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Investigating Bias in Maximum Likelihood Quantum State Tomography

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Maximum likelihood quantum state tomography yields estimators that are consistent, provided that the likelihood model is correct, but the maximum likelihood estimators may have bias for any finite data set. The bias of an estimator is the difference between the expected value of the estimate and the true value of the parameter being estimated. This paper investigates bias in the widely used maximum likelihood quantum state tomography. Our goal is to understand how the amount of bias depends on factors such as the purity of the true state, the number of measurements performed, and the number of different bases in which the system is measured. For that, we perform numerical experiments that simulate optical homodyne tomography of squeezed thermal states under various conditions, perform tomography, and estimate bias in the purity of the estimated state. We find that estimates of higher purity states exhibit considerable bias, such that the estimates have lower purity than the true states.

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I. INTRODUCTION

Quantum state tomography (QST) is the estimation of an unknown quantum state from experimental measurements performed on a collection of quantum systems all prepared in the same unknown state. QST is an important procedure for quantum computation and information [1], being used, for example, to learn properties of states prepared in experiments and for the validation of quantum gates in quantum process tomography.

In QST many identical copies of the system are prepared, each copy is independently measured, and the results of these measurements are used to estimate the system's quantum state ρ_{true} . A commonly used method to make the estimate is maximum likelihood estimation, in which one finds the state ρ_{ML} with the maximum likelihood given the measurement results [2]. The estimation is an optimization problem usually solved numerically using iterative algorithms, such as the expectation-maximization based $R\rho R$ [3] and gradient ascent algorithms. This optimization problem becomes more difficult as the dimension of ρ_{true} increases.

In this paper, we examine idealized simulated experiments with no systematic experimental errors, meaning that they are correctly described by the likelihood model. We analyze only the properties of the random measurement error and bias in the maximum likelihood estimator. Properties of this estimator have also been examined in [4–6]. The difference between the estimate's expected value and the true value of the parameter being estimated is called “bias”. Given a correct likelihood model and an informationally complete set of measurements [2], maximum likelihood estimators are consistent

and asymptotically unbiased [7], but they are typically biased for finite samples. This bias is caused by nonlinearity of the estimation procedure.

We could be tempted to avoid the bias problem by using linear inversion estimators, which are unbiased. However, common linear inversion estimators do not confine their estimates to physical state space [8], and linear estimators generally have larger mean squared error than maximum likelihood estimators [7].

In [4], the behavior of estimation errors in one-qubit state tomography was analyzed numerically using distances between the estimate and the true state. That analysis showed that for the tomography of a single qubit, the constraint that density matrices be positive semidefinite creates bias that increases as the length of the Bloch vector, a measure of distance from the state to the boundary of state space, approaches 1. However, that bias can be reduced if measurement operators are aligned with the Bloch vector. In [9], Monte Carlo simulations were used to study quantum state tomography of a few qubits measured in the bases of the Pauli operators. [9] showed that reconstruction schemes based on maximum likelihood and least squares both suffer from bias. The fidelity was systematically underestimated while the entanglement was overestimated.

In this paper we are interested in the tomography of continuous variable systems, whose bias has not yet been systematically investigated. We use numerical experiments to simulate optical homodyne tomography of squeezed thermal states under various conditions and perform maximum likelihood tomography on that data. Because [4] showed a relationship between bias and the length of a qubit's Bloch vector, we extend those results to higher dimensional systems by examining bias's dependence on purity, another measure of distance of a density matrix from the boundary of state space. We also inves-

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tigate how the amount of bias depends on factors such as the number of measurements performed, the number of different bases in which the system is measured, and the dimension of the Hilbert space. In Section II we review maximum likelihood estimation. In Section III we describe our numerical experiments and present our results. In Section IV we discuss the interpretation of our results and make some concluding remarks.

II. MAXIMUM LIKELIHOOD ESTIMATION

Continuous variable systems, such as a harmonic oscillator or a mode of light, live in infinite dimensional Hilbert spaces. Tomography cannot estimate the infinitely many parameters required to represent states in infinite dimensional spaces, so the standard approach in this case is to limit the number of unknown parameters, by truncating the Hilbert space at a maximum phonon or photon number n .

Let us consider N quantum systems, each of them prepared in a state described by a density matrix ρ_{true} . Each copy i has an observable labeled by θ_i measured with result x_i , for $i = 1, \dots, N$. In each measurement the observable is chosen by setting the phase θ_i of a local oscillator (a reference system prepared in a high amplitude coherent state). The outcome of the i -th measurement is described by a positive-operator-valued measure (POVM) element $\Pi(x_i|\theta_i) = \Pi_i$. The likelihood of a candidate density matrix ρ given the data set $\{(\theta_i, x_i) : i = 1, \dots, N\}$ is given by

$$\mathcal{L}(\rho) = \prod_{i=1}^N \text{Tr}(\Pi_i \rho), \quad (1)$$

where $\text{Tr}(\rho \Pi_i)$ is the probability, according to ρ , to obtain outcome x_i when measuring with phase θ_i .

The goal of maximum likelihood QST is to find the density matrix ρ_{ML} that maximizes the likelihood. In practice one usually maximizes the logarithm of the likelihood (the “log-likelihood”):

$$L(\rho) = \ln \mathcal{L}(\rho) = \sum_{i=1}^N \ln[\text{Tr}(\Pi_i \rho)], \quad (2)$$

which is maximized at the same density matrix as the likelihood. The log-likelihood function is concave, giving us a well-behaved optimization problem, such that the convergence to the unique solution will be achieved by most iterative optimization methods.

Our algorithm for likelihood maximization begins with several iterations of the $R\rho R$ algorithm followed by iterations of a regularized gradient ascent algorithm (RGA). After an initial period of fast convergence, we have observed significant slow-down in the $R\rho R$ algorithm after around $(n+1)^2/4$ iterations. To alleviate this problem, after $(n+1)^2/4$ $R\rho R$ iterations, we switch to the RGA. Let $\rho^{(k)}$ be the density matrix found after k iterations,

the first of which is provided by the last iteration of $R\rho R$. In the RGA, $\rho^{(k+1)}$ is parametrized as

$$\rho^{(k+1)} = \frac{(\sqrt{\rho^{(k)}} + A)(\sqrt{\rho^{(k)}} + A^\dagger)}{\text{Tr}[(\sqrt{\rho^{(k)}} + A)(\sqrt{\rho^{(k)}} + A^\dagger)]}, \quad (3)$$

where A may be any complex matrix of the same dimensions as ρ . This construction ensures that $\rho^{(k+1)}$ is a physical density matrix for any A . To choose A , a quadratic approximation of the log-likelihood is performed. A maximizes the quadratic approximation of the log-likelihood subject to the constraint that $\text{Tr}(AA^\dagger) \leq u$, where u is a positive number that the algorithm adjusts to ensure that the log-likelihood increases with each iteration.

All iterations halt when the stopping criterion of [10] signals that the $L(\rho_{\text{ML}}) - L(\rho^{(k)}) \leq 0.2$, where $L(\rho_{\text{ML}})$ is the maximum of the log-likelihood. By bounding the log-likelihood improvement that can be achieved with further iterations, we ensure that the last iteration produces an estimate that is “close” to ρ_{ML} , where that closeness is statistically relevant [10].

III. NUMERICAL EXPERIMENTS

Our numerical experiments simulated single mode optical homodyne measurements [11] of a state created by sending a squeezed vacuum state, with quadratures variances $s/2$ and $1/(2s)$, through a lossy medium with transmissivity t . These states are Gaussian states with zero means, which can be parametrized by their covariance matrices. Since we want to simulate states of different purities, we will express purity as a function of squeezing and transmissivity.

The covariance matrix of the state after the lossy medium is given by

$$\Sigma = t \begin{pmatrix} \frac{1}{2s} & 0 \\ 0 & \frac{s}{2} \end{pmatrix} + (1-t) \frac{\mathbb{I}}{2}, \quad (4)$$

where \mathbb{I} is the identity matrix. Purity is then given by [12]

$$\begin{aligned} p(s, t) &= \frac{1}{2\sqrt{\text{Det}(\Sigma)}} \\ &= \frac{1}{2\sqrt{(\frac{1}{2} - \frac{1}{4s} - \frac{s}{4})(t^2 - t) + \frac{1}{4}}}. \end{aligned} \quad (5)$$

Our numerical experiments begin with the choosing of a desired purity for the true state. We use Eq. (5) to obtain an (s, t) pair that produces the desired purity. The choice of (s, t) is not unique, so we use two strategies, described below, that give states that are close to the vacuum and highly squeezed states. We represent the pure squeezed state with squeezing s as ρ_{pure} , a density matrix in the photon number basis, truncated at n photons. We then simulate passage of the pure squeezed state through

a medium with transmissivity t by a quantum operation that is equivalent to appending an ancillary mode in the vacuum state, acting on the two modes with the beam splitter transformation, and tracing-out the ancillary mode. This quantum operation is expressed with the set of Kraus operators $\{E_i(t)|i = 1 \dots n\}$, and transforms ρ_{pure} into $\rho_{\text{true}} = \sum_{i=1}^n E_i(t)\rho_{\text{pure}}E_i(t)^\dagger$. This procedure gives us the density matrix of a state with the desired purity, represented in an n photon basis.

To compute the probability $P(x|\theta) = \text{Tr}(\rho_{\text{true}}\Pi(x|\theta))$ to obtain homodyne measurement result x at phase θ from state ρ_{true} , we derive a representation of $\Pi(x|\theta)$ also in the n photon basis. Let $|x\rangle$ be the x -quadrature eigenstate with eigenvalue x expressed in the photon number basis, and let $U(\theta)$ be the phase evolution unitary operator. For an ideal homodyne measurement, we would compute the probability as $\text{Tr}[\rho_{\text{true}}U(\theta)^\dagger|x\rangle\langle x|U(\theta)]$. However, real homodyne detectors suffer from photon loss. Because this loss is part of the measurement device, we include it in the POVM elements by expressing them as $\Pi(x|\theta) = \sum_{i=1}^n E_i(\eta)^\dagger U(\theta)^\dagger|x\rangle\langle x|U(\theta)E_i(\eta)$ [13]. By including the loss associated with the measurement device in the POVM elements, we can estimate the state of the system before that loss occurs. For all of our numerical experiments, we use $\eta = 0.9$, which is typical for state-of-the-art homodyne detectors. To produce random samples of homodyne measurement results, we use rejection sampling [14] from the distribution given by $P(x|\theta)$.

We use two different methods for choosing the phases at which the homodyne measurements are performed. In the first method, for each quadrature measurement a random phase is chosen. In the second method for a total of N measurements, measured at m different phases, we divide the upper-half-circle evenly among the m phases between 0 and π and measure N/m times at each phase. Measuring the quadrature only once for a very large number of phases is natural for experimental systems that slowly scan the phase while sampling quadratures. For other systems, it may be more convenient to fix the phase and repeatedly measure the quadrature before changing the phase. We expect these two strategies to behave differently for three reasons. (1) When measuring evenly spaced phases, we obtain a histogram of quadrature measurements that allows us to directly reconstruct the probability distribution of the quadrature at each of the phases, but when measuring random phases, our knowledge of the quadrature probability distribution at each phase is quite poor, but we obtain samples at many more phases. The statistics of the two strategies are quite different, and one might expect that estimates produce different biases. (2) [4] showed that bias is reduced if one measures a qubit in the direction of its Bloch vector. By increasing the number of phases at which we measure the optical mode, we increase the probability that we measure in a direction that points toward the boundary of state space, which might reduce bias. (3) To obtain a single maximum of the likelihood function, we require an informationally complete set of measurement operators.

If the number of phases is too small relative to the maximum number of photons n in the Hilbert space, we do not have an informationally complete set of measurement operators, and there will be a family of density matrices, all of which maximize the likelihood. According to [15], $n + 1$ different phases are required to reconstruct a state that contains at most n photons. The likelihood maximization algorithm identifies one of these density matrices, and there may be systematic error introduced in the process.

To calculate the mean purity, we reconstruct each state 50 times, each time obtaining the purity for the reconstructed state. We then calculate the arithmetic mean of the 50 purities to obtain the “mean reconstructed purity”. Our estimate of the purity bias is the difference between the mean reconstructed purity and the purity of the true state. The uncertainty in each bias estimate (shown as error bars in the figures) is the standard deviation of the mean of the reconstructed purity. The relative sizes of the magnitude of the bias ($\text{abs}(\text{bias})$) and the standard deviation of the 50 purities ($\text{std}(\text{purity})$) are also of interest, so we make some statements about them in the figure captions.

A. Nearly vacuum state

Let us start with tomography of a nearly vacuum state measured with randomly chosen phases. A state of a given purity with the weakest squeezing is reached when $t = 1/2$. To find the necessary squeezing, we solve Eq. (5) for s . Fig. 1 shows purity bias as a function of the true state purity for different numbers of measurements. Analyzing the graphs, we can see that, when fewer measurements are made, the highest purity states’ mean reconstructed purity is significantly lower than the true state purity. This is clear evidence of bias in the tomography algorithm. We can also see that as we increase the number of measurements, the variance and bias of the purity estimates decreases. For true state purities below 0.9, $\text{abs}(\text{bias})$ decreases with decreasing true state purity (when other parameters are fixed).

Fig. 2 shows color maps of the purity bias as a function of the number of measurements and the true state purity. These give us a qualitative description of purity bias for a larger parameter space than shown in Fig. 1. Fig. 3 shows the behavior of the purity bias as a function of the number of measurements for two fixed values of purity: 0.9 and 1. As we increase the number of measurements, the variance and bias of the purity estimates decreases, becoming approximately unbiased asymptotically, as expected. In Fig. 4 we show $\text{bias}/\text{std}(\text{purity})$ as a function of the number of measurements for the simulations shown in Fig. 3.

In Fig. 5, we use a nearly vacuum state, but rather than randomly choosing a phase for each measurement, we used only six evenly spaced phases. In Fig. 6, we plot the 8,000 measurement case for both measurement

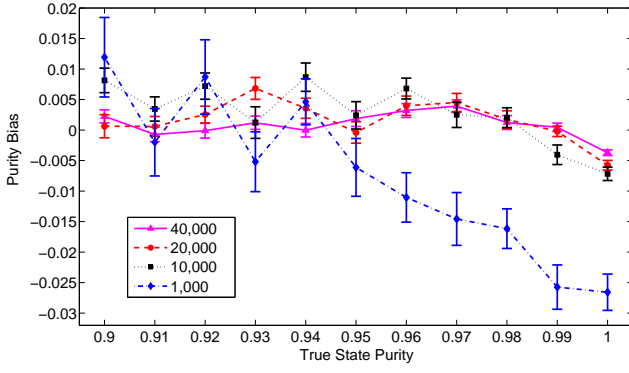
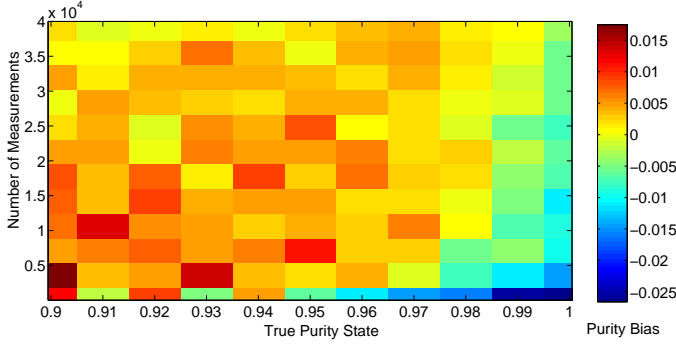
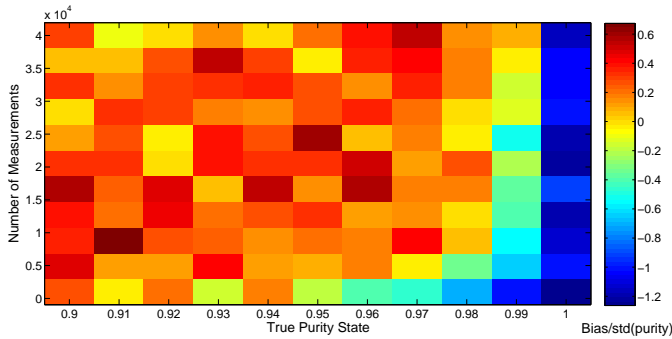


FIG. 1. Purity bias as a function of true state purity for a nearly vacuum state and random phases. Number of measurements: 40,000, 20,000, 10,000, and 1,000. Maximum photon number: 10. In the 40,000, 20,000, and 10,000 measurement cases, $\text{abs}(\text{bias})$ is considerably smaller than $\text{std}(\text{purity})$, except they are approximately equal when $\text{purity}=1$. In the 1,000 measurement case, $\text{abs}(\text{bias})$ and $\text{std}(\text{purity})$ are approximately equal at $\text{purity}=0.99$, and at $\text{purity}=1$ $\text{abs}(\text{bias})$ is larger than $\text{std}(\text{purity})$.



(a)



(b)

FIG. 2. Color map of the (a) purity bias and (b) purity bias measured in number of standard deviations of the purity estimates: $\text{bias}/\text{std}(\text{purity})$ as functions of the number of measurements and the true state purity for a nearly vacuum state measured with random phases. Maximum photon number = 10.

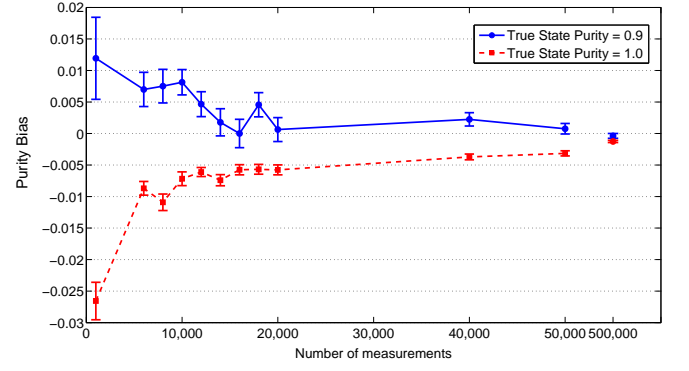


FIG. 3. Purity bias as a function of the number of measurements for a nearly vacuum state and measured with random phases. Maximum photon number: 10. Note that the horizontal axis has been shortened between 50,000 and 500,000 measurements.

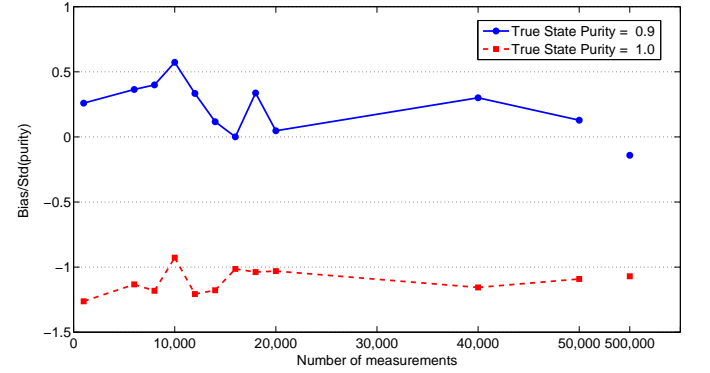


FIG. 4. Relative error of purity bias, $\text{bias}/\text{std}(\text{purity})$, as a function of the number of measurement for a nearly vacuum state and random phases. Maximum photon number: 10. Note that the horizontal axis has been shortened between 50,000 and 500,000 measurements.

schemes. Although only six phases is not informationally complete for the 10 photon Hilbert space in which we are performing the reconstruction, we see little effect on the purity bias. This is likely because the number of photons in the state is much smaller than 10.

To further explore the relationship between the number of phases and bias, in Fig. 7 we show the behavior of purity bias as a function of the chosen number of evenly spaced phases. Increasing the number of phases has very little effect on bias.

So far, we have presented results of density matrices reconstructed in a 10 photon Hilbert space. We now argue that 10 photons is sufficient to represent the nearly vacuum states that we have analyzed. A state will be well represented in a truncated Hilbert space of n photons, avoiding errors in the tomography, when the sum of probabilities of having n photons in this state is close to 1. For the nearly vacuum states, the number of photons in the state increases with decreasing purity. The nearly vac-

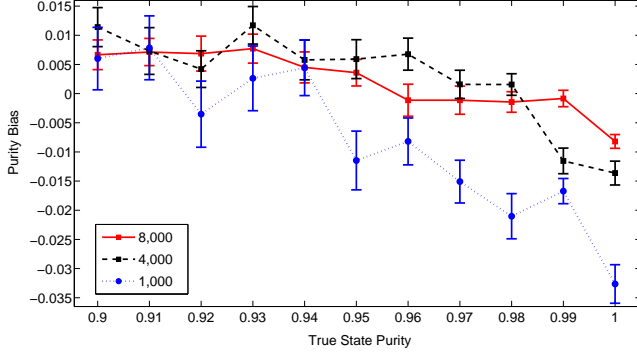


FIG. 5. Purity bias as a function of true state purity for a nearly vacuum state and six evenly spaced phases. Number of measurements: 8,000; 4,000; and 1,000. For 1,000 measurements $\text{abs}(\text{bias})$ is larger than $\text{std}(\text{purity})$ for true state purities 0.99 and 1.00. For all other cases shown $\text{abs}(\text{bias})$ is less than $\text{std}(\text{purity})$, though several points are very close.

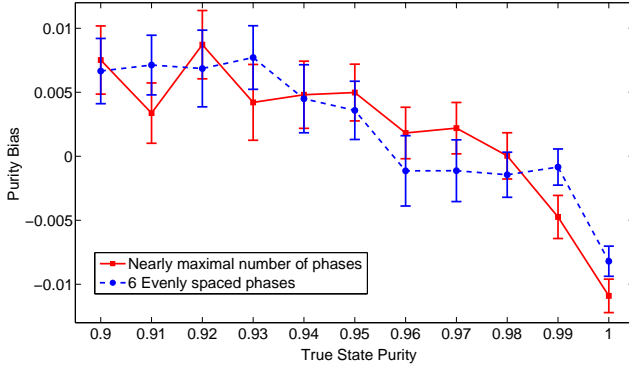


FIG. 6. Purity bias as a function of true state purity for a nearly vacuum state and both phase choosing methods: random phases and six evenly spaced phases. Number of measurements: 8,000. Maximum photon number: 10.

uum state with purity of 0.9 (the lowest that we report) has a probability of 1.15×10^{-5} to contain more than 10 photons, so a 10 photon Hilbert space should faithfully represent all of the nearly vacuum states. In Fig. 8 we show purity bias of density matrices reconstructed in 10 - 40 photon Hilbert spaces. We see that the use of larger Hilbert spaces has no effect on the purity bias. Fig. 8 also shows that when randomly choosing a phase for each of 8,000 measurements, more than sufficient phase information is gained to estimate the state even in a 40 photon Hilbert space. We explore the effect of measuring with an insufficient number of phases in Fig. 9, where we use only six evenly spaced phases to measure the nearly vacuum state. We reconstruct the density matrix in 10, 20, 30, and 40 photon Hilbert spaces, and we see that the results are very similar to those obtained when measuring at random phases.

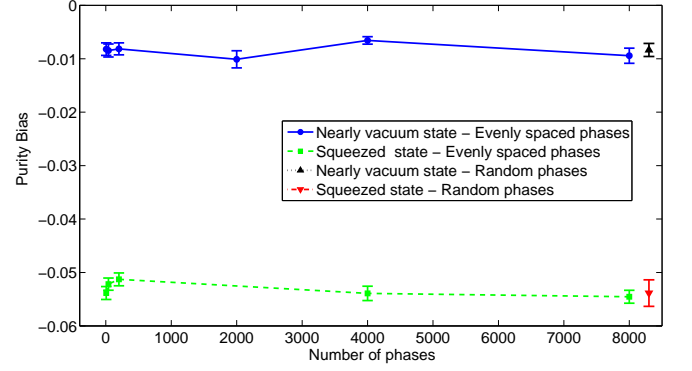


FIG. 7. Purity bias for reconstruction of states whose purity is 1 as a function of the number of evenly spaced phases at which the state is measured. Bias for the vacuum state is shown with blue circles, and bias for a squeezed state whose squeezed quadrature variance is $1/2$ of the vacuum variance is shown with green squares. Number of measurements = 8000. Maximum photon number = 10. The graph also shows the bias obtained when measuring 8000 random phases with the points just to the right of the 8000 evenly spaced phases point. Unlike other graphs in this paper, which use 50 simulated experiments to estimate bias, this graph uses 200 simulated experiments.

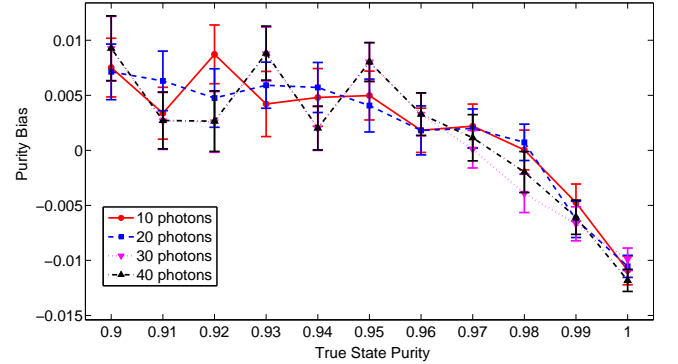


FIG. 8. Purity bias as a function of true state purity for a nearly vacuum state measured with random phases. Number of measurements: 8,000. Maximum photon number: 10, 20, 30 and 40. For all of these cases, we find $\text{abs}(\text{bias})$ larger than $\text{std}(\text{purity})$ only when the true state purity=1.

B. Highly squeezed states

To test the robustness of some of our claims, we now change the measured states from nearly vacuum states to highly squeezed states. Each state is created by sending a pure squeezed vacuum state, whose squeezed quadrature has variance $1/4$ of vacuum variance, through a lossy medium with one of the following transmissivities: $t = [0.5, 0.8, 0.9, 0.95, 0.99, 1]$. For each pair (s, t) , the purity is calculated using Eq. (5). The highly squeezed states contain more photons, so we truncate the Hilbert space at 20 photons. The highly squeezed state with the most photons has purity of 1 (and $t = 1$). That state's

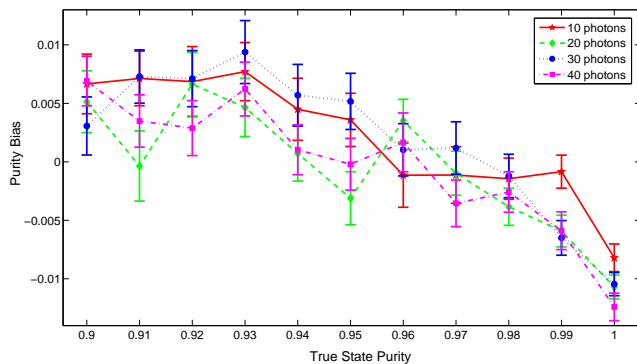


FIG. 9. Purity bias as a function of true state purity for a nearly vacuum state and 6 evenly spaced phases. Number of measurements: 8,000. Maximum photon number: 10, 20, 30 and 40.

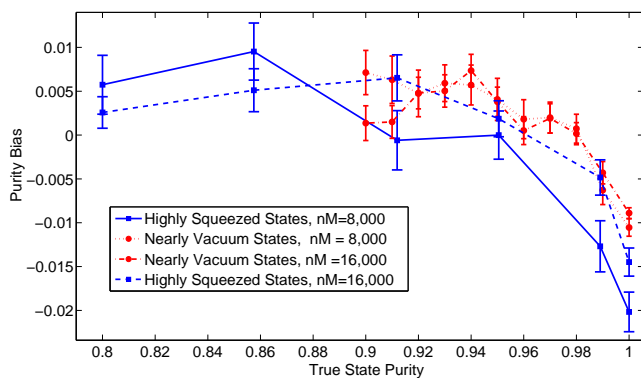


FIG. 10. Purity bias as a function of true state purity for nearly maximal number of phases and both nearly vacuum and highly squeezed states. A random phase is chosen for each measurement. Number of measurements: 16,000 and 8,000. Maximum photon number = 20. For reconstructing nearly vacuum states from 8,000 or 16,000 measurements $\text{abs}(\text{bias})$ is greater than $\text{std}(\text{purity})$ except when $\text{purity}=1$. The same is true for reconstructing highly squeezed states from 8,000 measurements. For reconstructing highly squeezed states from 16,000 measurements, $\text{abs}(\text{bias})$ is greater than $\text{std}(\text{purity})$ in all cases shown, except they are approximately equal when true state $\text{purity}=0.95$.

probability to contain more than 20 photons is 2.7×10^{-6} . The results for bias of highly squeezed states are similar to those of the nearly vacuum states.

In Fig. 10 we compare the estimated purities when measuring nearly vacuum and highly squeezed states, finding similar behavior in the two cases. It appears that bias is slightly higher for the highly squeezed states. Bias is clearly not a function of the true state's purity alone, but depends on other features of the true state. This dependence is not well understood. As more measurements are taken the biases decrease, and the gap between the bias of highly squeezed and nearly vacuum states decreases.

We also show the dependence of bias on the number of

evenly spaced phases used to measure a squeezed state in Fig. 7, seeing little relationship between bias and the number of phases, except there seems to be a slight increase in $\text{abs}(\text{bias})$ when very few phases are used.

IV. CONCLUSION

We have used idealized numerical experiments to generate simulated data under various conditions, performed tomography, and estimated bias in the purity of the results. The mean reconstructed purities of the highest purity states are significantly lower than the corresponding true state purities. This result shows clear evidence of bias in the tomography algorithm, even when the likelihood model is correct. In our simulations we did not see a strong relationship between purity bias and the number of phases used to measure the state, though it is possible that such a relationship for some combination of states and measurement conditions. The $\text{abs}(\text{bias})$ appears to be slightly larger for tomography performed on highly squeezed states than in nearly vacuum states.

In this work we have focused on the influence of the true state's purity on bias of the estimated purity, finding that more pure true states suffer from more bias toward lower purity states. This agrees with the results of [9]. However, whether this is a general property for all states is an open question. Our study has focused on bias in estimates of squeezed thermal states, but other states, especially non-Gaussian states, may have more or less bias. More numerical experiments on a greater diversity of states and using different measurement schemes would be informative as would exploration of bias in other parameters.

In many of our numerical experiments, we find that the bias in purity is significant compared to the standard deviation of the estimates of purity. This is particularly problematic if tools like the bootstrap are used to assign uncertainties in quantum state tomography. If a non-parametric bootstrap is used, every bootstrapped estimate will be similarly biased. If a parametric bootstrap is used, the original estimate is biased once and the bootstrapped estimates will be biased a second time. Bias correction methods exist for parametric bootstrap, but they require the bias to be consistent for different states [16]. This might be a reasonable approximation, but we have seen that it is not strictly true. Because of the problems caused by bias, it maybe helpful to use confidence intervals such as those described in [17–19] to assign uncertainties to estimated parameters. Unfortunately those methods produce confidence regions that are significantly larger (and more conservative) than those produced by bootstrap methods commonly used for quantum state tomography.

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