

Maximum-likelihood reconstruction of completely positive maps

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We present a method for the determination of the completely positive (CP) map describing a physical device based on random preparation of the input states, random measurements at the output, and the maximum-likelihood principle. In the numerical implementation the constraint of complete positivity can be imposed by exploiting the isomorphism between linear transformations from Hilbert spaces \mathcal{H} to \mathcal{K} and linear operators in $\mathcal{K} \otimes \mathcal{H}$. The effectiveness of the method is shown on the basis of some examples of reconstruction of CP maps related to quantum communication channels for qubits.

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I. INTRODUCTION

The problem of characterizing a physical device in the quantum domain and of reconstructing input-output relations has been recently addressed in a number of papers [1,2]. These issues are obviously interesting for technological purposes. For example, the practical determination of the transformations acting on quantum states is of great relevance in the new fields of quantum information, computation, and cryptography [3]. In this realm physical objects as optical fibers, parametric amplifiers, directional couplers, C-Not gates, quantum cloning machines, quantum communication channels, etc., should be characterized with very high precision. From the theoretical point of view a physical device is described in terms of a completely positive (CP) map. Hence, an experimental method of reconstructing a CP map would lead to a complete characterization. On the other hand, an effective and reliable technique for the determination of a CP map could allow us to check experimentally the correctness of the theoretical assumptions made in the description of the physical device. Finally, recall that the structure of CP maps naturally emerges in the theory of open systems [4]. It follows that an experimental technique to estimate a CP map also allows us to investigate the interaction between different systems, typically a system-reservoir interaction.

Here in this report we consider the general problem of reconstructing the CP map related to a physical device, without any assumptions on its mathematical form. We propose a method that resembles ordinary tomography for the use of random quantum measurements at the output, but also employs random input states, in order to have the richest statistics. The paper is organized as follows. Section II describes the general method, which is based on (i) the maximum-likelihood principle and (ii) a suitable parametrization of CP maps which is allowed by the isomorphism between linear transformations from Hilbert spaces \mathcal{H} to \mathcal{K} and linear operators in $\mathcal{K} \otimes \mathcal{H}$ [5,6]. Section III shows the application of the method for characterizing quantum communication channels. Section IV is devoted to the conclusions.

II. MEASURING QUANTUM DEVICES

The maximum-likelihood principle says that the best estimation of some unknown parameters is given by the values

that are most likely to generate the data one experimenter observes. Methods based on this principle have been used in the context of phase measurement [7], and to estimate the density matrix [8] and some parameters of interest in quantum optics [2]. The maximum-likelihood principle is quantified by a maximum search of a functional of the unknown parameters that corresponds to (the logarithm of) the theoretical probability of getting the data one has collected. In the following we derive the likelihood functional $\mathcal{L}(\mathcal{E})$ that links the experimental outcomes with the unknown CP map \mathcal{E} that characterizes the device. We consider a sequence of K independent measurements on the output, each described by a POVM $F_l(x_l)$, where x_l denotes the outcome at the l th measurement, and $l = 1, 2, \dots, K$. We denote by ρ_l the state at the input at the l th run. The probability of getting the string of outcomes $\vec{x} = \{x_1, x_2, \dots, x_K\}$ is then given by $p(\vec{x}) = \prod_{l=1}^K \text{Tr}[\mathcal{E}(\rho_l)F_l(x_l)]$. The maximum-likelihood principle states that the best estimate of the map \mathcal{E} maximizes $p(\vec{x})$ over the set of completely positive maps. More conveniently, one can search the maximum of the logarithm, namely, of

$$\mathcal{L}(\mathcal{E}) = \sum_{l=1}^K \ln \text{Tr}[\mathcal{E}(\rho_l)F_l(x_l)]. \quad (1)$$

The likelihood functional $\mathcal{L}(\mathcal{E})$ is concave, and in the present case it is defined on a convex set—the set of CP maps. It follows that the maximum is achieved by a single CP map, or by a closed convex subset of CP maps. In the last case one can infer that the data sample is not sufficiently large, or the set of measurements is not a *quorum* [9].

The maximization problem is constrained by complete positivity and trace-preserving properties of the map \mathcal{E} . A trace-preserving CP map is a linear map from operators in Hilbert space \mathcal{H} [$\dim(\mathcal{H}) = N$] to operators in \mathcal{K} [$\dim(\mathcal{K}) = M$] which can be written equivalently as follows:

$$\mathcal{E}(\rho) = \sum_k A_k \rho A_k^\dagger \quad (2)$$

$$= \text{Tr}_{\mathcal{H}}[(\mathbb{1}_{\mathcal{K}} \otimes \rho^T)S] \quad (3)$$

$$= \sum_{n=1}^{N^2} p_n U_n \rho U_n^\dagger, \quad (4)$$

where

$$\sum_k A_k^\dagger A_k = \mathbb{1}_{\mathcal{H}}, \quad (5)$$

$$S \geq 0 \quad \text{and} \quad \text{Tr}_{\mathcal{K}}[S] = \mathbb{1}_{\mathcal{H}}, \quad (6)$$

$$\text{Tr}[U_i^\dagger U_j] = \delta_{ij} \quad \text{and} \quad \sum_{n=1}^{N^2} p_n U_n^\dagger U_n = \mathbb{1}_{\mathcal{H}}, \quad (7)$$

and T denotes the transposition. Equation (2) is the well-known Kraus decomposition. Equation (3) exploits the isomorphism between linear maps from \mathcal{H} to \mathcal{K} and linear operators on the tensor-product space $\mathcal{K} \otimes \mathcal{H}$ [5,6,10,11]. The operator S can be written in terms of the map \mathcal{E} as follows:

$$S = \sum_{i=1}^{N^2} \mathcal{E}(V_i) \otimes V_i^* \quad (8)$$

where $*$ denotes the complex conjugation, and $\{V_i\}$ is any orthonormal basis for the space of linear operators on \mathcal{H} , namely $\text{Tr}[V_i^\dagger V_j] = \delta_{ij}$, and for any operator O one has $O = \sum_{i=1}^{N^2} \text{Tr}[V_i^\dagger O] V_i$. Notice also that for linearity [10,12] one has $S = \mathcal{E} \otimes \mathbb{1}(|\Psi\rangle\langle\Psi|)$, where $|\Psi\rangle$ represents the (unnormalized) maximally entangled state $|\Psi\rangle = \sum_{n=1}^N |n\rangle|n\rangle$.

Equation (3) can also be written as

$$\mathcal{E}(\rho) = \text{Tr}_{\mathcal{H}}[(\mathbb{1}_{\mathcal{K}} \otimes \rho) S^\Gamma], \quad (9)$$

where Γ denotes the partial transposition in \mathcal{H} , and then

$$S^\Gamma = \sum_{i=1}^{N^2} \mathcal{E}(V_i) \otimes V_i^\dagger. \quad (10)$$

Finally, Eq. (4) can be shown as follows. Chosen as an orthonormal basis $\{V_i\}$, Eq. (2) rewrites $\mathcal{E}(\rho) = \sum_{i,j=1}^{N^2} q_{ij} V_i \rho V_j^\dagger$, with $q_{ij} = \sum_k \text{Tr}[A_k V_i^\dagger] \text{Tr}[A_k V_j]$. The matrix Q with element q_{ij} is positive, and it can be diagonalized $Q = W D W^\dagger$ with W unitary. Then one has

$$\mathcal{E}(\rho) = \sum_{i,j=1}^{N^2} (W D W^\dagger)_{ij} V_i \rho V_j^\dagger = \sum_{n=1}^{N^2} p_n U_n \rho U_n^\dagger, \quad (11)$$

where $p_n = (D)_{nn} \geq 0$ and $\{U_n\}$ is the new orthonormal basis $U_n = \sum_{i,j=1}^{N^2} (W)_{ik} V_i$.

For $\mathcal{H} = \mathcal{K}$ the matrices A_k and U_n are squared. When referring to quantum communication channels, the channel is called bistochastic if also $\sum_k A_k A_k^\dagger = \mathbb{1}_{\mathcal{H}}$. Moreover, operators $\{U_n\}$ in Eq. (4) could be unitary, and in such case the (bistochastic) channel is said to be given by external random fields. For a qubit system ($\mathcal{H} = \mathcal{C}^2$) the set of bistochastic and external-random-field channels coincide [13].

The isomorphism between linear maps and operators established in Eqs. (3)–(8) or (9) and (10) has been useful for the study of positive maps [10,11] and to address the prob-

lem of separability of CP maps [14]. For our task—the maximization of $\mathcal{L}(\mathcal{E})$ —it is also crucial. The condition $S \geq 0$ allows one to write

$$S = C^\dagger C, \quad (12)$$

where C is an upper triangular matrix. Moreover, the diagonal elements of C can be chosen as positive. Such decomposition—referred to as Cholesky decomposition—is commonly used in linear programming [15]. Similarly, one has for the matrices ρ_l^T and the POVM's $F_l(x_l)$

$$\rho_l^T = R_l^\dagger R_l, \quad F_l(x_l) = A_l^\dagger(x_l) A_l(x_l). \quad (13)$$

From Eqs. (3), (12), and (13), the logarithmic-likelihood functional in Eq. (1) rewrites

$$\begin{aligned} \mathcal{L}(\mathcal{E}) &\equiv \mathcal{L}(C) = \sum_{l=1}^K \ln \text{Tr}[C^\dagger C (R_l^\dagger R_l \otimes A_l^\dagger(x_l) A_l(x_l))] \\ &= \sum_{l=1}^K \log \sum_{n,m=1}^{NM} |\langle\langle n|C(R_l^\dagger \otimes A_l^\dagger(x_l))|m\rangle\rangle|^2, \end{aligned} \quad (14)$$

where $\{|n\rangle\rangle\}$ denotes an orthonormal basis for $\mathcal{H} \otimes \mathcal{K}$. The expression obtained in Eq. (14) for the likelihood functional automatically satisfies the constraint of completely positivity. Furthermore, the terms appearing as an argument of the logarithm are explicitly positive, thus assuring the stability of numerical methods to evaluate $\mathcal{L}(C)$.

The trace-preserving condition is given in terms of the matrix S as $\text{Tr}_{\mathcal{K}}[S] = \mathbb{1}_{\mathcal{H}}$. This can be taken into account by using the method of undetermined Lagrange multipliers, then maximizing $\mathcal{L}'(\mathcal{E}) = \mathcal{L}(\mathcal{E}) - \text{Tr}[(\mathbb{1}_{\mathcal{K}} \otimes \mu) S]$, where μ is the undetermined matrix $\mu = \sum_{i,j=1}^N \mu_{ij} |i\rangle\langle j|$. The multipliers μ_{ij} cannot be easily inferred, except the condition $\text{Tr}[\mu] = K$. Writing S in terms of its eigenvectors as $S = \sum_i s_i^2 |s_i\rangle\rangle\langle\langle s_i|$, the maximum likelihood condition $\partial \mathcal{L}'(\mathcal{E}) / \partial s_i = 0$ implies

$$\sum_{i=1}^K \frac{\text{Tr}[(F_l(x_l) \otimes \rho_l) s_i |s_i\rangle\rangle\langle\langle s_i|]}{\text{Tr}[(F_l(x_l) \otimes \rho_l) S]} = \text{Tr}[(\mathbb{1}_{\mathcal{K}} \otimes \mu) s_i |s_i\rangle\rangle\langle\langle s_i|]. \quad (15)$$

Multiplying by s_i and summing over i gives $\text{Tr}[\mu] = K$. However, notice that the constraint $\text{Tr}[S] = N$ that follows from $\text{Tr}_{\mathcal{K}}[S] = \mathbb{1}_{\mathcal{H}}$ isolates a closed convex subset of the set of positive matrices. Hence, the maximum of the concave likelihood functional still remains unique under this looser constraint, and one can check *a posteriori* that the condition $\text{Tr}_{\mathcal{K}}[S] = \mathbb{1}_{\mathcal{H}}$ is fulfilled. The functional we maximize is then

$$\tilde{\mathcal{L}}(C) = \mathcal{L}(C) - \frac{K}{N} \text{Tr}[C^\dagger C], \quad (16)$$

where $\mathcal{L}(C)$ is given in Eq. (14), and the value of the multiplier has been obtained through a derivation similar to Eq. (15). The number of unknown real parameters is given by $(NM)^2$. The problem of maximization of functionals as Eq. (16) enters the realm of programming and numerical algebra optimization, where various techniques are known [15].

III. CHARACTERIZATION OF QUANTUM COMMUNICATION CHANNELS

In the following we show the effectiveness of our method on the basis of some examples of quantum communication channels for qubits, i.e., $\mathcal{H}=\mathcal{K}=\mathcal{C}^2$. In this case $(NM)^2=16$, and for such a relatively small number of parameters one can efficiently apply the method of downhill simplex [15,16] to find the maximum of the logarithmic-likelihood functional. This method has been reliable in the reconstruction of the density matrix of radiation field and spin systems [8]. The results in the following simulations have been obtained using random pure states at the input of the channel, along with a projective measurement in a random direction at the output.

The first example is the Pauli channel for qubits

$$\mathcal{E}_p(\rho) = \sum_{i=1}^4 p_i \sigma_i \rho \sigma_i, \quad (17)$$

where $\sum_{i=1}^4 p_i = 1$, $\sigma_0 \equiv 1$, and σ_i ($i=1,2,3$) denote the customary Pauli matrices. The positive matrix S_p reads

$$S_p = \begin{pmatrix} p_0+p_3 & 0 & 0 & p_0-p_3 \\ 0 & p_1+p_2 & p_1-p_2 & 0 \\ 0 & p_1-p_2 & p_1+p_2 & 0 \\ p_0-p_3 & 0 & 0 & p_0+p_3 \end{pmatrix}, \quad (18)$$

on the lexicographically ordered basis $|00\rangle, |01\rangle, |10\rangle, |11\rangle$, where $|0\rangle$ and $|1\rangle$ corresponds to the eigenstates of σ_z with eigenvalues 1 and -1 , respectively.

In Table I we reported the reconstructed matrix elements of S_p as obtained by a Monte Carlo simulation with $K=30\,000$ runs, for theoretical values $p_0=0.3$, $p_1=0.2$, $p_2=0.4$, and $p_3=0.1$. The trace-preserving property corresponds to the conditions $S_p(1,1)+S_p(3,3)=1$, $S_p(2,2)+S_p(4,4)=1$, and $S_p(1,2)+S_p(3,4)=0$, which are clearly satisfied. The estimated values compare very well with the theoretical ones.

For $p_1=p_2=p_3$ in Eq. (17), one obtains the depolarizing channel

$$\mathcal{E}_d(\rho) = \lambda \rho + \frac{1-\lambda}{2} 1, \quad (19)$$

with $\lambda = 1 - 4p_1$. In Fig. 1 (circles) we reported the statistical error $(\delta\lambda)_{ML}$ in the evaluation of the parameter λ versus the size K of the data sample (with the theoretical value $\lambda = 0.8$). The value of λ_{ML} has been inferred by the complete reconstruction of the matrix S_p . However, notice that one can also implement the maximum-likelihood method upon assuming the form of the CP map as in Eqs. (17) or (19). In such a case the space of parameters is reduced to 4 and 1, respectively. Figure 1 also shows the results obtained by a four-parameters estimation (triangles), thus by assuming an external-random-field channel. As shown by the interpolating line in the picture, in both cases one has an asymptotic

TABLE I. Maximum-likelihood estimation of real and imaginary parts of the matrix elements of S_p related to the Pauli channel in Eq. (17), for theoretical values $p_0=0.3$, $p_1=0.2$, $p_2=0.4$, and $p_3=0.1$. Random pure states and projective measurements along random directions have been used, with $K=30\,000$ runs. We compare the estimated values $S_p^{est}(i,j)$ with the theoretical values $S_p^{th}(i,j)$. The statistical error in the estimation of the matrix elements is around 0.01. For typical values and behavior of the statistical errors, see Fig. 1.

i	j	$S_p^{est}(i,j)$	$S_p^{th}(i,j)$
1	1	(0.388964638,0.)	0.4
1	2	(-0.011561621,-0.0160863415)	0
1	3	(-0.00103390675,-0.0164688228)	0
1	4	(0.188891975,-0.0241343938)	0.2
2	2	(0.617439461,0.)	0.6
2	3	(-0.182118262,0.000703314322)	-0.2
2	4	(-0.00825923682,0.020653044)	0
3	3	(0.606198593,0.)	0.6
3	4	(0.00111897098,0.0150693168)	0.
4	4	(0.389230293,0.)	0.4

inverse square-root dependence of the statistical error on the size of the data sample $(\delta\lambda)_{ML} \propto K^{-1/2}$, in accordance with the central limit theorem.

In the last example we consider a nonbistochastic channel, namely the amplitude damping channel

$$\mathcal{E}_a(\rho) = M_1 \rho M_1 + M_2 \rho M_2 \quad (20)$$

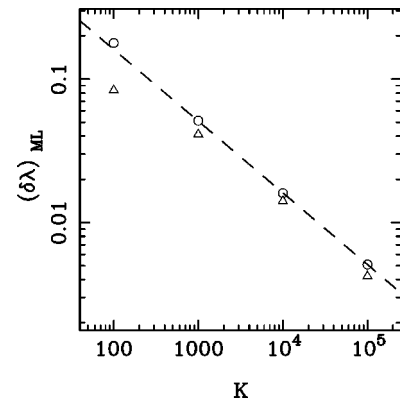


FIG. 1. Maximum-likelihood (ML) estimation of the CP map related to the depolarizing channel. The picture shows the value of the statistical error $(\delta\lambda)_{ML}$ in the estimation of the parameter λ (theoretical value $\lambda = 0.8$) versus the size K of the data sample. Circles referred to a ML reconstruction without assumptions on the form of the CP map; triangles are the results when assuming an external-random-field channel. As shown by the dotted interpolating line, the asymptotic dependence of the statistical error versus K is inverse square-root $(\delta\lambda)_{ML} \propto K^{-1/2}$, as it is demanded by the central limit theorem.

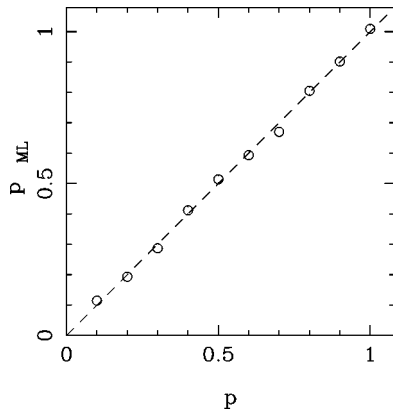


FIG. 2. Maximum-likelihood reconstruction of the CP map describing an amplitude damping channel. The value of the parameter p is inferred by reconstructing the positive matrix S_a in Eq. (22). Random pure states at the input and projection along random directions at the output have been used, with $K = 10\,000$ measurements. The diagonal dotted line represents perfect agreement with the theoretical values.

with

$$M_1 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{p} \end{pmatrix} \quad \text{and} \quad M_2 = \begin{pmatrix} 0 & \sqrt{1-p} \\ 0 & 0 \end{pmatrix}. \quad (21)$$

The corresponding positive matrix S_a writes

$$S_a = \begin{pmatrix} 1 & 0 & 0 & \sqrt{p} \\ 0 & 1-p & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \sqrt{p} & 0 & 0 & p \end{pmatrix}. \quad (22)$$

In Fig. 2 we have plotted the estimated value p_{ML} of parameter p versus its theoretical value, as inferred by the reconstruction of the matrix S_a through $K = 10\,000$ random measurements.

IV. CONCLUSIONS

We have proposed a method for reconstructing the completely positive map related to a physical device, based on the maximum likelihood principle. The method is very general, does not require *a priori* knowledge of the mathematical structure of the CP map, and can be adopted in many fields as quantum optics, spin systems, optical lattices, atoms, etc. We have shown some examples of the reconstruction of CP maps related to quantum communication channels, applying the downhill simplex method for the search of the maximum of the likelihood functional.

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