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Iterative algorithm for reconstruction of entangled states

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An iterative algorithm for the reconstruction of an unknown quantum state from the results of incompatible measurements is proposed. It consists of an expectation-maximization step followed by a unitary transformation of the eigenbasis of the density matrix. The procedure has been applied to the reconstruction of the entangled pair of photons.

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Predictions of advanced theories are more and more complex and more and more accurate. This may be recognized in the recent progress of quantum theory. In many applications, there is a need to determine the quantum state of the system. For this purpose, the quantum tomography has been developed. There is an extended bibliography concerning this topic covering various fields of possible applications [1]. However, all the varied and precise experiments that have been carried out over many years and that rely on quantum physics have not needed the total amount of information coded in the quantum state. This fact is reflected in the standard treatment of quantum tomography. When the standard quantum tomography is adopted for reconstruction of the state from realistic noisy data, one often runs into unphysical results. Standard methods are also known to be prone to the creation of various artifacts in the reconstructed state. All these flaws are usually paid little or no attention in the scientific literature. They are simply being regarded as unavoidable errors of reconstructions, which fall within the corresponding ''error bars.'' Here we would like to stress that the mentioned drawbacks of the standard tomographic techniques are actually much more serious, especially if the reconstructed state is to be of further use. This seems to be crucial for the potential application in quantum information. To quantify a fragile effect of entanglement, various entropic principles are used [2]. This feature is sensitive to semipositive definiteness of the reconstructed state—a necessary condition of successful reconstruction.

The purpose of this Rapid Communication is twofold. At first a simple iterative algorithm for maximum-likelihood (ML) estimation of the quantum state resembling ''climbing the hill of the likelihood'' will be derived. This result may be easily implemented numerically, and interpreted in quantum theory as generalized measurement. The algorithm will be illustrated for the example of reconstruction of an entangled state, representing an important example in quantum information processing.

Let us illustrate the motivation of quantum tomography considering the repeated measurement. Assume that we are given a finite number N of identical samples of the system, each in the same but unknown quantum state described by the density operator ρ. Given those systems, our task is to identify the unknown *true* state ρ from the results of measurements performed on them as accurately as possible. For simplicity, we will assume sharp measurements in the sense of von Neumann. As a result of each measurement, the state of the input system is projected into a pure state, which is the reading of the measuring apparatus. Let us assume, for concreteness, that M different outcomes of measurements have been observed. The relative frequencies f_j of occurrences of the observed results

$$\{|y_j\rangle\langle y_j|\}, \quad j=1,\ldots,M, \tag{1}$$

then comprise the data that the true state ρ should be inferred from. For the sake of simplicity, the measurement performed will be assumed as complete, i.e.,

$$H\equiv\sum_j \{|y_j\rangle\langle y_j|\}=1.$$

This condition will be released later to the case of incomplete measurements.

The probabilities of occurrences of various outcomes are generated by the true quantum state ρ according to the well-known handy quantum rule

$$p_j=\langle y_j|\rho|y_j\rangle. \tag{2}$$

If the probabilities p_j of getting a sufficient number of different outcomes $|y_j\rangle$ were known, it would be possible to determine the true state ρ directly by inverting the linear relation (2). This is the philosophy behind the ''standard'' quantum tomographic techniques. For example, in the rather trivial case of a spin one-half particle, the probabilities of getting three linearly independent projectors determine the unknown state uniquely. Here, however, a serious problem arises. Since only a finite number of systems can be investigated, there is no way how to find out these probabilities. The only data one has at disposal are the relative frequencies f_j, which sample the *principally* unknowable probabilities p_j. It is obvious that for a small number of runs the true probabilities p_j and the corresponding detected frequencies f_j may differ substantially. As a result of this, the modified realistic problem

$$f_j=\langle y_j|\rho|y_j\rangle \tag{3}$$

has generally no solution on the space of semipositive definite Hermitian operators describing physical states. Tomog-

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raphic methods based on the averaging of pattern functions; see, e.g., [1], are typical examples of linear methods that suffer from the above mentioned drawbacks.

Probabilistic interpretation of quantum theory suggests that a sort of statistical treatment of the observed data might be more natural and appropriate than the deterministic treatment described above. The philosophy of the proposed reconstruction method differs from the philosophy of standard methods. The basic question of the standard methods: ''What quantum state is determined by the measured data?'' is replaced by a more modest one: ''What quantum state is most likely in view of the measured data?''; this seems to be in accordance with the probabilistic interpretation of the quantum theory [3,4]. More specifically, instead of trying to invert the linear relation (3), we look for a density operator ρ_e that generates through Eq. (2) probabilities p_j that are as ''close'' to the observed frequencies f_j as possible. That is, we look for ρ_e that minimizes some measure of distance $d[\mathbf{f},\mathbf{p}(\rho)]$ between probabilities $\mathbf{p}$ and data $\mathbf{f}$.

At first sight it might seem that there is no reason to *prefer* one particular metric to another one—different metrics leading to different results. This ambiguity can be resolved by considering the formal description of the reconstruction process [5]. If the whole measurement and subsequent reconstruction are looked at as a single generalized measurement, then the *relation* between the actually performed measurement and resulting probability operator measure becomes particularly simple and easy to interpret for the metric known as the relative entropy or Kullback-Leibler divergence [6]:

$$d[\mathbf{f},\mathbf{p}] = -\sum_j f_j \ln p_j . \tag{4}$$

Adopting the metric (4) is equivalent to finding the maxima of the likelihood functional

$$\mathcal{L}(\rho) = \prod_j \langle y_j|\rho|y_j\rangle^{f_j}. \tag{5}$$

Thus we are led to the maximum-likelihood principle as the preferred way of doing the quantum state reconstruction.

ML methods are well known in the field of inverse problems and they have found many applications in reconstructions and estimations so far [7]. Unfortunately, except in the simplest cases, the maximization of the likelihood functional is a challenging problem on its own. A necessary condition for an extreme of the likelihood functional (5) can be derived in the form of the nonlinear operator equation for the density matrix ρ [3,8] and this equation may be interpreted as the closure relation for a quantum measurement. In the classical signal processing, an important role is played by the so-called linear and positive (LP) problems [9]. Since these are closely related to the problem of quantum state reconstruction, it is worthwhile to recall how the positive and linear problems can be dealt with using the ML approach.

Let us consider that the probabilities p_j of getting outcomes y_j are given by the following linear and positive relation:

$$p_j = \sum_i r_i h_{ij}, \quad \mathbf{p},\mathbf{r},\mathbf{h} > \mathbf{0}. \tag{6}$$

Here $\mathbf{r}$ is the vector describing the ''state'' of the system. For example, the reconstruction of a one-dimensional object from the noiseless detection of its blurred image could be accomplished by inverting the relation (6), where $\mathbf{r}$ and $\mathbf{p}$ would be the normalized intensities of the object and image, and $\mathbf{h}$ would describe the blurring mechanism. Again, here the presence of noise ($f_j \neq p_j$) tends to spoil the positivity of the reconstructed intensity $\mathbf{r}$.

The solution to LP problems in the sense of ML can be found using the expectation-maximization (EM) algorithm [9]. In the case of the discrete one-dimensional problem (6), the unknown object $\mathbf{r}$ is reconstructed by means of the following iterative algorithm [9]:

$$r_i^{(n)} = r_i^{(n-1)} \sum_j \frac{h_{ij} f_j}{p_j(\mathbf{r}^{(n-1)})}, \tag{7}$$

which is initialized with a positive vector $\mathbf{r}$ ($r_i > 0\ \forall i$).

The iterative algorithm (7) for solving the LP problems is convenient from the point of view of the numerical analysis. It is certainly much more convenient than the direct multidimensional maximization of the corresponding ML functional $\ln \mathcal{L} = \Sigma_j f_j \ln p_j$ [10]. This brings us back to the problem of quantum state reconstruction. It would be nice to have a similar iterative algorithm for dealing with the problem (3) [or equivalently for maximizing the ML functional (5)]. On the one hand, it is clear that the problem of quantum state reconstruction is not a linear *and* positive problem, since the quantum rule (2) cannot be rewritten in the form of Eq. (6) with a known positive kernel $\mathbf{h}$. As a consequence of this, the EM algorithm cannot be straightforwardly applied here. On the other hand, the reconstruction of the elements of the density matrix becomes a LP problem if the eigenbasis diagonalizing the density matrix is known. In this case, the unknown density matrix can be parametrized as follows:

$$\rho = \sum_k r_k |\phi_k\rangle\langle\phi_k|, \quad \rho|\phi_k\rangle = r_k|\phi_k\rangle, \tag{8}$$

where r_i are eigenvalues of ρ, the only parameters that remain to be determined from the performed measurement. Using the parametrization (8), the quantum rule (2) may be easily rewritten to the form of the LP problem Eq. (6).

This hints at splitting the quantum state reconstruction into two subsequent steps: the reconstruction of the eigenvectors of ρ in a fixed basis, which represents the classical part of the problem, followed by the ''rotation'' of the basis $\{|\phi_i\rangle\}$ in the ''right'' direction using the unitary transformation

$$|\phi_k'\rangle\langle\phi_k'| = U|\phi_k\rangle\langle\phi_k|U^\dagger. \tag{9}$$

Its infinitesimal form reads

$$U \equiv e^{i\epsilon G} \approx 1 + i\epsilon G. \tag{10}$$

Here G is a Hermitian generator of the unitary transformation and ϵ is a positive real number that is small enough to make the second equality in Eq. (10) approximately satisfied.

Consider now the total change of log likelihood caused by the change of diagonal elements of the density matrix and the rotation of the basis. Keeping the normalization condition $\mathrm{Tr}\,\rho=1$, the first-order contribution to the variation reads

$$\delta \ln \mathcal{L}=\sum_k \delta r_k(\langle \phi_k|R|\phi_k\rangle-1)+i\epsilon\,\mathrm{Tr}\{G[\rho,R]\}. \tag{11}$$

The operator R appearing here plays an important role in this treatment. It is a semipositively definite Hermitian operator comprising results of the measurement

$$R=\sum_j \frac{f_j}{p_j}|y_j\rangle\langle y_j|. \tag{12}$$

Notice that this operator depends on the old density matrix ρ through Eq. (2).

Inspection of Eq. (11) reveals a simple strategy on how to make the likelihood of the new state ρ' as high as possible [within limits of the validity of the linearization (10), of course]. In the first step, the first term on the right-hand side of Eq. (11) is maximized by estimating the eigenvalues of the density matrix, keeping its eigenvectors $|\phi_k\rangle$ constant. The iterative algorithm (7) described above can be straightforwardly applied to this LP problem. In the second step, the likelihood can further be increased by making the second term on the right-hand side of Eq. (11) positive. This is accomplished by a suitable choice of the generator of the unitary transformation (10). Remembering the norm induced by the scalar product defined on the space of operators, $(A,B)=\mathrm{Tr}\{A^\dagger B\}$, the generator G may be chosen as

$$G=i[\rho,R]. \tag{13}$$

Its form guarantees the non-negativity of the contribution to the likelihood and is optimal in the sense of the above introduced scalar product. Notice that this derivation holds only if the second-order contribution in ϵ to Eqs. (10) and (11) is negligible. From this an upper bound on the value of ϵ can be derived. ϵ can then be adaptively changed in each U step in order to minimize the computing time.

Now we have at our disposal all ingredients comprising the expectation-maximization algorithm followed by a unitary transformation (EMU) quantum state reconstruction algorithm that represents the main result of the present article. Starting from some positive initial density matrix ρ, this estimate is improved, first by finding new eigenvalues using the EM iterative algorithm (7), and then again by finding new eigenvectors by unitarily (U) transforming the old ones according to Eqs. (9), (10), and (13). These two steps are repeated. Continued repetition of the two steps, each monotonically increasing the likelihood of the current estimate, resembles climbing a hill. Convexity of the likelihood functional (5), $\mathcal{L}(\alpha\rho_1+(1-\alpha)\rho_2)\geqslant\alpha\mathcal{L}(\rho_1)+(1-\alpha)\mathcal{L}(\rho_2)$, $\alpha\in\langle 0,1\rangle$, guarantees that the global maximum is always attained.

The proposed EMU algorithm naturally leads to the previously introduced extremal equation for the density matrix [3,8]. The stationary point of the EMU algorithm is characterized by the vanishing variation of the log likelihood (11). Since the variations $\delta r_k,\epsilon$ are arbitrary parameters, this is equivalent to the Lagrange-Euler equation for density matrix

$$R\rho_e=\rho_e. \tag{14}$$

This nonlinear operator equation has recently been derived using the variational principle in Ref. [8] and using inequalities [3], and has been applied to the reconstruction of the state of a two-state system [11]. The iterative algorithm presented there, however, relied on a special parametrization and was not suitable for generalization. The EMU algorithm presented here provides us with a different route to Eq. (14), which is perhaps more appealing from the physical point of view, and suitable for implementation of the numerical algorithm. Notice, however, that this ''parameter estimation'' may be interpreted as a generalized measurement, since $R=1$ on the space where the reconstruction has been done.

These results should be modified in the case of incomplete detection. Provided that $H\neq 1$, the closure relation may be always recovered in the form

$$\sum_j H^{-1/2}\{|y_j\rangle\langle y_j|\}H^{-1/2}\equiv 1. \tag{15}$$

This corresponds to the renormalization of the probabilities $p_j=\langle y_j|\rho|y_j\rangle$ in the likelihood (5) to the normalized probabilities $p_j\rightarrow p_j/\Sigma_i p_i$. This formulation incorporates the case of incomplete detection. Notice that the extremal equation again possesses the form of Eq. (14) for the renormalized quantities $R\rightarrow R'=(H')^{-1/2}R(H')^{-1/2}$, $\rho_e\rightarrow\rho_e'=(H')^{1/2}\rho_e(H')^{1/2}$, $H'=\Sigma_j\{|y_j\rangle\langle y_j|\}/\Sigma_j p_j$. All the conclusions derived for complete measurements may be extended to this case of incomplete measurement as well. This formulation coincides with the estimation, provided that an assumption of Poissonian statistics is used. Assume that n_i samples the mean number of particles np_i, where p_i is as before the prediction of quantum theory for detection of the ith channel and n is the unknown mean number of particles. The relevant part of the log likelihood corresponding to the Poissonian statistics reads $\ln\mathcal{L}\propto\Sigma_i n_i\ln(np_i)-n\Sigma_i p_i$. The extremal equation for n may be easily formulated as the condition $n=\Sigma_i n_i/\Sigma_i p_i$. Inserting this estimate of unknown mean number of Poissonian particles into the log likelihood reproduces the renormalized likelihood function.

The proposed EMU algorithm has been applied to the reconstruction of the two-photon entangled state generated by the spontaneous downconversion source of White *et al.* [12]. White *et al.* measured the nominal Bell state $(|HH\rangle+|VV\rangle)/\sqrt{2}$ along 16 distinct directions: $\{|y_j\rangle\}=\{|HH\rangle, |HV\rangle, |VH\rangle, |VV\rangle, |HD\rangle, |HL\rangle, |DH\rangle, |RH\rangle, |DD\rangle, |RD\rangle, |RL\rangle, |DR\rangle, |DV\rangle, |RV\rangle, |VD\rangle, |VL\rangle\}$; H, V, D, R, and L being horizontal, vertical, diagonal, right circular, and

TABLE I. Eigenvectors of the reconstructed density matrix.

	$\|\phi_1\rangle$	$\|\phi_2\rangle$
$\|VV\rangle$	$0.696-0.027i$	$0.630+0.071i$
$\|VH\rangle$	$-0.050-0.020i$	$-0.284+0.174i$
$\|HV\rangle$	$-0.040+0.015i$	$-0.150-0.247i$
$\|HH\rangle$	$0.712-0.062i$	$-0.634-0.035i$

left circular polarization, respectively. Counted numbers of coincidences along these directions can be found in [12].

We have used the experimental data together with the proposed algorithm to reconstruct the *true* state generated by the source of entangled photon pairs. Due to various sources of errors, the true state is expected to differ from the nominal state. Notice that the chosen measurements are not complete, that is, $\Sigma_j |y_j\rangle\langle y_j|$ does not represent the resolution of unity. This has been taken into account.

Starting from the maximally mixed state $(|HH\rangle\langle HH|+|VV\rangle\langle VV|+|HV\rangle\langle HV|+|VH\rangle\langle VH|)/4$, new eigenvalues and eigenvectors of the density matrix are found using Eqs. (7) and (9). This has been repeated until a stationary point of the iteration process has been attained. The diagonal representation of the reconstructed density matrix reads

$$\rho_e^{\mathrm{ML}} = 0.962\,|\phi_1\rangle\langle\phi_1| + 0.038\,|\phi_2\rangle\langle\phi_2|. \qquad (16)$$

The other two eigenvalues are zero. The eigenvectors $|\phi_1\rangle$ and $|\phi_2\rangle$ are given in Table I.

The reconstructed density matrix (16) agrees well with the qualitative reasoning given in [12]. Namely, the reconstructed state is almost a pure state—a slightly rotated nominal Bell state. The apparent incompatibility of the nominal state with the registered data was interpreted in [12] as the result of possible slight misalignments of the axes of analysis systems with respect to the axes of the downconversion source. This is, of course, reflected in the reconstructed state (16), which quantifies such misalignments and might serve for hunting down the errors and calibrating the experimental setup. For such purposes the error analysis of the presented reconstruction technique becomes crucial. The results of numerical simulations suggest that the fidelity of the reconstructed state corresponding to tens of thousands of detections (like in [12]) is typically better than 0.99. A detailed estimation of statistical fluctuations will be presented elsewhere.

Notice also that the reconstructed density matrix (16) is semipositive definite. This should be contrasted with the result of standard reconstruction. Direct inversion of Eq. (3) yields the density matrix having the following diagonal representation: $r_1=1.022$, $r_2=0.068$, $r_3=-0.065$, $r_4=-0.024$ [13]. The corresponding eigenvectors need not be specified here. Apparently, direct inversion (standard tomography) leads to an unphysical nonpositive definite result. It is worth noting that the negative eigenvalues are comparable in magnitude with nondiagonal elements of ρ_e^{ML} in the H-V basis; see Table I. This is a nice example of a situation when standard methods fail even though rather high numbers of particles (tens of thousands) have been registered. ML reconstruction always provides physically sound results. Moreover, it represents genuine quantum measurement of the entangled state.

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