Optimized tomography for pure quantum states

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We describe a simple, optimized, self-correcting procedure for performing quantum pure state tomography. By analyzing the history of measurement outcomes at each step, the procedure returns the ‘most likely’ state after every measurement, as well as a suitable basis for the measurement that is to follow with the aim of maximizing the fidelity between the best guess and the unknown state. We illustrate the success of method by considering in detail the qubit case, and compare it against existing methods.

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I. INTRODUCTION

Quantum technology is a fast developing area of both experimental and theoretical research. It has well known applications in computation protocols \(^1\)–\(^6\), communication protocols \(^7\)–\(^12\), as well as in studying fundamental physical phenomena \(^13\)–\(^16\). Of particular interest is the devising of protocols for basic primitives that are meant to serve as building blocks for other, more involved, applications. One example is quantum state tomography (QST), whose purpose is to estimate the state of a quantum system, based on a measurement record of a finite ensemble of identical systems.

In recent years, much work has been devoted to constructing efficient protocols for QST, each emphasizing a different perspective of the process, e.g., studying the optimal measurement operators (optimal POVMs) to minimize the error due to statistical errors \(^17\)–\(^19\), allowing measurements on an ensemble of particles \(^20\)–\(^23\), and utilizing prior information about the state of the system (e.g., that the state is close to a pure state) together with compressive sampling techniques \(^24\)–\(^26\).

It is common practice in QST (and many other) protocols nowadays to have the quantum device run a program and to follow it by a post-processing step during which classical information is processed and conclusions are drawn. However, with advanced technologies and the growing control over quantum devices, comes the obvious need (and possibility) to integrate these two steps into one indivisible unit within which the program and the data-processing step are repeated successively feedbacking each other to form one efficient, fast, self-correcting, self-executing quantum protocol. Indeed, there has been a growing interest and actual progress in devising in situ protocols, in particular for QST of a single qubit system \(^27\)–\(^31\), with various degrees of automation where the measurement at later steps depends on the information acquired in previous steps. Some of these ideas were successfully implemented with current technology \(^28\)–\(^30\), \(^32\), \(^33\), and were shown to improve accuracy quadratically over common protocols \(^30\).

Nonetheless, despite these intricate protocols, it is not clear what the optimal QST protocols are in the various settings. Put differently, the question “What is the optimal sequence of measurements on a finite ensemble of identical systems in order to extract as much information as possible about the unknown state in the least amount of time?” remains open. This question becomes more significant nowadays where the opportunity of considering the implementation of self-learning protocols is becoming technologically more and more feasible, particularly in light of the fact that quantum systems are rather susceptible to decoherence.

In this paper we address the above question by offering an ‘optimizing protocol’ for the QST of pure states (postponing for the time being the case of arbitrary, mixed state QST). Pure states are of special interest, as state-of-the-art control over quantum devices allows a nearly coherent evolution of quantum systems. The physical setup we are considering is one in which an oven prepares and emits copies of an unknown quantum pure state of a given dimension \(d\), that we denote by \(|\psi\rangle\), at a constant rate. We are then given the task of providing an estimation of that state by performing orthogonal projective (von Neumann) single-copy measurements to determine it. The heart of the protocol we propose here is the computation of the ‘most likely’ candidate for the state emitted by the oven, followed by an optimization subroutine to determine an appropriate basis for the next measurement, based on the measurement record thus far. The proposed protocol is an optimized, fully-automated, self-correcting algorithm.

In what follows we describe the protocol as applied to systems of finite-dimensional Hilbert spaces. We then study the performance of the protocol and consider different situations to elucidate its guiding principles. We conclude with a summary and suggestions for possible follow-up research directions.
II. THE PROTOCOL

For the following, we shall be assuming for simplicity that no prior information is provided to us concerning the distribution over which the oven is emitting the pure states (the modifications required to address the general case will be discussed where appropriate). The main concept behind the protocol suggested here is to analyze, after each measurement, the entire history of measurement outcomes thus far, in order to establish at each step, the ‘most likely’ state for the unknown emitted state and, at the same time, to determine the basis states for the measurement on the next emitted copy. Based on this analysis, a measurement is then performed in the calculated optimized basis and the routine is repeated. By optimizing the measurement to be performed at each step, the proposed protocol maintains optimality throughout the procedure.

Next, we provide the steps of the protocol in detail. The reader is referred to Fig. 1 for a schematic diagram.

Step 1: At first, where no information about the state emitted by the oven has been acquired, the program executes a measurement in a randomly-chosen basis, and records the result.

Step 2: Based on all recorded measurement outcomes so far, the program computes the (pure) state most likely to have yielded the sequence of measurement outcomes. The details of this computation are given below. We shall denote this ‘best guess’ for the unknown state, or ‘most likely state’, after \( k \) measurements by \( |\psi_k\rangle \).

Step 3: After finding the most likely state, the program computes the optimal basis for the measurement that is to follow (this computation is also given below). As we shall argue, one of the basis states of the optimized measurement can be taken to be the most likely state.

Step 4: The program then executes a measurement in the ‘optimal basis’, and records the outcome.

Step 5: If the outcome of the \((k+1)\)-th measurement corresponds to the most likely state \( |\psi_k\rangle \), the basis of measurement is not changed, as the measurement basis remains optimal, and the program returns to Step 4. If conversely the outcome of the \((k+1)\)-th measurement does not yield the most likely state, the program returns to Step 2 to compute a new estimate for the state emitted by the oven and to adjust the basis of the measurement to follow.

A. Finding the most likely state

We now turn to address the details of computing the ‘most likely’ state. Let us consider the \( k \)-th iteration of the above protocol (note that one measurement is performed at each iteration on a single copy of the emitted state), and let \( S_k = \{ |\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_k\rangle \} \) be the sequence of \( k \) measurement outcomes obtained and recorded thus far. The most likely state, \( |\psi_k\rangle \), to have produced this sequence is, by definition, the state that maximizes the (infinitesimal) probability that the oven emitted \( |\tilde{\psi}\rangle \), conditioned on the sequence of measurement outcomes obtained so far, namely, \( dP(\psi|S_k) = p(\psi|S_k)|d\psi\). Here, \( p(\psi|S_k) \) is the corresponding probability density and \( d\psi \) is a Haar-measure over the pure-state manifold. Applying Bayes’ formula, the probability \( dP(\psi|S_k) \) may be written as \( dP(\psi|S_k) = P(S_k|\psi)dP(\psi)/P(S_k) \), where \( P(S_k|\psi) \), the probability of obtaining the outcome sequence \( S_k \) provided that the emitted state is \( |\tilde{\psi}\rangle \), is given through Born’s rule \( P(S_k|\tilde{\psi}) = \prod_{m=1}^{k} |\langle \phi_m|\tilde{\psi}\rangle|^2 \). The probability function \( dP(\psi) \) reflects our knowledge about the distribution over which the oven is choosing the states to emit, \( dP(\tilde{\psi}) = p(\tilde{\psi})d\tilde{\psi} \), and consequently, the probability of obtaining the sequence of measurement outcomes \( P(S_k) = \int P(S_k|\tilde{\psi})p(\tilde{\psi})d\tilde{\psi} \). Combining the above, we arrive at:

\[
dP(\psi|S_k) = \frac{p(\tilde{\psi})d\tilde{\psi}}{\int \prod_{m=1}^{k} |\langle \phi_m|\tilde{\psi}\rangle|^2 p(\tilde{\psi})d\tilde{\psi}} \prod_{m=1}^{k} |\langle \phi_m|\tilde{\psi}\rangle|^2.
\]

Now, since we are assuming that no prior information about the distribution over which the oven is emitting the states is given, i.e., that \( p(\tilde{\psi}) = \text{constant} \) [34], we can therefore eliminate \( p(\tilde{\psi}) \) from the above expression, which in turn allows us to identify the conditional probability density \( p(\psi|S_k) \) as

\[
p(\psi|S_k) = \frac{\prod_{m=1}^{k} |\langle \phi_m|\psi\rangle|^2}{\int \prod_{m=1}^{k} |\langle \phi_m|\psi\rangle|^2 d\psi}.
\]

The above expression is the one to be maximized in order to obtain the most likely state \( |\psi_k\rangle \). Equivalently, the most likely state can be obtained by maximizing the probability density

\[ p(\psi|S_k) \]

for the unknown state, or ‘most likely state’, after \( k \) measurements.

![Fig. 1](image_url) Schematics of the optimized pure state tomography protocol.
logarithm of $p(\tilde{\psi}|S_k)$, i.e.,

$$|\psi_k\rangle = \arg\max_{\psi} \log p(\tilde{\psi}|S_k) = \arg\max_{\psi} \sum_{m=1}^{k} \log |\langle \tilde{\psi}|\phi_m \rangle|^2.$$  

(3)

Note that here the denominator in the expression for $p(\tilde{\psi}|S_k)$ has been omitted as it is independent of $\tilde{\psi}$. Therefore, the most likely state, $|\psi_k\rangle$, maximizes the (log-)likelihood function of the sequence of $k$ measurements.

At this point, it is worth noting that the above calculation can readily be generalized to include the case where some a priori knowledge about the distribution over which the oven emits the states is given, in which case $p(\tilde{\psi})$ is no longer constant.

B. Optimizing the basis of measurement

Next, we describe the procedure aimed at optimizing the basis of the measurement-to-follow. We denote the orthonormal basis states of the $k$-th measurement, and which we need to optimize, by $B_k = \{|\tilde{e}_{k,1}\rangle, |\tilde{e}_{k,2}\rangle, \ldots, |\tilde{e}_{k,d}\rangle\}$. Suppose now that a measurement has been performed in the $B_k$ basis. Had the outcome been $|\tilde{e}_{k,n}\rangle$ (for some $1 \leq n \leq d$), the maximal log-likelihood value following that outcome would have been simply been

$$\mathcal{L}_{\tilde{e}_{k,n}} = \max_{\tilde{\psi}} \sum_{m=1}^{k-1} \log |\langle \tilde{\psi}|\phi_m \rangle|^2 + \log |\langle \tilde{\psi}|\tilde{e}_{k,n} \rangle|^2.$$  

(4)

Since however we do not know which of the $d$ outcomes will be obtained, in order to optimize the basis $B_k$ we must consider all possible outcomes and weigh them according to their chance of occurring, i.e., we need to maximize the maximal log-likelihood function averaged over all possible outcomes $B_k$:

$$\langle \mathcal{L} \rangle = \sum_{n=1}^{d} P(\tilde{e}_{k,n}|S_{k-1}) \mathcal{L}_{\tilde{e}_{k,n}},$$  

(5)

where $P(\tilde{e}_{k,n}|S_{k-1})$ is the probability of obtaining the state $|\tilde{e}_{k,n}\rangle$ as the outcome of the $k$-th measurement, given the measurement record $S_{k-1}$. The probability $P(\tilde{e}_{k,n}|S_{k-1})$ may be re-expressed as the probability of obtaining the outcome $|\tilde{e}_{k,n}\rangle$ conditioned on the oven emitting $|\tilde{\psi}\rangle$ and weighted by the probability that the emitted state is indeed $|\tilde{\psi}\rangle$ given the measurement record so far $S_{k-1}$, i.e.,

$$P(\tilde{e}_{k,n}|S_{k-1}) = \int P(\tilde{e}_{k,n}|\tilde{\psi}) p(\tilde{\psi}|S_{k-1}) d\tilde{\psi}.$$  

(6)

The optimal orthonormal basis for the $k$-th measurement, $B_k = \{|\tilde{e}_{k,1}\rangle, |\tilde{e}_{k,2}\rangle, \ldots, |\tilde{e}_{k,d}\rangle\}$, is thus by definition the basis that maximizes $\langle \mathcal{L} \rangle$, namely,

$$B_k = \arg\max_{\{\tilde{e}_{k,n}\}} \langle \mathcal{L} \rangle = \arg\max_{\{\tilde{e}_{k,n}\}} \sum_{n=1}^{d} \int p(\tilde{\psi}|S_{k-1}) |\langle \tilde{e}_{k,n}|\tilde{\psi} \rangle|^2 d\tilde{\psi} \times \max_{\psi} \left( \log p(\tilde{\psi}|S_{k-1}) + \log |\langle \tilde{\psi}|\tilde{e}_{k,n} \rangle|^2 \right),$$  

(7)

The solution to the above optimization problem would yield the basis of measurement for which the averaged maximum log-likelihood (over all possible measurement outcomes) is maximal.

While the optimization problem given in Eq. (7) is well-defined, finding the optimizing basis will, in general, be a fairly hard and time-consuming task. We therefore propose to ‘relax’ the above optimization problem to the simpler:

$$|e_{k,n}\rangle = \arg\max_{\psi} p(\tilde{\psi}|S_{k-1}),$$  

(8)

such that $|\langle \tilde{e}_{k,n}|\tilde{e}_{k,r} \rangle| = 0$ for all $1 \leq r \leq n - 1$. Within this approximation, the first basis state is simply $|e_{k,1}\rangle = \arg\max_{\tilde{\psi}} \prod_{m=1}^{k-1} |\langle \phi_m|\tilde{\psi} \rangle|^2 = |\psi_{k-1}\rangle$, i.e., it is the best guess for the state emitted by the oven based on the measurement record thus far, $S_{k-1}$, already computed in the previous step.

Eq. (8) is a good approximation to Eq. (7) when $p(\tilde{\psi}|S_{k-1})$ is peaked around a certain value. In this case, it is advantageous to ‘align’ one of the basis states with the peak of $p(\tilde{\psi}|S_{k-1})$ in order to maximize the cost function [Eq. (7)]. Since $p(\tilde{\psi}|S_{k-1})$ is a measure of how consistent $|\tilde{\psi}\rangle$ is with the measurement record $S_{k-1}$, as we gather more and more information about the emitted state, $p(\tilde{\psi}|S_{k-1})$ indeed becomes more and more sharply peaked around $|\tilde{\psi}\rangle$. As will also be illustrated in the next section, we shall see that the above approximation becomes valid very early on during the process, after only very few iterations.

In the next section we shall discuss several additional advantages to using the Eq. (8) as our measurement-basis optimization rule. However, it is worth pointing out that there should be no reason not to use the ‘unrelaxed’ optimization rule, Eq. (7), at least as the computational effort for doing so is reasonable.

One advantage of using the relaxed optimization condition, Eq. (8), is immediately apparent if the outcome of the $k$-th measurement is $|\psi_{k+1}\rangle = |\psi_{k-1}\rangle$. In this case $p(\tilde{\psi}|S_{k}) \sim p(\tilde{\psi}|S_{k-1}) |\langle \psi_{k-1}|\tilde{\psi} \rangle|^2$ and the most likely state obtained from the $k$ measurements thus far coincides with the most likely state of the previous step, i.e., $|\psi_k\rangle = |\psi_{k-1}\rangle$. Hence, the next measurement should include the outcome $|e_{k+1,1}\rangle = |\psi_k\rangle = |e_{k,1}\rangle$. In fact in this case without loss of generality we can take $B_{k+1} = B_k$ as all other basis states $|e_{k+1,n}\rangle$ with $n > 1$ yield $p(e_{k+1,n}|S_{k}) = 0$. Since our best guess $|\psi_k\rangle$ has a larger
and larger overlap with the emitted state as the procedure progresses, outcomes that correspond to best-guess-so-far $|\psi_k\rangle$ become more and more probable, which in turn implies a diminishing need for adjusting the measurement basis.

In what follows, we illustrate the efficiency of the proposed protocol compared with other tomographic procedures. To gain more insight into the rationale of the protocol, we discuss a few examples pertaining to qubit tomography in detail.

III. OPTIMIZED QUBIT TOMOGRAPHY

Let us now consider as a case study, the performance of the above protocol for the identification of a Haar-random pure qubit state $|\psi\rangle$. We note that for a qubit, the Hilbert space is two-dimensional, and therefore finding the most likely state at any iteration coincides with finding the optimal basis (as dictated by Eq. (8)) for the measurement of the next iteration. Furthermore, note that the maximization of the log-likelihood function, Eq. (3), is performed with respect to only two variables, e.g., the polar and azimuthal angles $\theta$ and $\phi$ of the orientation of the Bloch vector of the qubit.

A. Special cases

To gain insight into the details of the protocol, specifically to illustrate the validity of the relaxed optimization rule for obtaining the optimal basis of measurement, Eq. (8), in the proposed protocol, we first examine in some detail its first few iterations as they apply for the qubit case. Here, the first measurement is performed in a randomly chosen basis which we shall denote as $\{|\uparrow\rangle, |\downarrow\rangle\}$. Without loss of generality, let us assume that the outcome of that first measurement is $|\uparrow\rangle$. To determine the basis of measurement for the next iteration, one must first compute the probability density of obtaining $|\psi\rangle$ given that outcome, arriving at $p(\psi|\{\uparrow\}) = \cos^2(\theta/2)$, where $\theta$ is the polar angle of Bloch vector of $|\psi\rangle$. This probability density trivially yields the most likely state $|\psi\rangle = |\uparrow\rangle$. While the relaxed optimization rule, Eq. (8), dictates that we perform the next measurement in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis, a full optimization of Eq. (8) gives on the other hand an orthogonal direction $\{|\uparrow\rangle, -|\downarrow\rangle\}$ basis, where $|\pm\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \pm e^{i\varphi}|\downarrow\rangle)$ (without loss of generality we fix $\varphi = 0$). The probability density $p(\psi|\{\uparrow\})$ as well as the two measurement bases are depicted in Fig. 2. The above calculation reveals that in the first iteration, where very little is known about the emitted state, the full-optimization scheme gives fairly different, even contradicting, results, as to the next basis of measurement. In the second iteration, the outcome history $S_2 = \{|\uparrow\rangle, |\uparrow\rangle\}$ (equivalently $S_2 = \{|\uparrow\rangle, -|\downarrow\rangle\}$) yields the full-optimization (red) and relaxed (black) measurement bases that are depicted in Fig. 2. As can be clearly seen, already in the second iteration the relaxed and full optimization schemes are in very good agreement.

The third iteration measurement bases of the full and relaxed schemes are shown in Fig. 2. There, the full-optimization basis (red) and the ‘relaxed’ basis given by the protocol (black) are virtually on top of each other. Indeed, in line with the discussion following Eq. (8), we find that as the number of measurements increases, more information about the emitted unknown state is acquired (corresponding to $p(\psi|S_k)$ becoming more sharply peaked) preforming measurements in the basis in which the most likely state so far is one of the basis states, becomes more and more ‘informative’.

Next, we consider a scenario where the first $(k + 1)$ outcomes are $|\uparrow\rangle$ in the first $k$ measurements, followed by a $(k + 1)$-th measurement result of a $|\downarrow\rangle$ state. Note that this scenario follows the protocol directly: as long as the most likely state remains an outcome of a measurement, the measurement basis for the next iteration is not recomputed.

Now, the most likely state at the $(k + 1)$-th iteration is given by $|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle$, with $|\alpha|^2 + |\beta|^2 = 1$, where $\alpha$ is the solution to [c.f. Eq. (8)]

$$\hat{\alpha} = \arg \max_{\alpha} \left( f_1 \log |\alpha|^2 + (1 - f_1) \log(1 - |\alpha|^2) \right),$$

where we have defined $f_1 = \frac{k}{k + 1}$ and $f_\perp = 1 - f_1$ as the frequencies of $|\uparrow\rangle$ and $|\downarrow\rangle$, respectively.

The above equation can be easily solved and gives $\hat{\alpha} = \sqrt{\frac{1}{f_1}}$. It is worth pointing out that, interestingly, the log-likelihood function to be maximized takes the form of the (negative) binary entropy function $H(x) = -x \log x - (1 - x) \log(1 - x)$, with $0 \leq x \leq 1$.

The pure state that is most likely to yield the above sequence of results is in fact the family of states $|\psi\rangle = \sqrt{f_1}|\uparrow\rangle + e^{i\varphi} \sqrt{f_\perp}|\downarrow\rangle$. This family of states traces a circle on the Bloch-sphere representing the intersection of the sphere with a cone whose main axis is the state $|\uparrow\rangle$ and has an opening angle of $\theta = \arccos f_1$ (see Fig. 3). Since the maximizing state is degenerate, to construct the optimal basis for the following measure-
ment, one is free to choose $\varphi$ at will (here we choose $\varphi = 0$). The next-measurement basis in this case is therefore $\{\sqrt{F_1}|\uparrow\rangle + \sqrt{F_1}|\downarrow\rangle, \sqrt{F_1}|\uparrow\rangle - \sqrt{F_1}|\downarrow\rangle\}$. 

**B. The general case**

To test the performance of the method proposed here, we conducted $N_{\text{exp}} = 5000$ independent numerical experiments executing the ‘optimized tomography’ protocol for a large number of iterations ($N_{\text{iter}} = 2^{24}$). In each of these experiments, a Haar-random pure state $|\psi\rangle$ was generated, to simulate states emitted by the oven, followed by the application of the strategy discussed above. Measurements (one per iteration) were simulated numerically as well, using generation of random numbers to produce measurement outcomes with the appropriate probabilities, i.e., with probabilities $|\langle e_{k,n}|\psi\rangle|^2$. Here, $k$ is the measurement (or iteration) index and $n$ labels the basis states. In the qubit case, $n = 1, 2$. Throughout the execution of the protocol, the log-likelihood function, $\log p(\psi|S_k)$ of Eq. (2), was maximized whenever necessary using standard techniques (we found the Conjugate Gradient method to work very well) [37]. As noted earlier, in the qubit case, one needs to maximize over only two variables.

Using the infidelity,

$$ I = 1 - F = 1 - |\langle \psi|\psi_k\rangle|^2, $$

as our figure-of-merit to ascertain the success of our candidate state, we record the infidelity of our best-guess-so-far as a function of the number of trials, $N_{\text{iter}}$, averaging over the infidelities of the various experiments at each trial step, to obtain the average infidelity as the function of number of trials.

The scaling of the infidelity with the number of trials determines the performance of the method. The results are shown in Fig. 4 where we plot $\langle I(N_{\text{iter}})\rangle$ as a function of $N_{\text{iter}}$ (circles) on a log-log scale. We calculated the asymptotic behavior of the dependence to be

$$ \log_2 (I) = (-1.000 \pm 0.001) \log_2 N_{\text{iter}} + (1.00 \pm 0.01). $$

Figure 4 also shows how our proposed protocol compares with the ‘partially-adaptive’ strategy recently introduced by Mahler et al. [39] that has been shown to improve estimation accuracy quadratically. The strategy consists of a single adaptation step, where the first half of the qubits ($N_{\text{iter}}/2$) are measured in the eigenbasis of the Pauli operators, and based on the outcomes of this first phase, a best guess is generated. The eigenbasis of this best guess then serves as the basis of the measurements for the second half of the measurements [38]. While both methods scale similarly, namely inversely with the number of trials, the optimized protocol does somewhat better than the partially-adaptive protocol by a constant factor as the asymptote of the latter reads

$$ \log_2 (I) = (-1.000 \pm 0.001) \log_2 N_{\text{iter}} + (2.14 \pm 0.01). $$

Another line added to Fig. 4 is the average infidelity of the theoretical optimal collective measurement scheme on ensemble of $N_{\text{iter}}$ qubits [26]. The figure indicates that the proposed protocol is closer to the optimal average infidelity for any number of $N_{\text{iter}}$.

**C. Adjustment of measurement basis and numerical optimization**

At first glance, it may seem that the method presented here requires potentially-many adjustments to the basis of measurement, which in practice could be very time-
adjustments are logarithmically rare. This is illustrated in Fig. 5 which shows the infidelity as a function of number of iterations for five random experiments on a log-linear scale. The many plateaus observed in the infidelities of the experiment reflect same-measurement same-outcome streaks. The plateaus end with different-outcome results which requires an adjustment of the basis of the measurement as well a new calculation of the most likely state which in turns significantly lowers the infidelity (on average).

On a more quantitative note, we calculated the average number of measurement adjustments as a function of number of trials. The results are plotted in Fig. 6 showing a clear logarithmic dependence on the number of trials. The asymptotic fit reads \( y = (2.811 \pm 0.001) \log_2 N_{\text{iter}} + (-5.800 \pm 0.001) \) indicating that even if a change of the measurement basis is to be considered experimentally costly, these adjustments are logarithmically rare.

The fact that only a logarithmic amount of distinct outcomes and measurement adjustments is required also becomes important when storage of the history of measurement outcomes is concerned. Here, instead of storing the entire sequence \( S_k = \{ |\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_k\rangle \} \) one only needs to store the distinct outcomes together with their frequencies, i.e., \( S_k = \{ |\phi_1\rangle^{\otimes n_1}, |\phi_2\rangle^{\otimes n_2}, \ldots, |\phi_k\rangle^{\otimes n_k} \} \), where only distinct outcomes are included, \( k \) denotes the number of distinct outcomes at iteration \( k \), and \( n_m \) counts the number of times \( |\phi_m\rangle \) has been measured. In this notation the log-likelihood expression for maximization can be written as:

\[
\log p(\hat{\psi}|S_k) = \sum_{m=1}^k n_m \log |\langle \phi_m | \hat{\psi} \rangle|^2,
\]

which incidentally has been found to greatly facilitate the numerical maximization of the probability density.

IV. CONCLUSIONS AND FURTHER REMARKS

We described an optimized, fully-automated, self-adjusting, quantum state tomography procedure for pure states. The optimality of the protocol is achieved by requiring that at each step, the protocol yields the pure state that best captures our knowledge of the system together an information-optimized basis for the next measurement. This was achieved by maximizing, at each iteration, the appropriate likelihood function \[39\]. Moreover, unlike other methods, here no a priori knowledge of mutually-unbiased-bases is needed for the application of the protocol.

We illustrated the power of the technique in the case where the state to be found is a pure qubit state, and showed that our method is asymptotically closer to the theoretical bound than existing state-of-the-art adaptive procedures. Moreover, we showed that the number of learning, measurement-adjusting, steps is logarithmically rare, which makes the protocol attractive for a near-future implementation.
The protocol is designed to achieve optimality at every iteration, thus no post-processing of the data is required. It is therefore particularly interesting to apply as an in-situ procedure in integrated devices for quantum tomography. Such a device would act like a ‘robot’, correcting itself as needed to find the state emitted by an oven, based on the information it is gathering. In addition (and contrary to other methods) we note that the procedure offered here is optimized at every iteration. It can therefore be stopped at any stage, or after a chosen criterion of confidence or convergence is fulfilled, and no prior knowledge of the number of copies provided by the oven is necessary.

Finally, we note that the above method can be easily generalized to the cases where one is allowed to perform two- or more-particle measurements, or where prior information about the state-emitting oven is given. It would also be interesting to consider the possibility of generalizing the above protocol to the case of arbitrary mixed states. This case however will be reported elsewhere.

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[34] The constant equals $\frac{n^{-1}}{\sqrt{1-n^{-1}}}$.
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[36] Here we choose, for practical purposes, to take $\langle L \rangle$ to be the average over log-likelihood costs $\log p(\psi|S_k)$. This of course is not the only possible choice and in fact one could have equivalently taken $\langle L \rangle$ to be the average over likelihood functions $L = p(\psi|S_k)$. It is important to note however, that any good choice of $\langle L \rangle$ is expected to asymptotically converge to the same optimizing basis of measurement.
[37] In the qubit case, we have found that the log-likelihood function does not have local minima in which heuristic methods may get stuck.
[38] Denoting the basis of measurement by $|\uparrow \rangle$ and $|\downarrow \rangle$, and their frequencies of occurrence by $f_\uparrow$ and $f_\downarrow$, respectively, the pure state that best estimates $|\psi \rangle$ according to this procedure is $\sqrt{f_\uparrow}|\uparrow \rangle + \sqrt{f_\downarrow}|\downarrow \rangle$.
[39] In the future, one may even consider using quantum devices for the optimization step itself.