

## Quantum inference of states and processes

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The maximum-likelihood principle unifies inference of quantum states and processes from experimental noisy data. Particularly, a generic quantum process may be estimated simultaneously with unknown quantum probe states, provided that measurements on probe and transformed probe states are available. Drawbacks of various approximate treatments are also considered.

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### I. INTRODUCTION

The various quantum-state reconstruction techniques developed during recent years have made it possible to completely reconstruct an unknown state of a quantum-mechanical system, provided that many identical copies of the state are available. These reconstruction methods are nowadays routinely applied to the evaluation of the experiments where quantum states are generated, manipulated, and transmitted. The field was pioneered in the beginning of nineties in quantum optics, where the optical homodyne tomography has been devised for reconstruction of the quantum state of traveling light field [1–5]. Since then, many other reconstruction methods, applicable to various physical systems, have been developed [6–18]. The inference of quantum states plays very important role in the present-day experiments [19–22].

Most of the reconstruction methods, such as the direct sampling in optical homodyne tomography, are based on a direct linear inversion of the experimental data. This approach is conceptually simple and feasible. However, it may lead to certain unphysical artifacts such as the negative eigenvalues of the reconstructed density matrix. In order to avoid these unphysical artifacts, an estimation method, based on statistical maximum-likelihood principle, has been devised for the reconstruction of a generic quantum state [23–28]. This approach guarantees the positive semidefiniteness and trace normalization of the reconstructed density matrix. These necessary conditions are incorporated as constraints, i.e., as a certain prior information from the statistical point of view. Remarkably, the maximum likelihood estimation can be interpreted as a genuine generalized quantum measurement [24,26] and can be related to the information gained by optimal measurement and the Fisher information [29].

Given the current interest in the quantum-information processing, it is of paramount importance to reconstruct not only the quantum states but also the transformations of these states—the quantum-mechanical processes. The examination of quantum communication channels and the evaluation of the performance of quantum gates are examples of practical applicability of quantum-process reconstruction [30–37]. All necessary properties of the deterministic quantum transformations, namely, the complete positivity and trace preserva-

tion can be again incorporated within the maximum-likelihood approach as the appropriate constraints [38]. Compared with other reconstruction methods, the maximum-likelihood approach seems to be computationally more difficult. Therefore, several simplifications and approximations of the maximum-likelihood technique have been suggested recently [39,40].

In this paper we present a unified approach to the maximum-likelihood reconstruction of quantum states and quantum processes. Extremal equations for the reconstructed quantum state and for the quantum process are derived in Sec. II. These equations can easily be solved numerically by means of repeated iterations. Particular attention will be paid to the probing of the quantum process by entangled states which attracted considerable attention recently. In Sec. III we consider a realistic scenario where an unknown quantum transformation is probed by unknown states and the measurements are performed on both the input and output states. We propose a method for simultaneous estimation of the unknown probe states and the quantum process from the collected experimental data. The comparison of the exact maximum-likelihood method with the approximate ones is carried out in Sec. IV. Finally, the conclusions are given in Sec. V.

### II. RECONSTRUCTION OF QUANTUM PROCESS

Let us start with a brief review of the maximum-likelihood reconstruction of a quantum state. We assume a finite number  $N$  of identical samples of the physical system, each in the same but unknown quantum state described by the density operator  $\rho$ . Having these systems, our task is to infer the unknown quantum state  $\rho$  from the results of the measurements performed on them. We consider the positive operator-valued measure (POVM) [41]  $\Pi_l$  that yields probabilities  $p_l$  of individual outcomes,

$$p_l = \text{Tr}[\rho \Pi_l], \quad p_l \geq 0, \quad \sum_l p_l = 1. \quad (1)$$

If the POVM  $\Pi_l$  is tomographically complete, it is possible to determine the true state  $\rho$  directly by inverting the linear relations (1) between probabilities  $p_l$  and the elements of density matrix  $\rho$ . However, there is no way to find out the exact probabilities  $p_l$  since only a finite number  $N$  of samples of physical systems can be investigated. In the case of  $N_l$

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occurrences of outcomes  $\Pi_l$ , the relative detection frequencies  $f_l = N_l/N$  represent the only data that could be used for reconstructing the true state  $\rho$ . The maximum-likelihood approach to this reconstruction problem consists in finding a density operator  $\rho_{\text{est}}$  that generates, through Eq. (1), probabilities  $p_l$  that are as close to the observed frequencies  $f_l$  as possible [23,28],

$$\rho_{\text{est}} = \arg \max_{\rho} \mathcal{L}[f_l, p_l(\rho)], \quad (2)$$

$$\mathcal{L}[f_l, p_l(\rho)] = \sum_l f_l \ln p_l. \quad (3)$$

The measure  $\mathcal{L}[f_l, p_l(\rho)]$  of the distance between the probability distribution  $p_l$  and the detected relative frequencies  $f_l$  seems to be arbitrary. However, it can be shown that the reconstruction procedure can be interpreted as a generalized POVM measurement if the log-likelihood measure (3) is used [24,26]. The maximum-likelihood principle has been successfully applied to many problems of quantum-information processing, for example, to reconstruction of the spin state of an electron or polarization state of a photon [25], reconstruction of entangled spin state [28], estimation of quantum measurement [42], design of the optimal discrimination device for communication through a noisy quantum channel [43], and characterization of the universal cloning machine [44].

The challenging problem of maximization (2) of the log-likelihood functional (3) on the space of positive semidefinite operators  $\rho$ ,  $\text{Tr}[\rho] = 1$ , has been treated with the help of the numerical uphill simplex method [27]. A more analytical approach to the problem involves a formulation of nonlinear extremal operator equation for the density matrix that maximizes the log-likelihood functional [23,24,28],

$$\rho = \mu^{-1} R \rho, \quad R = \sum_l \frac{f_l}{p_l} \Pi_l, \quad (4)$$

where the Lagrange multiplier  $\mu$  reads

$$\mu = \text{Tr}[R\rho] = \sum_l f_l = 1. \quad (5)$$

The crucial advantage of Eq. (4) is that it is suitable for iterative solution, as has been demonstrated on many particular reconstruction problems. A combination of Eq. (4) and hermitian conjugate equation leads to the symmetric extremal equations in the manifestly positive semidefinite form [42]

$$\rho = \mu^{-2} R \rho R, \quad \mu = (\text{Tr}[R\rho R])^{1/2}. \quad (6)$$

The iterations

$$\rho^{(n+1)} = \mu^{(n)-2} R^{(n)} \rho^{(n)} R^{(n)} \quad (7)$$

preserve the positive semidefiniteness and trace normalization of the density operator  $\rho$ .

While density operator describes the state of physical system, the linear completely positive (CP) map describes the generic transformation of physical system from quantum state  $\rho_{\text{in}}$  to quantum state  $\rho_{\text{out}}$ . The mathematical formulation of CP maps relies on the isomorphism between linear CP maps  $\mathcal{M}_S$  from operators on the Hilbert space  $\mathcal{H}$  to operators on the Hilbert space  $\mathcal{K}$  and positive semidefinite operators  $S$  on Hilbert space  $\mathcal{H} \otimes \mathcal{K}$  [45–47],

$$\rho_{\text{out}} = \mathcal{M}_S[\rho_{\text{in}}] = \text{Tr}_{\mathcal{H}}[S \rho_{\text{in}}^T \otimes \mathbb{1}_{\mathcal{K}}], \quad (8)$$

where  $\mathbb{1}_{\mathcal{K}}$  is an identity operator on the space  $\mathcal{K}$  and  $T$  denotes the transposition in some fixed basis. The deterministic quantum transformations preserve the trace of the transformed operators,  $\text{Tr}_{\mathcal{K}}[\rho_{\text{out}}] = \text{Tr}_{\mathcal{H}}[\rho_{\text{in}}]$ . Since this must hold for any  $\rho_{\text{in}}$ , operator  $S$  must satisfy the condition

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

where  $\mathbb{1}_{\mathcal{H}}$  is an identity operator on space  $\mathcal{H}$ . Condition (9) effectively represents  $(\dim \mathcal{H})^2$  real constraints.

Making use of formalism (8) we may formulate the exact maximum-likelihood principle for estimated CP map  $S$  in a particularly simple and transparent form, and we can also straightforwardly extend the results obtained in Ref. [38] to the cases when the input and output Hilbert spaces have different dimensions.

Let  $\rho_m$  denote the various input states from space  $\mathcal{H}$ , which are used for the determination of the quantum process. Measurements described by POVMs  $\Pi_{ml}$  are carried out on each corresponding output state from space  $\mathcal{K}$ . Let  $f_{ml}$  denote the relative frequency of detection of the POVM element  $\Pi_{ml}$ . The estimated operator  $S$  should maximize the constrained log-likelihood functional [38,40]

$$\mathcal{L}_c[f_{ml}, p_{ml}(S)] = \sum_{m,l} f_{ml} \ln p_{ml} - \text{Tr}[\Lambda S], \quad (10)$$

$$p_{ml} = \text{Tr}[S \rho_m^T \otimes \Pi_{ml}], \quad (11)$$

where  $\Lambda = \lambda \otimes \mathbb{1}_{\mathcal{K}}$  and  $\lambda$  is the matrix of Lagrange multipliers that account for the trace-preservation condition (9). The extremal equations for  $S$  can be obtained by varying functional (10) with respect to  $S$ ,

$$\mathcal{L}_c[f_{ml}, p_{ml}(S + \delta S)] - \mathcal{L}_c[f_{ml}, p_{ml}(S)] = 0,$$

$$\text{Tr} \left[ \left( \sum_{m,l} \frac{f_{ml}}{p_{ml}} \rho_m^T \otimes \Pi_{ml} - \Lambda \right) \delta S \right] = 0, \quad (12)$$

for all  $\delta S$ , which leads to

$$S = \Lambda^{-1} K S, \quad K = \sum_{m,l} \frac{f_{ml}}{p_{ml}} \rho_m^T \otimes \Pi_{ml}. \quad (13)$$

Further, we have from Eq. (13) that  $S = S K \Lambda^{-1}$ . When we insert this expression in the right-hand side of the first formula in Eq. (13), we finally arrive at symmetrical expression suitable for iterations,

$$S = \Lambda^{-1} KSK \Lambda^{-1}. \quad (14)$$

The Lagrange multiplier  $\lambda$  must be determined from constraint (9). On tracing Eq. (14) over space  $\mathcal{K}$  we obtain quadratic equation for  $\lambda$ , which may be solved as

$$\lambda = (\text{Tr}_{\mathcal{K}}[KSK])^{1/2}. \quad (15)$$

The operator  $\Lambda$  is positive definite because  $KSK$  is positive-definite operator. The system of coupled Eqs. (14) and (15) may be conveniently solved numerically by means of repeated iterations, starting from some unbiased CP map, for example,  $S^{(0)} = \mathbb{1}_{\mathcal{H} \otimes \mathcal{K}} / (\dim \mathcal{K})$ . It is important to note that Eq. (14) preserves the positive semidefiniteness of  $S$  and also constraint  $\text{Tr}_{\mathcal{K}}[S] = \mathbb{1}_{\mathcal{H}}$  is satisfied at each iteration step.

The density matrix  $S$  representing the CP map  $\mathcal{M}_S$  can be, in fact, prepared physically in the laboratory if we first prepare a maximally entangled state on the Hilbert space  $\mathcal{H} \otimes \mathcal{H}$  and then apply a CP map to one part of this entangled state. In this way the quantum-process tomography can be transformed to the quantum-state tomography. More generally, this suggests that it may be useful to employ entangled quantum states as probes of an unknown quantum process [37].

Let  $\rho_{m,AB}$  denote the entangled state on the Hilbert space  $\mathcal{H}_A \otimes \mathcal{H}_B$  that serves as a probe of the CP map  $S$  that is applied to subsystem  $A$ . A joint generalized measurement described by the POVMs  $\Pi_{ml}$  is performed on the output Hilbert space  $\mathcal{K} \otimes \mathcal{H}_B$ . The log-likelihood functional has form (10); only the formula for probability  $p_{ml}$  changes to

$$p_{ml} = \text{Tr}_{\mathcal{H}_A \mathcal{H}_B \mathcal{K}}[(S \otimes \mathbb{1}_{\mathcal{H}_B})(\rho_{m,AB}^{T_A} \otimes \mathbb{1}_{\mathcal{K}})(\mathbb{1}_{\mathcal{H}_A} \otimes \Pi_{ml})], \quad (16)$$

where  $T_A$  stands for the partial transposition in subsystem  $A$ . Consequently, operator  $K$ , appearing in the extremal Eqs. (14) and (15) must be calculated as follows,

$$K = \sum_{m,l} \frac{f_{ml}}{p_{ml}} \text{Tr}_{\mathcal{H}_B}[(\rho_{m,AB}^{T_A} \otimes \mathbb{1}_{\mathcal{K}})(\mathbb{1}_{\mathcal{H}_A} \otimes \Pi_{ml})]. \quad (17)$$

Apart from these modifications of  $p_{ml}$  and  $K$ , one can proceed as before and solve Eqs. (14) and (15) by means of repeated iterations.

### III. QUANTUM-PROCESS MEASUREMENT BY UNKNOWN PROBE QUANTUM STATES

Up to now quantum states and processes have been treated independently. However, this is just a simplification typical of the realm of physical experiments. Widely accepted strategy as to how to approach a complex problem is to specify some partial subproblems, address them separately, and merge the solutions. This technique usually gives good answer in the technical sense. Though this is possible even in quantum theory, there are no fundamental reasons for such a factorization. To consider the full problem without splitting it into isolated subproblems is technically more advanced but could be advantageous. This strategy will be demonstrated on the synthesis of the problems treated sepa-

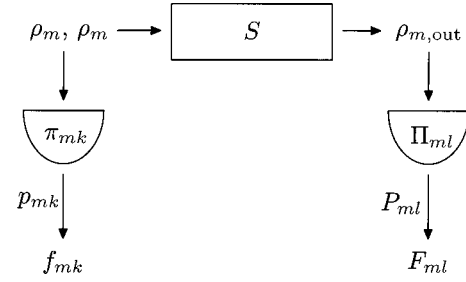


FIG. 1. Scheme of setup for the generalized measurement of quantum process using unknown quantum states as probes.

rately in the preceding section. Let us assume the estimation of the generic process with the help of a set of probe states, identity of which is also unknown. What is only known to the experimentalists is the output of certain measurements performed on the ensemble of probe states and on the ensemble of transformed probe states. In this sense all the considerations are done *ab initio*, since only results of generic measurements are required. A quantum object could be considered as known only to the extent specified by some preceding measurements. All the physically relevant results will be derived exclusively from the acquired data, where input states and their transformation are inseparably involved. States and their transformations should be considered as quantum objects. As such they are affected by quantum fluctuations, since in every experiment a certain portion of the noise will be present on the microscopic level.

In the following, the probe quantum states  $\rho_m$  will be treated as unknown mixed states and they will be inferred together with the unknown quantum process  $S$ . In accordance with the theory presented above, let us consider the set of probe states  $\rho_m$  on space  $\mathcal{H}$ . By means of unknown quantum process  $S$  these states are transformed onto output states  $\rho_{m,out}$  in space  $\mathcal{K}$ . The observation must be more complex now, involving the detection on the ensemble of both the input and the output states. For this purpose, the corresponding POVM elements will be denoted by  $\pi_{mk}$  and  $\Pi_{ml}$ . The diagram involving detected signals and measurements is shown in Fig. 1. Let  $f_{mk}$  denote the relative frequency of detection of the POVM element  $\pi_{mk}$  in the input space  $\mathcal{H}$  and  $F_{ml}$  denotes the relative frequency of detection of the POVM element  $\Pi_{ml}$  in the output space  $\mathcal{K}$ . Frequencies  $f_{mk}$  ( $\sum_k f_{mk} = 1$ ) and  $F_{ml}$  ( $\sum_l F_{ml} = 1$ ) approximate the true probabilities  $p_{mk}$  and  $P_{ml}$  of individual outcomes, respectively,

$$p_{mk} = \text{Tr}_{\mathcal{H}}[\rho_m \pi_{mk}],$$

$$P_{ml} = \text{Tr}_{\mathcal{K}}[\rho_{m,out} \Pi_{ml}] = \text{Tr}[S(\rho_m^T \otimes \Pi_{ml})], \quad (18)$$

where relation (8) was used. The estimated process  $S$  and probe states  $\rho_m$  should maximize the constrained log-likelihood functional

$$\begin{aligned} \mathcal{L}_c = & \sum_{m,k} f_{mk} \ln p_{mk} + \sum_{m,l} F_{ml} \ln P_{ml} - \sum_m \mu_m \text{Tr}[\rho_m] \\ & - \text{Tr}[\Lambda S]. \end{aligned} \quad (19)$$

The additivity of log likelihood reflects the independence of observations performed on the input and output states with the same degree of credibility. The Lagrange multipliers  $\mu_m$  and  $\Lambda = \lambda \otimes \mathbb{1}_{\mathcal{K}}$  fix necessary constraints—the trace normalization of the states,  $\text{Tr}[\rho_m] = 1$ , and the trace-preserving property (9) of process  $S$ .

The coupled extremal equations for the probe states  $\rho_m$  and for process  $S$  can be obtained by varying Eq. (19) with respect to independent variables  $\rho_m$  and  $S$ , which yields

$$\mu_m^{-2} R_m \rho_m R_m = \rho_m, \quad (20)$$

$$\Lambda^{-1} K S K \Lambda^{-1} = S, \quad (21)$$

where

$$R_m = \sum_k \frac{f_{mk}}{p_{mk}} \pi_{mk} + \text{Tr}_{\mathcal{K}} \left[ T_{\mathcal{H}} S \left( \mathbb{1}_{\mathcal{H}} \otimes \sum_l \frac{F_{ml}}{P_{ml}} \Pi_{ml} \right) \right], \quad (22)$$

$$K = \sum_{m,l} \frac{F_{ml}}{P_{ml}} \rho_m^T \otimes \Pi_{ml}, \quad (23)$$

and  $T_{\mathcal{H}}$  is operator of partial transposition in space  $\mathcal{H}$ , acting on space  $\mathcal{H} \otimes \mathcal{K}$ . The Lagrange multipliers can be determined from the appropriate constraints

$$\mu_m = (\text{Tr}_{\mathcal{H}} [R_m \rho_m R_m])^{1/2}, \quad (24)$$

$$\lambda = (\text{Tr}_{\mathcal{K}} [K S K])^{1/2}. \quad (25)$$

All necessary properties of the quantum states  $\rho_m$  and the quantum process  $S$  are satisfied during the iterative solution of the extremal equations (20)–(25).

In the rest of this section we illustrate the developed method on the estimation of a quantum process  $S$  that transforms one qubit state to another one,  $\dim \mathcal{H} = \dim \mathcal{K} = 2$ . The process  $S$  under consideration consists of a unitary  $\pi/4$  rotation in  $xz$  plane of the Bloch space and a subsequent non-unitary damping. The unitary part of the process can be represented by its action on orthogonal states  $|0\rangle$  and  $|1\rangle$  as

$$\begin{aligned} |0\rangle &\rightarrow \cos \theta |0\rangle + \sin \theta |1\rangle, \\ |1\rangle &\rightarrow \cos \theta |1\rangle - \sin \theta |0\rangle, \end{aligned} \quad (26)$$

where  $\theta = \pi/8$ . The nonunitary part of the process is described by operator  $dD + (1-d)E$ , where we chose  $d = 1/2$ . Process  $D = \mathbb{1}_{\mathcal{H} \otimes \mathcal{K}}/2$  is the totally depolarizing channel that maps all states to the maximally mixed state and  $E$  is the identity transformation. We have performed numerical simulations of  $\pi_{mk}$  and  $\Pi_{ml}$  measurements for  $M=20$  input probe states  $\rho_m$  and the corresponding transformed states  $\rho_{m,\text{out}}$ , respectively. The mixed states  $\rho_m$  have been randomly generated. We consider a convenient experimental realization where the same measurements are performed on all input as well as output states. In the present example, this POVM measurement consists of tomographically complete set of projective measurements in  $x$ ,  $y$ , and  $z$  directions, each made on  $N=1000$  identical samples of the probe states  $\rho_m$ , before

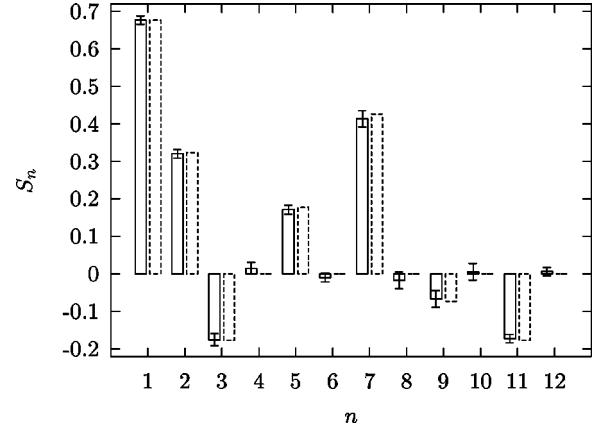


FIG. 2. Elements of the reconstructed quantum process (solid) are compared with the theoretical ones (dashed) for the rotating-damping channel and 20 various probe states.

and after transformation. Therefore, the total number  $6MN$  of the probe states have been used up. Theoretical probabilities  $p_{mk}$  and  $P_{ml}$  have been evaluated according to Eq. (18). They represent mean values of the multinomial distributions of the relative frequencies  $f_{mk}$  and  $F_{ml}$ . Corresponding variances are approximately given by  $p_{mk}(1-p_{mk})/N$  and  $P_{ml}(1-P_{ml})/N$ , respectively. The data  $f_{mk}$  and  $F_{ml}$  have been obtained by means of Monte Carlo simulation. Subsequently, we have iteratively solved extremal equations (20)–(25). Result of this procedure is shown in Fig. 2. Only 12 real independent elements of estimated process are plotted in form of vector  $\{S_n\}_{n=1}^{12}$ . The estimated values are well corresponding to the true ones. For the given fixed process and the POVM measurement we have repeated 10 000 times a simulation of the measurement and reconstruction of the process. Standard deviations of elements of the estimated process have been evaluated over the acquired ensemble and shown in Fig. 2 as appropriate error bars.

The simultaneous reconstruction discussed above yields a higher likelihood of estimated quantum objects than separate reconstructions of probe states and a quantum process. This seems to be a general rule. The likelihood  $\mathcal{L}_{\text{sim}}$  obtained by simultaneous reconstruction (20)–(25) of the quantum process  $S$  and the probe states  $\rho_m$  is always higher than the sum  $\mathcal{L}_{\text{seq}}$  of likelihoods  $\mathcal{L}_{\rho_m}$  obtained by the separate reconstructions (6) of the probe states  $\rho_m$  from data  $f_{mk}$ ,  $F_{ml}$  and likelihood  $\mathcal{L}_S$  of the estimated quantum process  $S$  (14)–(15), where the reconstructed probe states are utilized. Ratio  $\mathcal{L}_{\text{sim}}/\mathcal{L}_{\text{seq}}$ , averaged over an ensemble of possible experimental data, is plotted in Fig. 3 for several numbers of probe states and various numbers  $N$  of measurements. The true process  $S$  and the POVM measurements  $\pi_{mk}$ ,  $\Pi_{ml}$  are the same as in the previous example. A few percent improvement can be obtained by using the proposed simultaneous reconstruction method. For a small number  $N$  of measurements, so in the case of noisy data, the improvement becomes more obvious. The quantitative difference between simultaneous and sequential reconstruction procedures changes to qualitative one for a tomographically incomplete POVM measurement in the input or output space. Data ac-

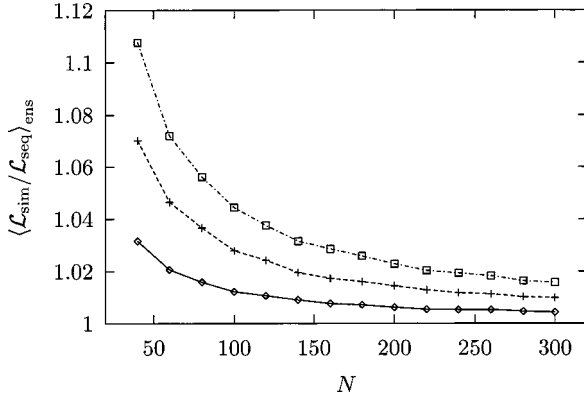


FIG. 3. The average ratio of the likelihood attained by simultaneous reconstruction of a quantum process and probe states and the likelihood attained by sequential one. The process is probed by 15 (diamond), 30 (plus), and 45 (square) quantum states. The ratio increases with the decreasing number  $N$  of measurements or with increasing number of probe states.

quired by such a measurement could be insufficient for the sequential reconstructions, however, they can be sufficient for the simultaneous one. For example, projective measurements in  $x$  and  $y$  directions in the input space and projective measurements in  $y$  and  $z$  directions in the output space represent this case. Thus, the presented simultaneous reconstruction technique is applicable to the problems where routine sequential methods fail.

#### IV. APPROXIMATE METHODS

Recently, approximate reconstruction methods based on the maximum likelihood have been presented. Two ways can be followed to modify the exact maximum-likelihood principle—either simplification of the distance measure (3) [39] or releasing some constraints on quantum states and processes [40].

For a large number  $N$  of identical samples of quantum states available for inspection the relative frequencies  $f_l$  fluctuate around the true values  $p_l$  according to the multidimensional Gaussian distribution that approximates the exact multinomial one,

$$\prod_l p_l^{f_l} \rightarrow \prod_l \exp\left[-\frac{(f_l - p_l)^2}{2\sigma_l^2}\right],$$

$$\sigma_l^2 \approx p_l(1 - p_l)/N. \quad (27)$$

Accordingly, the exact likelihood functional (3) can be replaced by the approximate one [39],

$$\sum_l f_l \ln p_l \rightarrow -\sum_l \frac{(f_l - p_l)^2}{2\sigma_l^2}. \quad (28)$$

The reconstruction based on this functional loses the essence of the generalized measurement, nevertheless, it preserves all physical properties of estimated quantum states. The Gaussian limit of the likelihood method has been recently applied to the reconstruction of polarization-entangled states of light

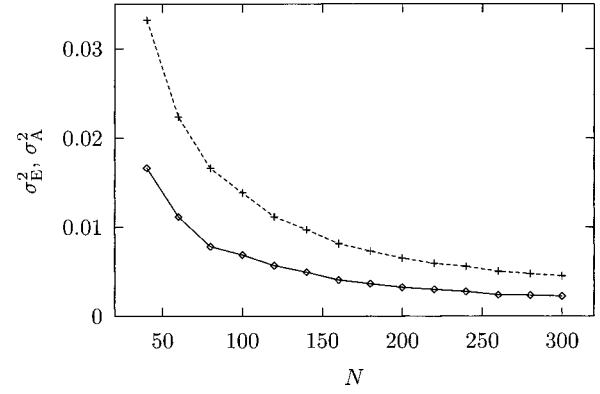


FIG. 4. Variance  $\sigma_E^2$  (diamond) of the exact maximum-likelihood reconstruction of a unitary quantum process and variance  $\sigma_A^2$  (plus) of the approximate one for various numbers  $N$  of measurements.

[48–50]. Unlike this, the approximate reconstruction of quantum processes proposed in Ref. [40] uses the exact likelihood functional (10), however, it decreases the number of constraints incorporated by the Lagrange multipliers. The  $(\dim \mathcal{H})^2$  necessary conditions that guarantee the correct normalization of the estimated process are replaced by a single condition,  $\text{Tr}[S] = \dim \mathcal{H}$ . This is equivalent to assuming that the Lagrange multiplier  $\lambda$  is proportional to identity operator.

In order to compare explicitly the exact maximum-likelihood estimation of quantum process [38] with approximate method presented in Refs. [40,44], we have carried out extensive numerical simulations. Quantitative comparison of the two approaches was based on the variances of estimates  $S_E$  (exact) and  $S_A$  (approximate),

$$\sigma_E^2 = \langle \text{Tr}[(S_E - S_{\text{true}})^2] \rangle_{\text{ens}},$$

$$\sigma_A^2 = \langle \text{Tr}[(S_A - S_{\text{true}})^2] \rangle_{\text{ens}}, \quad (29)$$

where  $\langle \dots \rangle_{\text{ens}}$  denotes averaging over an ensemble of all possible experimental data and  $S_{\text{true}}$  denotes the true CP map. For a given fixed CP map, input states, and output measurements, we have repeated 1000 times a simulation of the measurements and reconstruction of CP maps  $S_E$  and  $S_A$ . Subsequently, we have calculated variances (29) as statistical averages over the acquired ensemble. We have found that the exact maximum-likelihood estimation yields, in all cases, much lower variance than approximate approach. This is a direct consequence of the fact that the exact treatment takes into account all constraints imposed by quantum-mechanical laws on the estimated operator  $S$ . A typical example is shown in Fig. 4. In this case, the quantum process is a unitary transformation (26) of a single qubit. Six different input states are considered—eigenstates of three Pauli matrices  $\sigma_x$ ,  $\sigma_y$ , and  $\sigma_z$ .  $3N$  copies of each input state are used. On each corresponding output state, a spin projection along axes  $x$ ,  $y$ , and  $z$  is measured  $N$  times. As can be seen in Fig. 4, the variance  $\sigma_E^2$  is approximately twice smaller than variance  $\sigma_A^2$ . In fact, for CP maps which do not represent unitary transformations, such as damping channels, the difference may be even stron-

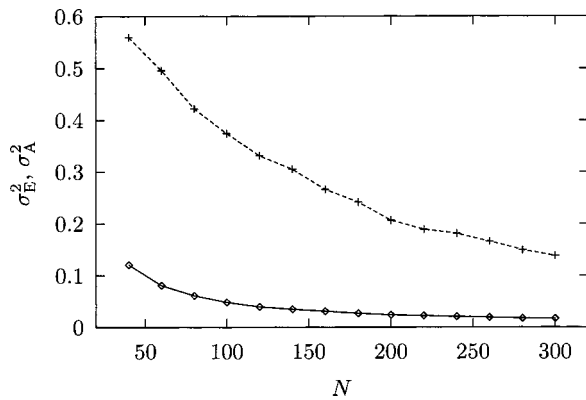


FIG. 5. Variance  $\sigma_E^2$  (diamond) of the exact maximum-likelihood reconstruction of a rotating-damping channel and variance  $\sigma_A^2$  (plus) of the approximate one for various numbers  $N$  of measurements.

ger. The variances  $\sigma_E^2$  and  $\sigma_A^2$  in the case of rotating-damping channel with  $d=3/4$  are shown in Fig. 5.

## V. CONCLUSIONS

The unified approach to inference of quantum states and quantum processes from experimental noisy data has been presented. The proposed technique, based on the maximum-likelihood principle, preserves all properties of the states and

the processes imposed by quantum mechanics. This method is very versatile and can handle data from many different experimental configurations such as the probing of quantum processes with entangled states or a simultaneous reconstruction of an unknown process and unknown states that are used to probe this process. The extremal equations (6), (14), (15), and (20)–(25) for the most likely quantum state and process can be very efficiently solved numerically by means of repeated iterations. The exact maximum likelihood estimation of quantum objects has been compared with the approximate methods. The approximate ones yield estimates whose variance is typically substantially larger than in the case of the exact approach. This comparison clearly illustrates the importance of keeping all the constraints imposed by quantum theory. Loosely speaking, there is always a choice—either to acquire less portion of the data and then to adopt more sophisticated algorithm for its evaluation or vice versa. The efficient and precise reconstruction technique discussed in the present paper can find applications in design and evaluation of quantum-information devices and contemporary quantum experiments with photons as well as with electrons, neutrons, and other objects.

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