Process reconstruction: From unphysical to physical maps via maximum likelihood

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We show that the method of maximum likelihood (MML) provides us with an efficient scheme for the reconstruction of quantum channels from incomplete measurement data. By construction this scheme always results in estimations of channels that are completely positive. Using this property we use the MML for a derivation of physical approximations of unphysical operations. In particular, we analyze the optimal approximation of the universal NOT gate as well as the physical approximation of a quantum nonlinear polarization rotation.

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I. INTRODUCTION

Any quantum dynamics [1,2]—i.e., the process that is described by a completely positive (CP) map of a quantum-mechanical system—can be probed in two different ways. Either we use a single entangled state of a bipartite system [3], or we use a collection of linearly independent single-particle test states [4,5] (forming a basis of the vector space of all Hermitian operators). Given the fragility of entangled states in this paper we will focus our attention on the process reconstruction using only single-particle states.

The task of a process reconstruction is to determine an unknown quantum channel (a "black box") using correlations between known input states and results of measurements performed on these states that have been transformed by the channel (see Fig. 1).

The linearity of quantum dynamics implies that the channel $\mathcal{E}$ is exhaustively described by its action $\varrho_j \to \varrho_j' = \mathcal{E}[\varrho_j]$ on a set of basis states—i.e., a collection of linearly independent states ϱ_j—that play the role of *test states*. Therefore, to perform a reconstruction of the channel $\mathcal{E}$ we have to perform a complete state tomography [1] of ϱ_j'. The number of test states equals d^2, where $d = \dim \mathcal{H}$ is the dimension of the Hilbert space associated with the system. Consequently, in order to reconstruct a channel we have to determine $d^2(d^2-1)$ real parameters—i.e., 12 numbers in the case of qubit $(d=2)$.

In what follows we will assume that test states can be prepared on demand perfectly. Nevertheless, the reconstruction of the channel $\mathcal{E}$ can be affected by the lack of required information due to the following reasons: (i) each test state is represented by a finite ensemble of identically prepared test particles (e.g., qubits), and correspondingly, measurements performed at the output can result in an approximate estimation of transformed test states; (ii) the set of test states is not complete; and (iii) incomplete measurements on transformed test states are performed. In these cases some of the parameters that determine the map $\mathcal{E}$ cannot be deduced from the measured data. In order to accomplish the channel reconstruction additional criteria have to be considered.

In this paper we will pay attention to case (i), which is typical for experiments—one cannot prepare an infinite ensemble of identically prepared particles, so the frequencies of the measured outcomes are only approximations of probability distributions. Consequently, the reconstruction of output states ϱ_j' might lead us to unphysical conclusions about the action of the quantum channel. As a result we can find a negative operator ϱ_j', or a channel $\mathcal{E}$, which is not CP [1,2].

In what follows we will introduce and compare two schemes as to how to perform a single-qubit channel reconstruction with insufficient measurement data. First, we will consider a rather straightforward "regularization" of the reconstructed unphysical map. Second, we will exploit the method of *maximum likelihood* (MML) to perform an estimation of the channel. We will use these methods to perform a reconstruction of single-qubit maps based on numerical simulation of the antiunitary *universal* NOT *operation* (UNOT) [7,9]. This is a linear, but not a CP, map, and we will show how our regularization methods will result in optimal physical approximations of the UNOT operation. We will conclude that the MML is a tool that provides us with approximations of nonphysical operations. In order to demonstrate the power of this approach we will also apply it to obtain an approximation of a nonlinear quantum-mechanical map, the so-called *nonlinear polarization rotation* (NPR) [10].

Our paper is organized as follows: In Sec. II we briefly describe basic properties of single-qubit channels. In Sec. III we show how qubit channels can be estimated and approximated via a simple regularization procedure. We apply this estimation procedure in Sec. IV to derive a physical approximation of the universal NOT gate. In Sec. V we show how the method of maximum likelihood can be applied for an estimation of quantum channels and we rederive the approximation of the universal NOT gate. In Sec. VI we use the MML to approximate the nonlinear polarization rotation of a single qubit. We conclude our paper with some comments on the estimation of two-qubit quantum gates.

II. STRUCTURE OF QUBIT CHANNELS

Quantum channels are described by linear trace-preserving CP maps $\mathcal{E}$ defined on a set of density operators

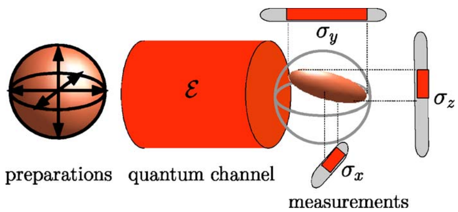

FIG. 1. (Color online) A schematic representation of a reconstruction of a single-qubit channel. Input (test) states of the single-qubit channels are represented by the Bloch sphere (the state space of a single qubit). At the output of the single-qubit channel (modeled as an ellipsoid—i.e., the Bloch sphere that is "deformed" by the action of the channel) a complete measurement of test states is performed. The complete measurement is performed via the projective measurement of σ operators. Based on correlations between input and output states of the test qubits the action of the quantum channel (a CP map) is determined (estimated).

[1,2,11]. The complete positivity is guaranteed if the operator $\Omega_{\mathcal{E}}=\mathcal{E}\otimes\mathcal{I}[P_+]$ is a valid quantum state (P_+ is the projection onto a maximally entangled state). Any qubit channel $\mathcal{E}$ can be imagined as an affine transformation of the three-dimensional Bloch vector $\vec{r}$ (representing a qubit state)—i.e., $\vec{r}\to\vec{r}\,'=T\vec{r}+\vec{t}$, where T is a real 3×3 matrix and $\vec{t}$ is a translation [11]. This form guarantees that the transformation $\mathcal{E}$ is Hermitian and trace preserving. The CP condition defines (nontrivial) constraints on possible values of involved parameters. In fact, the set of all CP trace-preserving maps forms a specific convex subset of all affine transformations. Representing the qubit states by four-dimensional vectors $\vec{v}_\varrho=(1,\vec{r})$, where the first element corresponds to normalization of the state Tr $\varrho=1$, one can express the action of the channel $\mathcal{E}$ in more compact matrix form

$$\mathcal{E}[\varrho]=\begin{pmatrix}1 & \vec{0}\\ \vec{t} & T\end{pmatrix}\begin{pmatrix}1\\ \vec{r}\end{pmatrix}=\begin{pmatrix}1\\ \vec{t}+T\vec{r}\end{pmatrix}. \qquad (1)$$

In other words the qubit channels form 4×4 matrices of the affine form.

The matrix T can be written in the so-called singular-value decomposition—i.e., $T=R_U D R_V$ with R_U,R_V corresponding to orthogonal rotations and $D=\mathrm{diag}\{\lambda_1,\lambda_2,\lambda_3\}$ being diagonal where λ_k are the singular values of T. This means that any map $\mathcal{E}$ is a member of a less-parametric family of maps of the "diagonal form" $\Phi_{\mathcal{E}}$—i.e., $\mathcal{E}[\varrho]=U\Phi_{\mathcal{E}}[V\varrho V^\dagger]U^\dagger$ where U,V are unitary operators. The reduction of parameters is very helpful, and most of the properties (including complete positivity) of $\mathcal{E}$ are reflected by the properties of $\Phi_{\mathcal{E}}$. The map $\mathcal{E}$ is CP only if $\Phi_{\mathcal{E}}$ is. Let us note that $\Phi_{\mathcal{E}}$ is determined not only by the matrix D, but also by a new translation vector $\vec{\tau}=R_U\vec{t}$; i.e., under the action of the map $\Phi_{\mathcal{E}}$ the Bloch sphere transforms as $r_j\to r_j'=\lambda_j r_j+\tau_j$.

A special class of CP maps is composed of the unital maps, which transform the total mixture into itself. In this case $\vec{t}=\vec{\tau}=\vec{0}$, and the corresponding map $\Phi_{\mathcal{E}}$ is uniquely specified by just three real parameters. The positivity of the transformation $\Phi_{\mathcal{E}}$ results in conditions $|\lambda_k|\leqslant 1$, while to fulfill the CP condition we need that to have the four inequalities $|\lambda_1\pm\lambda_2|\leqslant|1\pm\lambda_3|$ be satisfied. These conditions specify a tetrahedron lying inside a cube of all positive unital maps. In this case the extreme points represent four unitary transformations I, σ_x, σ_y, and σ_z (see Fig. 2).

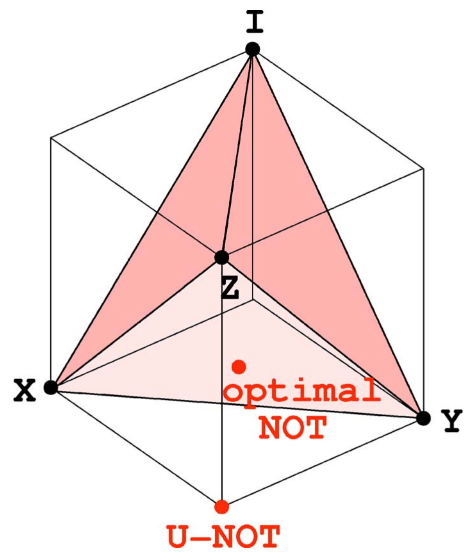

FIG. 2. (Color online) Unital CP maps are embedded in the set of all positive unital maps (cube). The CP maps form a tetrahedron with four unitary transformations in its corners (extremal points), I, x, y, and z, corresponding to the Pauli σ matrices. The unphysical UNOT operation ($\lambda_1=\lambda_2=\lambda_3=-1$) and its optimal completely positive approximation quantum universal NOT gate ($\lambda_1=\lambda_2=\lambda_3=-1/3$) are shown.

III. QUBIT CHANNEL ESTIMATION AND ITS REGULARIZATION

Reconstructions of states and processes share many common features. Therefore we briefly recall basic concepts of the state reconstruction using *finite* ensembles of identically prepared states. In this case one can obtain from estimated mean values of the observable a *negative* density operator of a qubit, $\varrho=\frac{1}{2}(I+\vec{r}\cdot\vec{\sigma})$, with $|\vec{r}|>1$. The reconstructed operator has always unit trace, but the associated vector $\vec{r}$ can point *out* of the Bloch sphere. One can argue that the proper physical state is the closest one to the reconstructed operator—i.e., a pure state with $\vec{r}_c$ pointing into the same direction. Formally it corresponds to a multiplication $\vec{r}$ by some constant k—i.e., $\vec{r}_c=k\vec{r}$ (see, e.g., Ref. [12]). The correction by k can be expressed as

$$\varrho_c=k\varrho+(1-k)\frac{1}{2}I=\frac{1}{2}(I+k\vec{r}\cdot\vec{\sigma}), \qquad (2)$$

and it can be understood as a convex addition of the total mixture $\frac{1}{2}I$ represented by the center of the Bloch sphere—i.e., $\vec{0}=(0,0,0)$. In other words, the correction consists of the addition of completely random and equally distributed events (clicks) to outcome statistics—i.e., an *addition of random noise*.

As we have seen from above, an important role in the state reconstruction is played by the total mixture $\frac{1}{2}I$, which is an average over all possible states. An average over all CP maps is the map $\mathcal{A}$, which transforms the whole state space into the total mixture—i.e., $\mathcal{A}[\varrho]=\frac{1}{2}I$ [13].

The reconstruction of qubit channels consists of the known preparation of (at least) four linearly independent test states ϱ_j and a state reconstruction of the corresponding four output states ϱ_j'. The process estimation based on the correlations $\varrho_j \rightarrow \varrho_j'$ is certainly trace preserving and positive (if all ϱ_j' are positive), though complete positivity might be problematic. The average channel $\mathcal{A}$ can be used to correct ("regularize") improper estimations $\mathcal{E}$ to obtain a CP qubit channel $\mathcal{E}_c$:

$$\mathcal{E}_c = k\mathcal{E} + (1-k)\mathcal{A} = \begin{pmatrix} 1 & \vec{0} \\ k\vec{t} & kT \end{pmatrix}. \tag{3}$$

This method of channel regularization uses the same principle as the method for states; i.e., it is associated with the addition of random noise to the data.

Let us try to estimate what is the critical value of k—i.e., the amount of noise that surely corrects any positive map. Trivially, it is enough to set $k=0$. In this case we completely ignore the measured data and the corrected map is $\mathcal{A}$. However, we are interested in some nontrivial lower bound—i.e., in the largest possible value of k that guarantees complete positivity. Let us consider, for simplicity, that the map under consideration is unital. Then the worst case of a positive map that is not CP is represented by the universal NOT operation.

IV. UNIVERSAL NOT GATE

The logical NOT operation can be generalized into the quantum domain as a unitary transformation $|0\rangle \rightarrow |1\rangle$, $|1\rangle \rightarrow |0\rangle$. However, this map is basis dependent and does not transform all qubit states $|\psi\rangle$ into their (unique) orthogonal complements $|\psi_\perp\rangle$. Such universal NOT ($\mathcal{E}_{\mathrm{NOT}}: |\psi\rangle \rightarrow |\psi_\perp\rangle$) is associated with inversion of the Bloch sphere—i.e., $\vec{r} \rightarrow -\vec{r}$, which is not a CP map. It represents an unphysical transformation specified by $\lambda_1=\lambda_2=\lambda_3=-1$. The distance (see Fig. 2) between this map and the tetrahedron of completely positive maps is extremal; i.e., it is the most unphysical map among linear transformations of a single qubit and can be performed only approximatively. A quantum "machine" that optimally implements an approximation of the universal NOT has been introduced in Refs. [6–8] and experimentally realized by de Martini *et al.* [9]. The machine is represented by a map $\widetilde{\mathcal{E}}_{\mathrm{NOT}}=\mathrm{diag}\{1,-1/3,-1/3,-1/3\}$. The distance [13] between the UNOT and its optimal physical approximation reads

$$d(\widetilde{\mathcal{E}}_{\mathrm{NOT}},\widetilde{\mathcal{E}}_{\mathrm{NOT}}) = \int_{states} \mathrm{d}\varrho \mathrm{Tr}|(\widetilde{\mathcal{E}}_{\mathrm{NOT}} - \widetilde{\mathcal{E}}_{\mathrm{NOT}})[\varrho]| = 1/3. \tag{4}$$

The CP conditions imply that the minimal amount of noise necessary for a regularization of the universal NOT gate corresponds to the value of $k=1/3$—i.e., $\lambda_1=\lambda_2=\lambda_3=-1/3$ (see Fig. 2). The channel representing this point corresponds to the best CP approximation of the universal NOT operation—i.e., to the optimal universal NOT machine originally introduced in Refs. [6–8].

One way how to interpret the "regularization" noise is to assume that the qubit channel is influenced by other quantum systems (the physics behind the dilation theorem [7]).

The reason why we have to consider the noise in a reconstruction of quantum maps is that we deal with incomplete measurement statistics (e.g., test states are represented by finite ensembles). As a result, the reconstructed assignment $\varrho_j \rightarrow \varrho_j' = \mathcal{E}[\varrho_j]$ is determined not only by the properties of the map $\mathcal{E}$ but also by the character of the estimation procedure. In this situation, the map itself can be unphysical, but if we require that the estimation procedure be such that the complete positivity of the estimated map is guaranteed, then the result of the estimation is a physical approximation of an unphysical operation. In order to proceed we assume the method of maximum likelihood.

V. METHOD OF MAXIMUM LIKELIHOOD

The MML is a general estimation scheme [14,15] that has already been considered for the reconstruction of quantum operations from incomplete data. It has been studied by Fiurášek and Hradil [16] and by Sachci [17] (criticized in Ref. [18]). The task of the maximum likelihood in the process reconstruction is to find a map $\mathcal{E}$ for which the *likelihood* is maximal. By definition we assume that the estimated map has to be CP. Let us now briefly describe the principal idea in more detail.

Given the measured data represented by the couples ϱ_k and F_k (ϱ_k is one of the test states and F_k is a positive operator corresponding to the outcome of the measurement used in the kth run of the experiment) the likelihood functional is defined by the formula

$$L(\mathcal{E}) = -\ln \prod_{k=1}^{N} p(k|k) = -\sum_{k=1}^{N} \ln \mathrm{Tr}\mathcal{E}[\varrho_k]F_k, \tag{5}$$

where N is the total number of "clicks" and we used $p(j|k) = \mathrm{Tr}\mathcal{E}[\varrho_k]F_j$ for the conditional probability of using the test state ϱ_k and observe the outcome F_j. The aim is to find a physical map $\mathcal{E}_{est}$ that maximizes this function—i.e., $L(\mathcal{E}_{est}) = \max_{\mathcal{E}} L(\mathcal{E})$. This variational task is usually performed numerically.

Numerical results

Our approach is different from those described in Refs. [16–18] in the way we find the maximum of the functional defined in Eq. (5). The parametrization of $\mathcal{E}$ itself, as defined in Eq. (3), guarantees the trace-preserving condition. Hence only the CP condition must be checked separately during the numerical maximalization. Instead of using the Lagrange multipliers (and increasing thereby the number of parameters for the numerical procedure), we introduce the CP condition as an external boundary for a Nelder-Mead simplex algorithm. The maximalization itself is performed by the Mathematica 5.0 built-in function with the following parameters.

(i) *Method=Nelder Mead.* We chose the *simplex algo-*

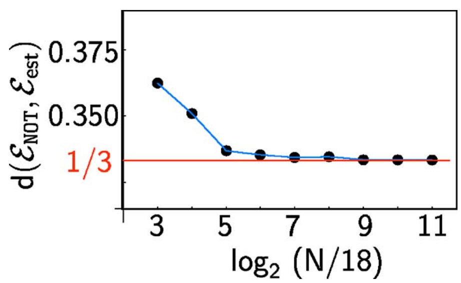

FIG. 3. (Color online) The distance $d(\mathcal{E}_{\mathrm{NOT}},\mathcal{E}_{est})$ as a function of the number of measured outcomes, N, in logarithmic scale. We used six input states (eigenvectors of σ_x, σ_y, and σ_z) and measured σ_x, σ_y, and σ_z. The distance converges to the theoretical value 1/3, which corresponds to the optimal universal NOT.

rithm because it gives the most stable results with the smallest memory requirements.

(ii) *Shrink ratio and contract ratio*=0.95. These parameters are normally taken somewhere around 0.5. Their values close to unity induce a rather slow "cooling" of the process and prevents it from falling into a local maximum. So the global minimum can be determined reliably. The price to pay is usually a longer time of the numerical search.

(iii) *Reflect ratio*=1.5. This parameter is bigger than the standard choice but it helps us to enhance the probability of finding the global maximum.

As an input we use the eigenstates of σ_x, σ_y, and σ_z as the collection of six test states. The data are generated as (random) results of three projective measurements σ_x, σ_y, and σ_z applied in order to perform the output-state reconstruction. In order to analyze the convergence of the method we have performed the reconstruction for a different number of detected events ("clicks") and compare the distance between the original map $\mathcal{E}_{\mathrm{NOT}}$ and the estimated map $\mathcal{E}_{est}$. The result is plotted in Fig. 3, where we can see that the distance converges to 1/3 as calculated in Eq. (4). For $N=100\times 18$ clicks—i.e., each measurement is performed 100 times per particular input state—the algorithm leads us to the map

$$\mathcal{E}_{est}=\begin{pmatrix} 1 & 0 & 0 & 0 \\ -0.0002 & -0.3316 & -0.0074 & 0.0203 \\ 0.0138 & -0.0031 & -0.3334 & 0.0488 \\ -0.0137 & 0.0298 & -0.0117 & -0.3336 \end{pmatrix}, \quad (6)$$

which is very close $[d(\mathcal{E}_{est},\mathcal{E}_{app})=0.0065]$ to the best approximation of the NOT operation—i.e., $\mathcal{E}_{app}=\mathrm{diag}\{1,-1/3,-1/3,-1/3\}$.

We conclude that for large N the MML reconstruction gives us the same result as a theoretical prediction derived in Ref. [7]. From here it follows that the MML helps us not only to estimate the map when just incomplete data are available, but also serves as a tool to derive physical approximations of unphysical maps. The reconstruction procedure guarantees that the estimation and approximation is physical. In order to illustrate the power of this approach we will find an approximation of the nonlinear quantum mechanical transformation that is even "more" unphysical than the linear though antiunitary UNOT operation.

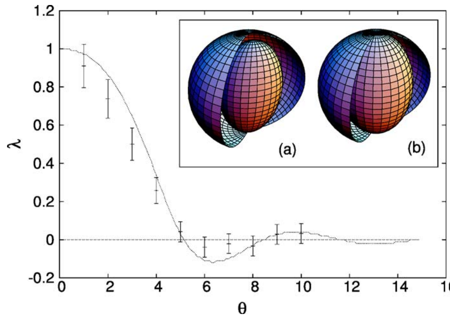

FIG. 4. (Color online) We present analytical as well as numerical results of an approximation of a nonlinear map $\mathcal{E}_\theta$ for different values of the parameter θ (measured in radians). The numerical ("experimental") results shown in the graph in terms of a set of discrete points with error bars are obtained via the MML. The theoretical approximation $\widetilde{\mathcal{E}}_\theta$ of the nonlinear NPR map is characterized by the parameter λ, which is plotted (solid line) in the figure as a function of the parameter θ. In the inset (a) is the Bloch sphere transformation for $\theta=3$ obtained by MML and in (b) the same transformation obtained analytically.

VI. NONLINEAR POLARIZATION ROTATION

Let us consider the nonlinear transformation of a qubit defined by the relation [10]

$$\mathcal{E}_\theta[\varrho]=e^{i(\theta/2)\langle\sigma_z\rangle_\varrho\sigma_z}\varrho e^{-i(\theta/2)\langle\sigma_z\rangle_\varrho\sigma_z}. \quad (7)$$

Unlike the universal NOT this map is nonlinear. Four test states are not sufficient to allow us to determine the action of nonlinear maps. Consequently, the fabricated data must use all possible input states (covering the whole Bloch sphere) as test states, but still we use only three different measurements performed on outcomes that are sufficient for the state reconstruction. We note that a straightforward regularization via the addition of noise cannot result in a CP map unless the original map is not completely suppressed by the noise; i.e., the regularization leads to a trivial result $\mathcal{E}=\mathcal{A}$. However, as we shall see, the maximum likelihood approach gives us a reasonable and nontrivial approximation of the transformation (7).

First, we present an analytic derivation of a physical approximation of $\mathcal{E}_\theta$. This approximation is the closest physical map $\widetilde{\mathcal{E}}_\theta$—i.e., $d(\widetilde{\mathcal{E}}_\theta,\mathcal{E}_\theta)=\min$. The map $\mathcal{E}_\theta$ exhibits two symmetries: the continuous U(1) symmetry (rotations around the z axis) and the discrete σ_x symmetry (rotation around the x axis by π). The physical approximation $\widetilde{\mathcal{E}}_\theta$ should possess these properties as well. Exploiting these symmetries the possible transformations of the Bloch vector are restricted as follows: $x\to\lambda x$, $y\to\lambda y$, and $z\to pz$. In the process of minimalization the parameter p behaves trivially and equals unity. It means that $\widetilde{\mathcal{E}}_\theta$ is of the form $\mathcal{E}_\lambda=\mathrm{diag}\{1,\lambda,\lambda,1\}$. Our task is to minimize the distance $d(\mathcal{E}_\theta,\mathcal{E}_\lambda)=\int d\varrho|\mathcal{E}_\theta[\varrho]-\mathcal{E}_\lambda[\varrho]|$ in order to find the physical approximation $\widetilde{\mathcal{E}}_\theta$—i.e., the functional dependence of λ on θ.

We plot the parameter λ that specifies the best physical approximation of the NPR map in Fig. 4. In the same figure we also present the result of a maximum likelihood estimation of the NPR map based on a finite number of "measurements." Here, for every point (θ), the nonlinear operation was applied to 1800 input states that have been chosen randomly (via a Monte Carlo method). These input states have been transformed according to the nonlinear transformation (7). Subsequently simulations of random projective measurements have been performed. With these "experimental" data a maximization procedure was performed as described in the previous section. The resulting approximation specified by a value of λ (error bars shown in the graph represent the variance in outcomes for subsequent runs with different test states, but the same procedure parameters) transforms the original Bloch sphere as is shown in the inset for particular value $\theta=3$. Figure 4(a) corresponds to the result obtained by MML, and Fig. 4(b) has been obtained via analytic calculations. We see that the original Bloch sphere is transformed into an ellipsoid, one axis of which is significantly longer than the remaining two axes, which are of a comparable length. The mean of these two lengths corresponds to the parameter λ, which specifies the map. We conclude that the MML is in excellent agreement with our analytical calculations.

VII. CONCLUSIONS

In this paper we have shown that the method of maximum likelihood can be efficiently used for derivation of physical approximations of unphysical maps (both non-CP linear maps as well as nonlinear quantum-mechanical transformations). We have applied this method for approximating qubit transformations (the universal NOT gate and the nonlinear polarization rotation). It would be desirable to apply this method for the estimation and approximation of quantum-mechanical maps of higher-dimensional systems (qudits) or multiqubit systems (quantum registers). This would allow us to estimate, approximate, and quantify the performance of multiqubit gates. Unfortunately, quantum channels of d-dimensional systems are parametrized by $d^2(d^2-1)$ parameters and even in the case of a general two-qubit gate the number of parameters that have to be determined is equal to 240, which makes the problem numerically untractable when a totally unknown two-qubit gate is estimated. On the other hand, the number of parameters can be dramatically reduced when some *a priori* information about the action of the gate is available. We will address this problem elsewhere.

In our paper we have considered that the input states of test particles are prepared perfectly; i.e., the action of the initial-state preparator is totally known. Certainly, this is an approximation of a real situation, when test states are prepared with finite precision. This additional source of uncertainty has to be taken into account in realistic estimation procedures of quantum channels.

ACKNOWLEDGMENTS

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