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RECONSTRUCTION OF THE DENSITY MATRIX AS A CONSTRAINED OPTIMIZATION PROBLEM*

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We present a numerical algorithm for the maximum-likelihood estimation of the density matrix, and apply it to the homodyne tomography of a single-mode radiation field. The algorithm is based on a specific form of the Gauss decomposition for positive definite Hermitian matrices. Results from Monte Carlo simulated experiments are presented.

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Over past several years a great deal of interest has been paid to the reconstruction of the complete quantum state from experimental data [1]. Theoretical research in this field, apart from designing new measurement schemes, explores also the problem of extracting the optimal amount of information from data available in a realistic experimental setup. In this communication, we present a numerical algorithm for reconstructing the density matrix using the maximum-likelihood method [2, 3]. We discuss this algorithm in the context of quantum homodyne tomography [4, 5], which is actually the most successful method for quantum state reconstruction, and, in fact, the unique technique that has been so far experimentally implemented to measure nonclassical states of light [4, 6].

The realistic homodyne measurement of the quadrature $\hat{x}_\theta = (\hat{a}e^{-i\theta} + \hat{a}^\dagger e^{i\theta})/\sqrt{2}$ is described by the positive operator-valued measure

$$\hat{\mathcal{H}}(x;\theta) = \frac{1}{\sqrt{\pi(1-\eta)}} \exp\left(-\frac{(x-\sqrt{\eta}\hat{x}_\theta)^2}{1-\eta}\right), \tag{1}$$

where η is the detector efficiency. After repeating the measurement N times, we obtain a set of pairs $(x_i;\theta_i)$ consisting of the outcome x_i and the local oscillator phase θ_i for the ith run, where $i = 1, \ldots, N$.

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In the maximum-likelihood approach, these data are used to construct the likelihood functional [2]

$$\mathcal{L}(\hat{\varrho}) = \prod_{i=1}^{N} \mathrm{Tr}[\hat{\varrho}\,\hat{\mathcal{H}}(x_i;\theta_i)] \tag{2}$$

defined on the manifold of density matrices. The maximum-likelihood estimate of the quantum state is then defined as the density matrix $\hat{\varrho}_{\mathrm{ML}}$ that maximizes the likelihood functional.

Quantum state estimation using the maximum-likelihood method, despite its elegant formulation, presents in general a highly nontrivial constrained optimization problem. The central difficulty lies in the appropriate parameterization of the manifold of density matrices. The parameter space should be of the lowest possible dimension in order to preserve the maximum of the likelihood functional as a single isolated point. Moreover, the expression of quantum expectation values in terms of this parameterization should enable fast evaluation of the likelihood functional, as this step is performed many times in the course of numerical maximization.

Here, we introduce a parameterization of the manifold of density matrices which provides an efficient algorithm for maximizing the likelihood functional. We shall represent the density matrix $\hat{\varrho}$ in the form

$$\hat{\varrho} = \hat{T}^{\dagger}\hat{T} \tag{3}$$

which automatically guarantees that $\hat{\varrho}$ is positive definite and Hermitian. The remaining condition of unit trace $\mathrm{Tr}\hat{\varrho} = 1$ will be taken into account in the maximization procedure using the method of Lagrange multipliers.

To achieve the minimal parameterization, we shall assume that $\hat{T}$ is a lower-triangular matrix with real elements on the diagonal and complex ones below. This form of $\hat{T}$ is motivated by the Cholesky decomposition known in numerical analysis [7], and exists for an arbitrary positive definite Hermitian matrix. For the M-dimensional Hilbert space, the number of free real parameters in the matrix $\hat{T}$ is $M + 2M(M-1)/2 = M^2$, which equals the number of independent real parameters for a Hermitian matrix. This confirms that our parameterization is minimal.

The above parameterization of the manifold of density matrices allows one to apply readily one of the standard maximization procedures. In practice, instead of using the likelihood function $\mathcal{L}(\hat{\varrho})$, it is convenient to evaluate its logarithm. Thus the function subjected to maximization is given by

$$L(\hat{T}) = \sum_{i=1}^{N} \log \mathrm{Tr}[\hat{T}^{\dagger}\hat{T}\hat{\mathcal{H}}(x_i;\theta_i)] - \lambda\,\mathrm{Tr}(\hat{T}^{\dagger}\hat{T}) \tag{4}$$

where λ is a Lagrange multiplier. It can be easily shown that λ equals the total number of measurements N [8]. Of course, for a light mode it is necessary to truncate the Hilbert space to a finite dimensional basis.

We have applied the present approach to a set of Monte Carlo experiments. We have simulated a homodyne detection for some quantum states, and applied the maximum-likelihood algorithm to reconstruct the density matrix in the Fock basis, truncated upon defining the maximum number of photons. We have used the downhill simplex method [9] to find the maximum of the function $L(\hat{T})$. Results of the reconstruction for a coherent state and a squeezed vacuum are presented in Fig. 1.

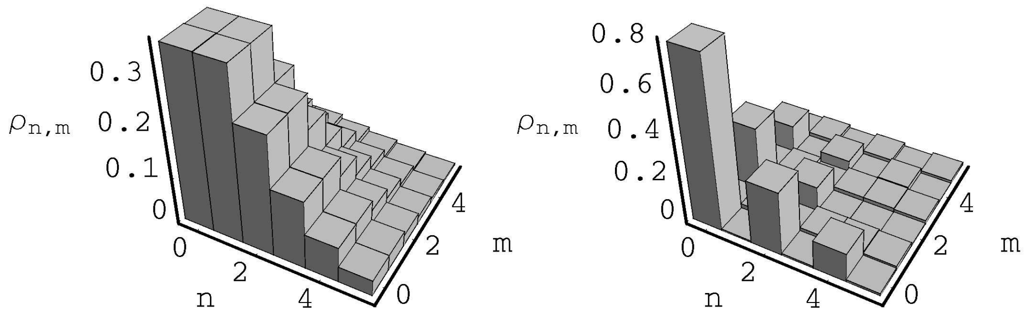

Fig. 1. Monte Carlo simulation of the tomographic reconstruction of the density matrix using the maximum likelihood technique. On the left the density matrix for a coherent with $\langle a^\dagger a\rangle = 1$ average photon, and on the right for a squeezed vacuum with $\langle a^\dagger a\rangle = 0.5$ photons. In both simulated experiments $N_\phi = 100$ phases with $N_x = 5000$ data each have been used. The truncation of the Hilbert space has been set to $N_H = 5$, and we considered a quantum efficiency $\eta = 0.8$ at the photodetectors.

In numerical calculations, it is convenient to use an expression for the quantum expectation value $\mathrm{Tr}[\hat{T}^\dagger\hat{T}\hat{\mathcal{H}}(x_i;\theta_i)]$ which is explicitly positive definite. This protects the algorithm against occurrence of a negative number as an argument of the logarithm function, which may in principle happen when $\mathrm{Tr}[\hat{T}^\dagger\hat{T}\hat{\mathcal{H}}(x_i;\theta_i)]$ is very close to zero. A simple calculation yields the expression:

$$\mathrm{Tr}[\hat{T}^\dagger\hat{T}\hat{\mathcal{H}}(x_i;\theta_i)] = \sum_{k=0}^{M-1}\sum_{j=0}^{k}\left|\sum_{n=0}^{k-j}\sqrt{\binom{n+j}{n}\eta^n(1-\eta)^j}\langle k|\hat{T}|n+j\rangle\langle n|x_i\rangle e^{in\theta_i}\right|^2 \quad (5)$$

where

$$\langle n|x\rangle = \frac{1}{\pi^{1/4}}e^{-\frac{1}{2}x^2}\frac{H_n(x)}{\sqrt{n!\,2^n}}$$

are eigenstates of the harmonic oscillator in the position representation ($H_n(x)$ being the n-th Hermite polynomial). This formula has another advantage from the point of view of numerical calculations: the argument of the most inner sum involves a product of terms dependent only on η, x, or θ. After discretization of x and θ, each of these three terms can be evaluated once and efficiently stored as a two-dimensional array without extensive memory usage.

In conclusion, we have presented an effective implementation of the maximum likelihood method to the tomographic reconstruction of the density matrix of a light mode. Our approach is based on a suitable parameterization for the density matrix, which allows to use a minimal set of parameters and avoids negative values in the evaluation of the log-likelihood function. Our method can be readily generalized [8] to the reconstruction of quantum states of other systems like spins or trapped ions.

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