = \min_{\sigma \in \Gamma(\mathcal{H}_{\phi}^{\perp})} \text{Tr}(\rho_{out} - \sigma)^2.
$$
 (16)

Thereby, $\Gamma(\mathcal{H}_{\phi}^{\perp})$ denotes the linear convex set of all density operators formed by convex sums of pure states of the Hilbert space $\mathcal{H}_{\phi}^{\perp}$. This measure is based on the well-known Hilbert-Schmidt norm for Hilbert-Schmidt operators *A* and *B*, i.e., $||A-B|| = \sqrt{\text{Tr}(A-B)^2}$. We omitted the square root as it is unimportant for our purposes. As shown in Appendix C 1, the minimal distance of (16) can also be expressed in the more convenient form

$$
D(\rho_{out}|\phi^{\perp}) = 2\langle \phi | \rho_{out}^2 | \phi \rangle - \frac{2}{3} \langle \phi | \rho_{out} | \phi \rangle^2. \tag{17}
$$

Correspondingly, the largest achievable distance, i.e.,

$$
\Delta(U_{\alpha}) = \sup_{\phi \in \Omega_{\alpha}} D(\rho_{out} | \phi^{\perp}) = \sup_{\phi \in \Omega_{\alpha}} \left\{ 2 \langle \phi | \rho_{out}^{2} | \phi \rangle - \frac{2}{3} \langle \phi | \rho_{out} | \phi \rangle^{2} \right\},
$$
\n(18)

is a convenient error measure characterizing the quality of the NOT operation for a given class of input states with a given degree of entanglement. This error measure has two important properties (for details see Appendix C 2). First, the positivity of density operators implies that it is zero if and only if the NOT operation is ideal for all input states $|\phi\rangle$ $\in \Omega_{\alpha}$, i.e.,

$$
\Delta(U_{\alpha}) = 0 \quad \Leftrightarrow \sup_{|\phi\rangle \in \Omega_{\alpha}} \langle \phi | \rho_{\text{out}} | \phi \rangle = 0. \tag{19}
$$

Second, this error measure is invariant under the unitary group $U(4)$. For the covariant processes of (11) this implies that the distance $D(\rho_{out}, \phi^{\perp})$ is unbiased with respect to all states from the class Ω_{α} . Thus, for these processes we can omit the supremum in (18) and we can calculate the error as the distance (17) associated with an arbitrarily chosen state of the class Ω_{α} .

Therefore, in general the construction of an optimal quantum NOT operation is equivalent to minimizing the error measure $\Delta(U_\alpha)$ over all possible processes. In the following the resulting optimal error measure will be denoted by Δ_{α} $=\inf_{U_{\alpha}}\Delta(U_{\alpha}).$

1. Noncovariant quantum NOT operations for maximally entangled qubit pairs

Before dealing with the general case let us focus on quantum NOT operations for the special class of maximally entangled pure input states $\Omega_{1/\sqrt{2}}$. In this special case one is able to construct even perfect quantum NOT operations which map an arbitrary pure input state onto a pure output state but which are typically not covariant.

In order to determine the general structure of all physically feasible quantum NOT operations U for ME states let us impose the natural additional requirement that, if the quantum NOT operation U is applied twice the resulting operation is proportional to the identity operator. Therefore, the quantum NOT operation U we are looking for should satisfy the following requirements:

(1) Orthogonality: It maps an arbitrary pure state onto a pure state according to

$$
\langle \phi | \mathcal{U} | \phi \rangle = 0 \quad \forall \, | \phi \rangle \in \Omega_{1/\sqrt{2}}; \tag{20}
$$

(2) unitarity,

$$
\mathcal{U}\mathcal{U}^{\dagger} = I; \tag{21}
$$

(3) cyclic property

$$
\mathcal{U}^2 = \lambda I \quad \text{where} \quad \lambda \in \mathbf{C}.\tag{22}
$$

For our analysis we take advantage of the special basis states (sometimes referred to as the magic base) [13]

$$
|e_1\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle), \quad |e_2\rangle = \frac{i}{\sqrt{2}}(|00\rangle - |11\rangle),
$$

$$
|e_3\rangle = \frac{i}{\sqrt{2}}(|01\rangle + |10\rangle), \quad |e_4\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle),
$$
 (23)

in which all maximally entangled two-qubit states can be written as real-valued linear combinations of these basis states. Clearly, the concurrence of an arbitrary normalized two-qubit superposition state $|\Gamma\rangle = \sum_i \gamma_i |e_i\rangle$ with complex values of γ is given by

$$
C(|\Gamma\rangle\langle\Gamma|) = \left|\sum_{i} \gamma_i^2\right|.\tag{24}
$$

Hence, for ME states this concurrence has to be equal to unity. This happens if and only if all coefficients γ are real valued. In this sense all ME states form a four-dimensional real Hilbert space. Expressing condition (20) in this magic base it turns out that all possible quantum NOT operations form a vector space of real-valued 4×4 antisymmetric matrices. The dimension of this vector space equals 6 and a possible basis is given by the matrices

$$
U_{1} = \begin{pmatrix}\n0 & 1 & 0 & 0 \\
-1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & -1 & 0\n\end{pmatrix},
$$
\n
$$
U_{2} = \begin{pmatrix}\n0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
0 & -1 & 0 & 0 \\
-1 & 0 & 0 & 0\n\end{pmatrix},
$$
\n
$$
U_{3} = \begin{pmatrix}\n0 & 0 & 1 & 0 \\
0 & 0 & 0 & -1 \\
-1 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0\n\end{pmatrix},
$$
\n
$$
V_{1} = \begin{pmatrix}\n0 & 1 & 0 & 0 \\
-1 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 \\
0 & 0 & 1 & 0 \\
0 & 0 & -1 & 0 \\
-1 & 0 & 0 & 0\n\end{pmatrix},
$$
\n
$$
V_{2} = \begin{pmatrix}\n0 & 0 & 0 & 1 \\
0 & 0 & -1 & 0 \\
0 & 1 & 0 & 0 \\
-1 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0\n\end{pmatrix},
$$
\n
$$
V_{3} = \begin{pmatrix}\n0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
-1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0\n\end{pmatrix}.
$$
\n(26)

This set of matrices has the following interesting algebraic properties:

$$
\{U_i, U_j^{\dagger}\} = -\{U_i, U_j\} = 2\delta_{ij}I, \quad U_i^T = -U_i,
$$

$$
U_i U_j = -\delta_{ij}I + \varepsilon_{ijk}U_k,
$$

$$
\{V_i, V_j^{\dagger}\} = -\{V_i, V_j\} = 2\delta_{ij}I, \quad V_i^T = -V_i,
$$

$$
V_i V_j = -\delta_{ij} I + \varepsilon_{ijk} V_k, \quad [U_i, V_j] = 0. \tag{27}
$$

As a consequence every linear operation with the property (20) is a linear superposition of U_i , V_i , i.e.,

$$
\mathcal{U} = \sum_{i=1}^{3} \alpha_i U_i + \beta_i V_i, \quad \alpha_i, \beta_i \in \mathbf{R}.
$$
 (28)

The property (27) and requirement (21) imply the relation

$$
I = UU^{\dagger} = \sum_{i=1}^{3} \alpha_{i}^{2} U_{i} U_{i}^{\dagger} + \beta_{i}^{2} V_{i} V_{i}^{\dagger} + \sum_{(ij)} [\alpha_{i} \alpha_{j} (U_{i} U_{j}^{\dagger} + U_{j}^{\dagger} U_{i})
$$

+ $\beta_{i} \beta_{j} (V_{i} V_{j}^{\dagger} + V_{j}^{\dagger} V_{i}) + \sum_{i,j=1}^{3} \alpha_{i} \beta_{j} (U_{i} V_{j}^{\dagger} + V_{j} U_{i}^{\dagger})$
= $\left(\sum_{i=1}^{3} \alpha_{i}^{2} + \beta_{i}^{2}\right) I - 2 \sum_{i,j=1}^{3} \alpha_{i} \beta_{j} U_{i} V_{j}.$ (29)

Taking into account the structure of the matrices $U_i V_j$ this yields the conditions

$$
\alpha_i \beta_j = 0 \Longrightarrow \begin{cases} \alpha_i = 0 \land \sum_{i=1}^3 \beta_i^2 = 1, \\ \beta_i = 0 \land \sum_{i=1}^3 \alpha_i^2 = 1. \end{cases}
$$
 (30)

The quantum NOT operation satisfying requirements (20) – (22) has the general structure

$$
\left(\mathcal{U} = \sum_{i=1}^{3} \alpha_i U_i \quad \text{with } \sum_{i=1}^{3} \alpha_i^2 = 1, \quad \alpha_i \in \mathbf{R}\right)
$$

$$
\vee \left(\mathcal{U} = \sum_{i=1}^{3} \beta_i V_i \quad \text{with } \sum_{i=1}^{3} \beta_i^2 = 1, \beta_i \in \mathbf{R}\right). \quad (31)
$$

In both cases the condition (22) is satisfied automatically, i.e.,

$$
\mathcal{U}^2 = -I. \tag{32}
$$

Therefore, for maximally entangled two-qubit states the ideal quantum NOT operation is not unique. Its most general form is given by (31) .

2. Optimal covariant quantum NOT operations

Let us construct optimal quantum NOT operations for arbitrary classes of pure two-qubit input states of a given degree of entanglement Ω_{α} . In this case a similar strategy can be used as the one used for the construction of optimal universal quantum copying processes $[12]$. Similarly, it can be shown (for details, see Appendix C 2) that for any optimal quantum NOT operation U_{α} , always an equivalent covariant shown (for details, see Appendix C 2) that for any optimal
quantum NOT operation U_{α} , always an equivalent covariant
quantum process (11), say $\widehat{U_{\alpha}}$, can be found which satisfies the covariance condition (2). Thus, this latter quantum NOT process yields the same optimal error measure Δ_{α} for all possible two-qubit input states $|\phi\rangle \in \Omega_{\alpha}$. This basic observation allows us to restrict our search for the optimal quantum NOT operation for an arbitrary class Ω_{α} to covariant quantum processes of the form of (11) which minimize the error measure (18).

The error measure of the output state (8) with respect to the normalized pure two-qubit input state $|\phi\rangle = \alpha |\uparrow \uparrow \rangle$ $+\beta \downarrow \downarrow$ is given by

$$
\Delta(Z = V + X, Y) = \frac{1}{12} \{ [1 + Z(1 - 4\alpha^2 \beta^2) + Y(1 + 8\alpha^2 \beta^2)]^2 + 6\alpha^2 \beta^2 (1 - 4\alpha^2 \beta^2)(Z - 2Y)^2 \}.
$$
 (33)

In Appendix D it is shown that for all classes of states Ω_{α} all optimal quantum NOT processes are determined by points (V, X, Y) of the triangle *ABC* of Fig. 1. Therefore, for an optimal quantum NOT process the operator K_{00} of the Kraus representation (11) vanishes. Thus, minimizing the quantity (33) with respect to points of the triangle *ABC* yields the final solution. Depending on the value of α two cases can be distinguished. For $\alpha \le \alpha_0$ with α_0

 $=\sqrt{(1-\sqrt{1-4K})}/2 \approx 0.1836$ and $K=(8-3\sqrt{6})/20$ the minimal error

$$
\Delta_{\alpha} = \frac{1}{243} (4 + 160\alpha^2 \beta^2 - 128\alpha^4 \beta^4)
$$
 (34)

is obtained. The resulting optimal quantum NOT operation is independent of the parameter α and is characterized by the point $(V=-\frac{1}{3}, X=-\frac{1}{3}, Y=\frac{1}{9})$. It turns out that this particular optimal quantum NOT process U_{SEP} consists of two one-qubit optimal covariant universal-NOT (UNOT) processes *u*¹ applied to each of the qubits separately, i.e., $U_{SEP} = u^1 \otimes u^1$ with

$$
u^{1}(\rho) = \frac{1}{3}(2I - \rho).
$$
 (35)

These latter optimal one-qubit UNOT quantum processes were studied in detail in [5]. According to (11) a Kraus representation of the optimal two-qubit quantum NOT operation U_{SEP} is given by

$$
U_{SEP}(\rho_{in}) = \sum_{i,j=1}^{3} K_{ij}\rho_{in}K_{ij}^{\dagger} \quad \text{with } K_{ij} = \frac{1}{3}\sigma_i \otimes \sigma_j. \quad (36)
$$

Optimal quantum NOT processes with $\alpha \ge \alpha_0$ yield an error of magnitude

$$
\Delta_{\alpha} = \frac{4\alpha^2 \beta^2 (1 - 4\alpha^2 \beta^2)}{2 + 35\alpha^2 \beta^2 - 100\alpha^4 \beta^4}
$$
(37)

and they are characterized by points (V, X, Y) on the straight line

$$
Y = -\frac{1}{3} \frac{2 - 31\alpha^2 \beta^2 + 20\alpha^4 \beta^4}{-2 - 35\alpha^2 \beta^2 + 100\alpha^4 \beta^4},
$$

\n
$$
X + V = Z = \frac{2}{3} \frac{4 - 29\alpha^2 \beta^2 - 20\alpha^4 \beta^4}{-2 - 35\alpha^2 \beta^2 + 100\alpha^4 \beta^4}, \quad X, V \ge -\frac{1}{3}.
$$

 (38) Each triple of parameters (V, X, Y) from this one-parameter Each triple of parameters (V, A, I) from this one-parameter
line segment defines the Kraus representation (11) of the
optimal two-qubit quantum NOT operation $\widehat{U}_{\alpha}(V)$ for a paroptimal two-qubit quantum NOT operation $\widehat{U}_{\alpha}(V)$ for a particular class of states Ω_{α} .

These considerations show that an ideal covariant two-

qubit quantum NOT process with zero-valued error measure can only be obtained for maximally entangled states. Such a process is characterized by any point (V, X, Y) satisfying the conditions $Y = -\frac{1}{3}$, $X + V = Z = \frac{2}{3}$ $(X, V \ge -\frac{1}{3})$. Therefore, ideal covariant two-qubit quantum NOT processes form a oneparameter family. This reflects the fact that there is a huge class of noncovariant ideal quantum NOT operations (31). Each element U of this class corresponds to some covariant counterpart \hat{U} with the same error (18) (see Appendix C 2). Thus, for maximally entangled states the ideal covariant twoqubit NOT operations are characterized by the parameter range $-\frac{1}{3}$ ≤ *V* ≤ 1. A Kraus representation of these processes is given by

with

$$
K_{0i} = \frac{1}{2} \left(\frac{1}{3} + V \right)^{1/2} \sigma_i \otimes I, \quad K_{i0} = \frac{1}{2} (1 - V)^{1/2} I \otimes \sigma_i.
$$
\n(40)

 $(K_{0i}\rho_{in}K_{0i}^{\dagger} + K_{i0}\rho_{in}K_{i0}^{\dagger})$

, (39)

 $U_{ME}(V)(\rho_{in}) = \sum_{i=1}^{n}$

3

The error Δ_{α} achieves its maximal value for $\alpha^2 \beta^2 = \frac{1}{10}$, i.e., $\alpha_{max} = \sqrt{\frac{1}{2} - \sqrt{\frac{3}{20}}}$. The corresponding maximal error is given by $\Delta_{\alpha_{max}} = \frac{4^{20}}{75}$ and its associated quantum processes are characterized by the points (V, X, Y) with $Y = -\frac{1}{15}$ and $X + V$ $=Z=-\frac{2}{15}$ $(X, V \ge -\frac{1}{3})$. One of the processes satisfying these conditions is the four-dimensional covariant UNOT process \mathcal{G}_{NOT} introduced in Ref. [4]. This particular covariant twoqubit UNOT process minimizes the error with respect to all possible two-qubit pure input states independent of their degree of entanglement. This special process is characterized by the parameters $X=V=Y=-\frac{1}{15}$ and it maps an arbitrary two-qubit input state ρ onto the output state

$$
\rho_{out} = \mathcal{G}_{NOT}(\rho) = \frac{1}{15}(4I - \rho).
$$
 (41)

In summary, the smallest achievable errors Δ_{α} for these optimal covariant two-qubit quantum NOT processes \hat{U}_α are given by

$$
\Delta_{\alpha} = \begin{cases}\n\frac{1}{243}(4 + 160\alpha^2\beta^2 - 128\alpha^4\beta^4), & U_{SEP} = u^1 \otimes u^1 \quad \text{for } \alpha \le \alpha_0, \\
\frac{4\alpha^2\beta^2(1 - 4\alpha^2\beta^2)}{2 + 35\alpha^2\beta^2 - 100\alpha^4\beta^4}, & \widehat{U_{\alpha}}(V) \quad \text{for } \alpha \ge \alpha_0, \\
\frac{4}{75}, & U_{\alpha_{max}} = \mathcal{G}_{\text{NOT}} \quad \text{for } \alpha = \alpha_{max}, \\
0, & U_{ME}(V) \quad \text{for } \alpha = \frac{1}{\sqrt{2}}.\n\end{cases}
$$
\n(42)

Their dependence on the degree of entanglement α is depicted in Fig. 2.

The optimal way to complement two-qubit pure separable states with $\alpha=0$ is to perform one-qubit covariant UNOT quantum operations on each qubit independently. The resulting minimum error for separable states is given by $\Delta_0 = \frac{4}{243}$. This quantum process also yields the minimal error for twoqubit pure states with $\alpha \le \alpha_0$. But the minimum error Δ_{α} increases monotonically with the degree of entanglement up to the critical value $\alpha_0 \approx 0.1836$ with $\Delta_{\alpha_0} \approx 0.0373$. For $\alpha \ge \alpha_0$ the covariant processes $\widehat{U_\alpha}(V)$ are optimal. These pro- $\geq \alpha_0$ the covariant processes $U_\alpha(V)$ are optimal. These processes reach their maximum error at $\alpha_{max} = \sqrt{\frac{1}{2} - \sqrt{\frac{3}{20}}}$ and for maximally entangled states with $\alpha = 1/\sqrt{2}$ the error vanishes.

These results demonstrate that only in the case of ME states is one able to construct ideal covariant quantum NOT processes. This implies that there are no noncovariant ideal quantum NOT processes for nonmaximally entangled pure states. This can be proved indirectly. Suppose that such processes existed. In this case we were able to construct to each ideal noncovariant quantum NOT process a corresponding covariant process (compare with Appendix C 2). However, this is in direct contradiction with our findings. Moreover, this fact also tells us that there is no magic base for sets of states Ω_{α} $(\alpha \neq \frac{1}{\sqrt{2}})$. Only maximally entangled states make up a real subspace of the Hilbert space of two qubits. This emphasizes once more the special character of the set of maximally entangled states in comparison with all other pure entangled states.

IV. GENERAL REPRESENTATION OF UNIVERSAL TWO-QUBIT PROCESSES

Based on the results of Sec. III all possible completely positive covariant two-qubit processes as defined by (11) can be represented by convex combinations of four basic quantum processes which correspond to the corners of the tetrahedron *ABCD* of Fig. 1. For this purpose let us briefly summarize the graphical representation of these completely positive covariant quantum maps. According to the results of Appendix D all optimal two-qubit quantum NOT operations have to be presented by points of the triangle *ABC*. Thereby, point $B=(V=-\frac{1}{3}, X=-\frac{1}{3}, Y=\frac{1}{9})$ characterizes a quantum NOT operation minimizing the error (18) for classes of states Ω_{α} with $\alpha \leq \alpha_0$. Points on straight lines specified by the parameters (38) characterize optimal quantum NOT processes minimizing the error (18) for the classes of states Ω_{α} with α $\geq \alpha_0$. In particular, points with *Y* = − $\frac{1}{3}$, *X* + *V* = *Z* = $\frac{2}{3}$ (*X*, *V* ≥ $-\frac{1}{3}$) define optimal quantum NOT processes for maximally entangled states. The line segments *AD* and *CD* correspond to the restrictions $V=1$ and $X=1$. Therefore, they specify completely positive covariant processes which do not change the reduced density operator of the first or the second qubit. The process corresponding to the point *D* leaves both reduced density operators unchanged. So it represents the identity operations. Furthermore, the processes represented by the points $(A=V=1, X=-\frac{1}{3}, Y=-\frac{1}{3})$ and $(C=V=-\frac{1}{3}, X=1, Y$ $=-\frac{1}{3}$ are ideal covariant quantum NOT operations for maximally entangled states and moreover they do not change the

FIG. 2. The minimum error (18) and the errors of the three relevant UNOT processes and their dependence on the degree of entanglement α . The solid line represents the optimal minimum error. The dashed line U_{SEP} corresponds to an independent application of two one-qubit covariant UNOT operations u^1 to each qubit from the entangled pair. The dash-dotted line U_{ME} corresponds to the ideal covariant UNOT map for maximally entangled states. The dotted line represents the minimum achievable error for an unknown two-qubit pure state if its degree of entanglement is unknown.

reduced density operators of the first and second qubits. Therefore, we have the correspondences

$$
U_{ME}^{(1)} \leftrightarrow A, \quad U_{SEP} \leftrightarrow B, \quad U_{ME}^{(2)} \leftrightarrow C, \quad I \leftrightarrow D. \quad (43)
$$

In terms of these special quantum processes all possible completely positive covariant two-qubit processes can be represented as convex combinations. Thus, a two-qubit quantum operation (1) is completely positive and satisfies the covariance condition (2) if and only if it can be expressed as a linear convex combination of these basic quantum operations, i.e., (43),

$$
\Pi_{a_1, a_2, a_3, a_4} = a_1 I + a_2 U_{SEP} + a_3 U_{ME}^{(1)} + a_4 U_{ME}^{(2)},
$$

\n
$$
a_i \ge 0 \quad \text{and} \quad \sum_{i=1}^4 a_i = 1.
$$
 (44)

V. CONCLUSION

A classification was presented of all possible completely positive covariant two-qubit quantum processes which satisfy the covariance condition (2). It could be shown that any of these processes can be represented by a convex sum of four special covariant two-qubit quantum processes some of which had already been discussed in the literature previously. On the basis of this general classification all possible completely positive covariant quantum processes were constructed that describe quantum NOT operations acting on pure two-qubit states of a particular degree of entanglement in an optimal way. It was shown that for maximally entangled pure

two-qubit input states even an ideal covariant quantum NOT operations can be constructed. Furthermore, for this particular class of input states it is possible to find the general structure of all possible ideal quantum NOT operations.

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APPENDIX A: IRREDUCIBLE TENSOR OPERATORS

In this appendix basic properties of irreducible tensor operators of the group $SU(2)$ are summarized. These irreducible tensor operators are convenient tools for implementing the covariance condition (2).

Rotation properties of quantum states described by the continuous group $O(3)$ or its universal covering group $SU(2)$ are conveniently analyzed by representing the density operator of this quantum state in irreducible tensor components. In terms of orthonormal angular momentum eigenstates *Jm* with −2*J*,−2*J*+1,... *m* ...,2*J*−1,2*J* and *J* being half integer or integer) a set of irreducible tensor operators $T(J_1J_2)_{KQ}$ (with $|J_1-J_2| \le K \le J_1+J_2$ and $-K, -K+1, \ldots$ $\leq q \leq \dots, K-1, K$ is defined by [11,14]

$$
T(J_1, J_2)_{Kq} = \sum_{m_1 m_2} (-1)^{J_1 - m_1} \sqrt{2K + 1} \begin{pmatrix} J_1 & J_2 & K \\ m_1 & -m_2 & -q \end{pmatrix}
$$

 $\times |J_1 m_1\rangle \otimes \langle J_2 m_2|.$ (A1)

The orthogonality and completeness relations of the 3*j* symbol appearing in (A1) imply the orthonormality relations

$$
\operatorname{Tr} [T(J_1, J_2)_{Kq} T(J_1', J_2')_{K'q'}^{\dagger}] = \delta_{J_1 J_1'} \delta_{J_2 J_2'} \delta_{KK'} \delta_{qq'}.
$$
 (A2)

Here, Tr denotes the trace over the Hilbert space spanned by the direct sum of the angular momentum subspaces involved. Therefore, the irreducible tensor operators of $(A1)$ may be viewed as special examples of complete orthogonal sets of operators which have particularly simple transformation properties with respect to the rotation group. These transformation properties are described by the relation

$$
UT(J_1J_2)_{KQ}U^{\dagger} = \sum_{q} T(J_1J_2)_{Kq}D(U)_{qQ}^{(K)},
$$
 (A3)

with $D(U)_{qQ}^{(K)}$ $\binom{K}{a}$ denoting rotation matrix elements [14]. These latter matrix elements satisfy the orthogonality relation

$$
\int D(\gamma \beta \alpha)_{mm'}^{(j)*} D(\gamma \beta \alpha)_{MM'}^{(J)} \sin \beta d\beta d\alpha d\gamma
$$

=
$$
\frac{8 \pi^2}{2J+1} \delta_{jJ} \delta_{mM} \delta_{m'M'}.
$$
 (A4)

Here, α , β , and γ denote the Euler angles characterizing a particular rotation. According to (A3) the quantum numbers J_1, J_2 , and K characterize a particular irreducible representation of the rotation group.

As the tensor operators of (A1) form a complete set any operator including the density operator ρ can be decomposed according to

$$
\rho = \sum_{J_1 J_2 Kq} \text{Tr} \{ T(J_1 J_2)_{Kq}^{\dagger} \rho \} T(J_1 J_2)_{Kq}.
$$
 (A5)

In the special case of two qubits with angular momenta *J* $=\frac{1}{2}$, for example, in such a decomposition the irreducible tensor operators $T(\frac{1}{2}, \frac{1}{2})_{Kq}$ (with $K \in \{0, 1\}$ and $-K \leq q \leq K$) appear for each qubit. Their explicit form is given by (4). Obviously, the set of tensor products of irreducible tensor operators is also a complete set of operators on the two-qubit Hilbert space and we can express an arbitrary two-qubit density operator in the form of (3) . With the help of the relation (A4), finally, it is straightforward to prove that the most general form of an output state satisfying the covariance condition (2) is given by (5) .

APPENDIX B: COMPLETE POSITIVITY

In this appendix the basic steps imposed on covariant two-qubit quantum processes by complete positivity are discussed. This can be done in a convenient way with the help of the theorem of Jamiolkovski and Choi $[17-19]$ whose contents is summarized in the following.

Let *H* be an *n*-dimensional Hilbert space with an inner product, say $\langle \cdot | \cdot \rangle$, and let $\mathcal{B}(H)$ be the associated n^2 -dimensional Hilbert space of linear operators on H whose inner product (\cdot, \cdot) is defined by the relation (A, B) $=Tr(A^{\dagger}B)$ for all $A, B \in \mathcal{B}(H)$. Furthermore, let $\mathcal{L}(H_1, H_2)$ be the vector space of linear transformations from an n_1 -dimensional Hilbert space H_1 to an n_2 -dimensional Hilbert space H_2 and let $I \in \mathcal{L}(\mathcal{B}(H), \mathcal{B}(H))$ denote the linear identity operation acting on $\mathcal{B}(H)$. A linear transformation $T \in \mathcal{L}(\mathcal{B}(H_1), \mathcal{B}(H_2))$ is called completely positive if the tensor product $T \otimes I$ maps an arbitrary positive operator A $\in B(H_1 \otimes H)$ onto a positive operator $B \in B(H_2 \otimes H)$ [1].

The problem of answering the question whether a given linear operation is completely positive or not can be solved with the help of a theorem due to Jamiolkovski and Choi [17–19]. This theorem states the following.

Theorem 1. Let $\{|u_i\rangle\}$ be an arbitrary orthonormal basis in the Hilbert space H_1 and $P_{ij} = |u_i\rangle\langle u_j|$ be the corresponding standard orthonormal basis in the Hilbert space $\mathcal{B}(H_1)$. Then a linear operation $T \in \mathcal{L}(\mathcal{B}(H_1), \mathcal{B}(H_2))$ is completely positive if and only if the linear operator $\mathcal{J}(T) = \sum_{ij} T(P_{ij}) \otimes P_{ij}$ is positive.

With the help of this theorem we can determine for which parameters (V, X, Y) the covariant quantum process $\Pi_{V, X, Y}$ is completely positive. The covariance condition (2) associates an arbitrary input state (6) with the output state (7) . We can express this relation between the input and output states by the linear transformation

$$
\rho_{out} = \Pi_{V,X,Y}(\rho_{in}(\vec{P}, \vec{Q}, \mathcal{M})) = \sum_{i,j=0}^{3} l_{ij}L_{ij}\rho_{in}(\vec{P}, \vec{Q}, \mathcal{M})L_{ij}^{\dagger}
$$
\n(B1)

with

$$
l_{00} = \frac{1}{16}(1 + 3X + 3V + 9Y), \quad l_{i0} = \frac{1}{16}(1 + 3X - V - 3Y),
$$

$$
l_{0i} = \frac{1}{16}(1 + 3V - X - 3Y), \quad l_{ij} = \frac{1}{16}(1 - X - V + Y),
$$
(B2)

and with

$$
L_{00} = I \otimes I, \quad L_{i0} = \sigma_i \otimes I,
$$

$$
L_{0i} = I \otimes \sigma_i, \quad L_{ij} = \sigma_i \otimes \sigma_j.
$$
 (B3)

If $l_{ij} \ge 0$ for all $i, j \in \{x, y, z\}$ the covariant process $\Pi_{V, X, Y}$ is completely positive and the Kraus operators can be written in the form (11) . Therefore the conditions (9) are sufficient to guarantee the complete positivity of the operator Π_{VXY} . That these conditions are also necessary follows from Theorem 1. With the aid of (B1) one can check easily that the eigenvalue spectrum of the operator $\mathcal{J}(\Pi_{V,X,Y}) = \sum_{ij=1}^{4} \Pi_{V,X,Y}(P_{ij}) \otimes P_{ij}$ is given by

$$
\sigma(\mathcal{J}(\Pi_{V,X,Y})) = \left\{ \frac{1}{4} (1 + 3X + 3V + 9Y), \frac{1}{4} (1 + 3X - V - 3Y), \frac{1}{4} (1 - X - V - Y) \right\}
$$

+ Y \left\} (B4)

Hence, the covariant process $\Pi_{V,X,Y}$ is completely positive if and only if the conditions (9) are satisfied.

APPENDIX C: THE ERROR MEASURE AND ITS COVARIANT OPTIMALITY

In this appendix the relation (17) is proved for the error measure and it is shown that this error measure does not depend on the pure two-qubit input state selected but only on its degree of entanglement. Furthermore, for the sake of completeness we recapitulate the proof that whenever there is an optimal quantum NOT operation at all, then there exists also an associated covariant one.

1. Basic properties of the error measure

Let us first of all prove Eq. (17). We start from an arbitrary two-qubit density operator ρ . Let us denote the eigenvectors of its restriction onto the three-dimensional subspace orthogonal to $|\phi\rangle$, $\mathcal{H}_{\phi}^{\perp}$, by $|\phi_1\rangle$, $|\phi_2\rangle$, and $|\phi_3\rangle$. The orthonormal vectors $|\phi\rangle$, $|\phi_1\rangle$, $|\phi_2\rangle$, and $|\phi_3\rangle$ form an orthonormal basis in which this density operator takes the form

$$
\rho = \begin{pmatrix}\n\lambda_1 & \lambda_2 & \lambda_3 & \lambda_4 \\
\lambda_2^* & \beta_1 & 0 & 0 \\
\lambda_3^* & 0 & \beta_2 & 0 \\
\lambda_4^* & 0 & 0 & \beta_3\n\end{pmatrix}
$$
\nwith $\lambda_1 + \sum_{i=1}^3 \beta_i = 1$, $\lambda_1, \beta_i \ge 0$. (C1)

The coefficients λ_i and β_i are restricted by the requirement of positivity of ρ . In this base an arbitrary quantum state that is located entirely in the orthogonal subspace spanned by the states $|\phi_1\rangle$, $|\phi_2\rangle$, and $|\phi_3\rangle$ can be represented by a matrix of the form

$$
\sigma = \begin{pmatrix}\n0 & 0 & 0 & 0 \\
0 & \alpha_{11} & \alpha_{12} & \alpha_{13} \\
0 & \alpha_{12}^* & \alpha_{22} & \alpha_{23} \\
0 & \alpha_{13}^* & \alpha_{23}^* & \alpha_{33}\n\end{pmatrix}
$$
\nwith $\sum_{i=1}^3 \alpha_{ii} = 1$, $\alpha_{ii} \ge 0$. (C2)

Again the coefficients α_{ij} have to be consistent with the positivity of σ . In this notation the measure $D(\rho|\phi^{\perp})$ assumes the form

$$
D(\rho|\phi^{\perp}) = \min_{\sigma \in \Gamma(\mathcal{H}_{\phi}^{\perp})} \text{Tr}(\rho - \sigma)^{2} = \min_{\sigma \in \Gamma(\mathcal{H}_{\phi}^{\perp})} [\text{Tr}(\rho^{2}) - 2\text{Tr}(\rho\sigma)
$$

+
$$
\text{Tr}(\sigma^{2})] = \min_{\sigma \in \Gamma(\mathcal{H}_{\phi}^{\perp})} \left(\text{Tr}(\rho^{2}) - 2\sum_{i=1}^{3} \beta_{i}\alpha_{ii} + \sum_{i=1}^{3} \alpha_{ii}^{2} + 2\sum_{i,j=1; i < j}^{3} |\alpha_{ij}|^{2} \right) = \min_{\sigma \in \text{diag}\Gamma(\mathcal{H}_{\phi}^{\perp})} \left(\text{Tr}(\rho^{2}) - 2\sum_{i=1}^{3} \beta_{i}\alpha_{ii} + \sum_{i=1}^{3} \alpha_{ii}^{2} \right). \tag{C3}
$$

In the last equation we used the fact that the minimum is achieved on the set of density matrices $\Gamma(\mathcal{H}_{\phi}^{\perp})$ which are diagonal in the base $|\phi\rangle$, $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$. The set of these density operators we denoted by diag $\Gamma(\mathcal{H}_{\phi}^{\perp})$. Therefore, the quantity (C3) has to be minimized with respect to nonnegative coefficients α_{ii} constrained by the condition $\sum_{i=1}^{3} \alpha_{ii} = 1$. Using the method of Lagrangian multipliers one obtains the minimum at the point $\alpha_{ii} = \beta_i + \frac{1}{3}\lambda_1$ and its value is given by

$$
D(\rho|\phi^{\perp}) = 2\sum_{i=2}^{4} |\lambda_i|^2 + \frac{4}{3}\lambda_1^2 = 2\sum_{i=2}^{4} |\langle \phi | \rho | \phi_i \rangle|^2 + \frac{4}{3} \langle \phi | \rho | \phi \rangle^2.
$$
 (C4)

This expression can also be rewritten in the equivalent form

$$
D(\rho|\phi^{\perp}) = 2\left(\sum_{i=2}^{4} \langle \phi|\rho|\phi_i\rangle\langle\phi_i|\rho|\phi\rangle + \langle \phi|\rho|\phi\rangle\langle\phi|\rho|\phi\rangle\right) - \frac{2}{3}\langle \phi|\rho|\phi\rangle^2 = 2\langle \phi|\rho^2|\phi\rangle - \frac{2}{3}\langle \phi|\rho|\phi\rangle^2.
$$
 (C5)

This form [compare with (17)] explicitly exhibits the independence of this measure on the diagonalization procedure used in its derivation.

From Eq. (17) it is straightforward to prove that the distance $D(\rho | \phi^{\perp})$ for covariant processes (11) is unbiased with respect to all states from a given class Ω_{α} . Suppose we have an arbitrary covariant process Π and an input state $|\phi\rangle$ $\epsilon \in \Omega_{\alpha}$. We denote its associated output state by ρ_{ϕ} [ρ_{ϕ} $= \Pi(|\phi\rangle\langle\phi|)]$. Let us now take another input state $|\psi\rangle \in \Omega_{\alpha}$ connected with the state $|\phi\rangle$ by a unitary transformation *U* $= U_1 \otimes U_2$ [$U_1, U_2 \in SU(2)$]. The distance $D(\rho_{\psi}, \psi^{\perp})$ between this state and its associated output state $\rho_{\psi} = \Pi(|\psi\rangle\langle\psi|)$ is given by

$$
D(\rho_{\psi}, \psi^{\perp}) = 2\langle \psi | \rho_{\psi}^{2} | \psi \rangle - \frac{2}{3} \langle \psi | \rho_{\psi} | \psi \rangle^{2}
$$

$$
= 2\langle \psi | \Pi (|\psi \rangle \langle \psi|)^{2} | \psi \rangle - \frac{2}{3} \langle \psi | \Pi (|\psi \rangle \langle \psi|) | \psi \rangle^{2}
$$

$$
= 2 \langle \phi | U^{\dagger} \Pi (U | \phi \rangle \langle \phi | U^{\dagger})^{2} U | \phi \rangle
$$

$$
- \frac{2}{3} \langle \phi | U^{\dagger} \Pi (U | \phi \rangle \langle \phi | U^{\dagger}) U | \phi \rangle^{2}.
$$
 (C6)

With the help of the covariance condition (2) this expression can be rewritten in the form

$$
D(\rho_{\psi}, \psi^{\perp}) = 2\langle \phi | U^{\dagger} U \Pi (|\phi\rangle\langle \phi|)^{2} U^{\dagger} U |\phi\rangle - \frac{2}{3} \langle \phi | U^{\dagger} U \Pi (|\phi\rangle)
$$

$$
\times \langle \phi |) U^{\dagger} U |\phi\rangle^{2} = D(\rho_{\phi}, \phi^{\perp}). \tag{C7}
$$

Hence, a covariant quantum operation yields the same error (17) for all states of a given entanglement class Ω_{α} .

2. Optimality of covariant maps

Let us prove the statement that an optimal quantum NOT operation can always be represented by a corresponding covariant quantum map with the same error. This proof is based on the well-known approach used by Werner $\lceil 12 \rceil$ in the context of optimal cloning of arbitrary *d*-dimensional quantum states. The crucial point of this proof is the fact that for an arbitrary and in general noncovariant quantum NOT operation U_{α} acting on two qubits one can define its associated average *U*_{α} acting on two qubits one \widehat{U}_{α} over all group operations

$$
\widehat{U_a}(\rho) = \int dU_1 dU_2 (U_1^{\dagger} \otimes U_2^{\dagger}) U_a (U_1 \otimes U_2 \rho U_1^{\dagger} \otimes U_2^{\dagger}) (U_1
$$

$$
\otimes U_2), \qquad (C8)
$$

where $dU_1 dU_2$ denotes the normalized left invariant Haar measure of the group $SU(2) \otimes SU(2)$. The resulting quantum operation is also an admissible NOT operation and, in addi-

tion, it also satisfies the covariance condition (2). For a quantum NOT operation U_α our error measure reads

$$
\Delta(U_{\alpha}) = \sup_{|\phi\rangle \in \Omega_{\alpha}} D(\rho_{out}|\phi^{\perp}) = \sup_{|\phi\rangle \in \Omega_{\alpha}} \left(2\langle \phi | \rho_{out}^{2} | \phi \rangle - \frac{2}{3} \langle \phi | \rho_{out} | \phi \rangle^{2} \right).
$$
 (C9)

This error is a convex function of the quantum operation *U*. This can be seen by considering a convex combination of two arbitrary two-qubit quantum operations, say V_1 and V_2 , and an arbitrary two-qubit pure input state, say $\sigma = |\phi\rangle\langle\phi|$. The distance $D(\rho_{out} | \phi^{\perp})$ satisfies the inequality

$$
D(\eta V_1(\sigma) + (1 - \eta) V_2(\sigma) | \phi^{\perp}) = \eta D(V_1(\sigma) | \phi^{\perp}) + (1 - \eta) D(V_2(\sigma) | \phi^{\perp}) - \eta (1 - \eta) D(V_1(\sigma) + V_2(\sigma) | \phi^{\perp})
$$

\n
$$
\leq \eta D(V_1(\sigma) | \phi^{\perp}) + (1 - \eta) D(V_2(\sigma) | \phi^{\perp}) \qquad (C10)
$$

and is therefore convex. Our error measure Δ is defined as the supremum of a set of convex expressions in U_{α} and hence is also convex. This implies the inequality

$$
\Delta(\widehat{U_a}) \le \Delta(U_a). \tag{C11}
$$

Therefore, optimal quantum NOT operations which minimize the error can always be found in the form of covariant quantum processes satisfying (2).

APPENDIX D: DETERMINATION OF THE OPTIMAL TWO-QUBIT QUANTUM NOT OPERATION

In this appendix the optimal two-qubit quantum NOT operations are determined for all values of the entanglement parameter $0 \le \alpha \le 1/\sqrt{2}$. For this purpose we have to minimize the error of (33) under the constraints of complete positivity as given by the relations (9) .

Let us first of all consider the case of nonentangled states, i.e., $\alpha = 0$. The lower bound of the error (33) can be derived with the help of inequality (9), i.e., $Y \ge -\frac{1}{9} - \frac{1}{3}(X+V)$, which yields

$$
\Delta(Z = V + X, Y) \ge \frac{4}{3} \left(\frac{1}{6} (Z)(1 - 10\alpha^2 \beta^2) + \frac{2}{9} (1 - \alpha^2 \beta^2) \right)^2.
$$
\n(D1)

Minimizing the right-hand side of inequality (D1) with respect to the parameters *X* and *V* yields the minimal error

$$
\Delta_0 = \frac{4}{243} \tag{D2}
$$

for $X = V = -\frac{1}{3}$. Hence, from relations (9) we obtain the result $Y = \frac{1}{9}$.

The same approach can be used for maximally entangled states with $\alpha = 1/\sqrt{2}$. Now, an estimation of a lower bound can be based on inequality (9) rewritten in the form $X+V$ $\geq -\frac{1}{3} - 3Y$. The resulting lower bound is given by

$$
\Delta(Z = V + X, Y) \ge \frac{4}{3} \left(\frac{1}{6} (1 + 2\alpha^2 \beta^2) + \frac{1}{2} Y(-1 + 10\alpha^2 \beta^2) \right)^2.
$$
\n(D3)

The minimization of this lower bound leads to the minimal error

$$
\Delta_{1/\sqrt{2}} = 0. \tag{D4}
$$

It is achieved for quantum processes characterized by parameters (V, X, Y) which are elements of the line segment $Y =$ $-\frac{1}{3}$, *X* + *V* = *Z* = $-\frac{1}{3}$, and *X* + *V* = $\frac{2}{3}$.

Let us now consider the general case $\alpha \in (0, 1/\sqrt{2})$. Local extrema of relation (33) are determined by the conditions

$$
\frac{\partial \Delta (Z = V + X, Y)}{\partial Z} = 0 \quad \land \quad \frac{\partial \Delta (Z = V + X, Y)}{\partial Y} = 0
$$

$$
\Rightarrow V = X = Y = -\frac{1}{3}.
$$
 (D5)

The point $V = X = Y = -1/3$ at which this local minimum is reached is not contained in the tetrahedron *ABCD*. Therefore, the minimum error has to be attained at points of the triangles which form the surface of the tetrahedron *ABCD*. It can be checked in a straightforward way that the minima for all values of $\alpha \in (0, 1/\sqrt{2})$ are contained in the triangle *ABC*. This latter triangle is defined by the relation *Z*=*X*+*V*=−3*Y* $-\frac{1}{3}$ with $-\frac{1}{3} \le Y \le \frac{1}{9}$ and $-\frac{1}{3} \le X, V \le 1$. With the help of the substitution $Z=-3\tilde{Y}-\frac{1}{3}$ in (33) we obtain a quadratic function of *Y* which is minimal at the point

$$
Y_{min} = -\frac{1}{3} \frac{2 - 31\alpha^2 \beta^2 + 20\alpha^4 \beta^4}{-2 - 35\alpha^2 \beta^2 + 100\alpha^4 \beta^4}.
$$
 (D6)

This condition is valid for all values of $\alpha \in (0, 1/\sqrt{2})$. However, the relation $Y \le 1/9$ is valid only as long as $\alpha \ge \alpha_0$ with $\alpha_0 = \sqrt{(1-\sqrt{1-4K})/2}$ and $K = (8-3\sqrt{6})/20$. The minimal error in the range $\alpha \le \alpha_0$ is achieved by the largest *Y* value satisfying the condition $Y \le 1/9$, i.e., by $Y = 1/9$. As a result we obtain the relation

$$
\Delta_{\alpha} = \begin{cases}\n\frac{1}{243}(4 + 160\alpha^2\beta^2 - 128\alpha^4\beta^4), & Y = \frac{1}{9}, X = V = -\frac{1}{3}, X + V = -3Y - \frac{1}{3} \quad \text{for } \alpha \le \alpha_0, \\
\frac{4\alpha^2\beta^2(1 - 4\alpha^2\beta^2)}{2 + 35\alpha^2\beta^2 - 100\alpha^4\beta^4}, & Y_{min}, X + V = -3Y - \frac{1}{3}, \quad \text{for } \alpha \ge \alpha_0.\n\end{cases}
$$
\n(D7)

From (D7) we can easily determine the value of α for which Δ_{α} is maximal. This happens at $\alpha_{max} = \sqrt{1/2} - \sqrt{3}/20$. The corresponding maximum error is given by $\Delta_{\alpha_{max}} = \frac{4}{75}$ and the

associated optimal quantum NOT operation is characterized by the parameter range *Y* =−1/15, *X*+*V*=−2/15 with −1/3 $\leq X, V \leq 1.$

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