RECONSTRUCTION OF DIAGONAL ELEMENTS OF DENSITY MATRIX USING MAXIMUM LIKELIHOOD ESTIMATION¹

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The data of the experiment of Schiller et al., *Phys. Rev. Lett.* **77**(1996) 2933, are alternatively evaluated using the maximum likelihood estimation. The given data are fitted better than by the standard deterministic approach. Nevertheless, the data are fitted equally well by a whole family of states. Standard deterministic predictions correspond approximately to the envelope of these maximum likelihood solutions.

1. Introduction

Quantum state provides the complete information about quantum systems. Recently quantum tomography has been devised for prediction of quantum state on the basis of homodyne detection with rotated basis of quadrature operators [1,2,3]. The technique has been applied to analysis of realistic measurement and now, quantum state reconstruction is routinely used in various applications [4].

Nevertheless, potential problems of deterministic schemes has been reported. The positive definiteness of the reconstructed density matrix is not guaranteed within deterministic data inversion yielding some nonphysical predictions. Positive definiteness can be preserved using information theory [5]. The approach based on the maximum likelihood (MaxLik) estimation is closely related to the standard treatment. Instead of the question: "What quantum state is determined by these data?" the question consistent with quantum theory reads: "What quantum state seems to be most likely ?" The

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Fig. 1. Homodyne detection and reconstructed data for coherent state

general formulation of the MaxLik problem was given in [6,7]. The extremum density matrix is given by nonlinear operator equation

$$\hat{R}(\hat{\rho})\hat{\rho} = \hat{\rho},\tag{1}$$

where

$$\hat{R} = \sum_{i} \frac{f_i}{\rho_{ii}} \hat{\Pi}_i, \quad \rho_{ii} = \operatorname{Tr}(\hat{\rho}\hat{\Pi}_i).$$
(2)

Here $\hat{\Pi}_i$ represents the projectors corresponding to (in general unsharp) nonorthogonal measurement. The measured relative frequencies are denoted here as f_i , $\sum_i f_i = 1$. The state may be reconstructed on the subspace where the projectors provide the resolution of identity operator $\hat{R} = \hat{1}$. Although the form of equation (??) suggests an iterative solution, it is not easy since the iterations need not be convergent in general. Solution simplifies significantly provided that the projectors $\hat{\Pi}_i$ commute. The diagonal elements of density matrix in common commuting basis may be estimated very effectively, as showed by Banaszek [8,9]. This numerical approach will be used here for evaluation of the diagonal elements of density matrix for the experiment reported by Schiller et. al [3]. All the necessary steps of general reconstruction scheme will be demonstrated on this example.



Fig. 2. Reconstruction of diagonal elements for coherent state

2. Reconstruction

The diagonal elements of density matrix only will be reconstructed. Data corresponding to the random-phase homodyne detection [10] are sufficient for this purpose. Projectors enumerated by position are given as

$$\hat{\Pi}(x) = \frac{1}{2\pi} \int_0^{2\pi} d\theta |x,\theta\rangle \langle x,\theta|.$$
(3)

They commute and are complete on the full interval $x \in (-\infty, \infty)$. Nevertheless, any realistic measurement will register only a finite sampling of discrete decomposition. Denoting the position of a particular bin in x-coordinate as x_i , the projectors in number state basis read

$$\hat{\Pi}(x_i) = \Delta x \sum_{n=0}^{\infty} \sum_{k=0}^{n} \Phi_k(x_i) \eta^k (1-\eta)^{n-k} \binom{n}{k} |n\rangle \langle n|,$$
(4)

$$\Phi_k(x) = \frac{1}{2^k k! \sqrt{\pi}} e^{-x^2} H_k^2(x).$$
(5)

Here η denotes the efficiency of counting of photoelectrons, enumerated by index k and Δx is the width of the bin. This detection of discretized quadrature components reproduces the identity operator as

$$\hat{R} = \sum_{i} \hat{\Pi}(x_i).$$
(6)



Fig. 3. Histogram of relative entropies and moments of particle number operator for various MaxLik estimates.

Diagonal elements of \hat{R} in number state basis shows the subspace where this operator equals approximately to identity. Here the reconstruction may be done applying the MaxLik procedure. Relative entropy (log of likelihood function)

$$K(\rho/f) = -\sum_{i} f_i \ln \frac{\rho_{ii}}{f_i} \ge 0$$
(7)

shows how the given state approaches the ideal condition $\rho_{ii} = f_i$. Provided that this condition is met, the relative entropy equals to zero. In the following the relative entropy will be evaluated for various states and given data f_i . For comparison, the relative entropy will be expressed in % with respect to the entropy of measured data, $S(f) = -\sum_i f_i \ln f_i$.

The data corresponding to measurement of coherent and squeezed state will be considered explicitly. All the calculations has been done for an overall efficiency $\eta = 0.85$ here. The Fig. 1 plots the data measured by random-phase homodyning and reconstructed data using deterministic and MaxLik approaches. The reconstruction of diagonal elements of density matrix in number state basis is plotted in the Fig. 2. Deterministic reconstruction yields slightly nonphysical results indicated by several negative diagonal elements obtained. A typical MaxLik estimation of diagonal elements is plotted in the upper right panel. However, the estimates depend on the starting point of the iteration process. The procedure has been repeated 100 times with different starting points. The average of all estimates is plotted in left bottom panel of the Fig. 2.



Fig. 4. Homodyne detection and reconstructed data for squeezed state

Diagonal elements R(n) plotted in the right bottom panel of the Fig. 2 deliminate the subspace for reconstruction as $n_{edge} = 50$.

The MaxLik estimates fit the measured data obviously better. While the relative entropy for the deterministic "state" is about $K(\rho/f) \approx 1.6\%$ of the value S = 4.717, the relative entropy of the MaxLik estimates fluctuates around the value 0.31% of the entropy S only. The histogram of relative entropies is plotted in the left upper panel of the Fig. 3. Significantly, all these states fit well the input data and there is no observable difference in fitted data statistics. Other panels show the uncertainty of moments for various MaxLik estimates (denoted by index $_{AV}$). The x-coordinate represents the deviation of the moments $\langle \hat{n}^k \rangle / \langle \hat{n}^k \rangle_{AV} - 1$ for k = 1, 10, 50. All the low moments are estimated very sharply within the accuracy $10^{-2}\%$. However, the 50-th moments already fluctuate within 30%. The average number of particles is estimated here as $\bar{n}_{MaxLik} \approx 29.6$. The value obtained from the deterministic approach is $\bar{n}_{det} \approx 25.6$, i.e. 30.1 considering efficiency η .

Similar analysis may be done for the data corresponding to squeezed state. The histogram of random-phase homodyne detection and reconstructed data are plotted in the Fig. 4. The dimension of subspace for reconstruction is about $n_{edge} = 100$ (not plotted here). The reconstructed diagonal elements are shown in the Fig. 5. The deterministic reconstruction has been considered on too small subspace as seen on the upper left panel. The MaxLik estimation has been done 100 times on a 75 dimensional subspace, because the higher dimension is out of the range of our program. While



Fig. 5. Reconstruction of diagonal elements for squeezed state



Fig. 6. Histogram of relative entropies and moments of particle number operator for various MaxLik estimates

deterministic estimation is characterized by the relative entropy $K_{sq}(\rho/f) \approx 15\%$ of the value S = 4.02, the relative entropy of MaxLik estimates fluctuating around the value 0.15% are considerably better. The histogram of relative entropies is plotted in the upper left panel of the Fig. 6, the other panels show the uncertainty in moments of various MaxLik estimates. The value of moments is again related to the averaged MaxLik estimate as in the Fig. 3.

3. Conclusion

The MaxLik procedure fits the measured data better than the deterministic scheme, but the results are not single valued. Instead of a single state predicted by the deterministic scheme, there is a family of states fitting the data equally well. Hence the MaxLik state reconstruction is more uncertain in comparison to the deterministic prediction. However, this uncertainty corresponds to the probabilistic nature of quantum theory. Measured data do not determine an unique state and the reconstruction has to take it into account.

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