Asymptotic Efficiency and Finite Sample Performance of Frequentist Quantum State Estimation

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We undertake a detailed study of the performance of maximum likelihood (ML) estimators of the density matrix of finite-dimensional quantum systems, in order to interrogate generic properties of frequentist quantum state estimation. Existing literature on frequentist quantum estimation has not rigorously examined the finite sample performance of the estimators and associated methods of hypothesis testing. While ML is usually preferred on the basis of its asymptotic properties - it achieves the Cramer-Rao (CR) lower bound - the finite sample properties are often less than optimal. We compare the asymptotic and finite-sample properties of the ML estimators and test statistics for two different choices of measurement bases: the average case optimal or mutually unbiased bases (MUB) and a representative set of suboptimal bases, for spin-1/2 and spin-1 systems. We show that, in both cases, the asymptotic standard errors of the ML estimators grossly underestimate the estimation error in finite samples, rendering inference based on the asymptotic properties of the ML unreliable and misleading for experimentally realistic sample sizes. The results indicate that in order to fully exploit the information geometry of quantum states and achieve smaller reconstruction errors, the use of Bayesian state reconstruction methods - which, unlike frequentist methods, do not rely on asymptotic properties - is necessary, since the estimation error is typically lower due to the incorporation of prior knowledge.

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I. INTRODUCTION

Perhaps the most fundamental problem in quantum statistical inference (QSI) is the reconstruction of the density matrix of a quantum system on the basis of a finite number of quantum observations. Due to the rapidly growing interest in quantum computation and quantum control, the ability to retrieve the maximum amount of information about a quantum state based on the smallest number of measurements is a subject of paramount importance. The accuracy of all derivative forms of QSI, including process estimation, is ultimately determined by that of the underlying state estimation.

Methods for quantum state estimation can be formally subdivided into three categories. The first, tomographic inversion [1], is the least computationally expensive and most popular technique. However, tomographic inversion cannot enforce the constraints on the density matrix during estimation, and hence the estimates produced are often not physically meaningful. The second class consists of frequentist techniques of inference based on a likelihood function, the most notable of which is maximum likelihood (ML) estimation [2]. This class of methods avoids the problems associated with tomography and is asymptotically more efficient than the latter (as explained in Section III E). However, it delivers distributional results for the estimators of the parameters of interest under the assumption of an infinite number of measurements. Hence, for finite sample sizes, the estimated confidence intervals for the parameters may have actual coverages quite different from the corresponding asymptotic ones and, as is well known in the statistics literature, this divergence typically tends to become more pronounced as the number of parameters and non-linearity of the model increases. All forms of frequentist inference, including tomographic inversion and ML estimation, require a complete observation level, i.e. \( N^2 - 1 \) linearly independent observable operators where \( N \) is the Hilbert space dimension, in order to estimate all the parameters. The third type, Bayesian estimation [3, 4, 5, 6, 7], which is based on updating a prior plausibility distribution of the parameters based on observed data, lends itself readily to both incomplete observation levels and a finite number of measurements. Moreover, the estimation error that arises in Bayesian methods is typically lower, reflected in shorter lengths of Bayesian confidence intervals compared to their frequentist counterparts, due to the use of such priors 1.

1 The principle of entropy maximization (PEM) is an estimation methodology that can consistently estimate all parameters with an incomplete observation level, since it implicitly assumes a prior plausibility distribution over the parameter space. However, it has been shown that the von Neumann entropy employed...
In this paper, we investigate the finite sample properties of ML estimators of the density matrix of finite-dimensional, spin-1/2 (one qubit) and spin-1 quantum systems. Among frequentist estimation techniques, ML is usually preferred on the basis of its asymptotic properties - (i) the ML estimator is asymptotically efficient in the sense that its asymptotic variance achieves the Cramer-Rao lower bound for consistent estimators, (ii) likelihood based testing approaches are optimal, in the sense of the Neyman-Pearson Fundamental Lemma and the Large Deviation Principle, for a broad class of hypothesis testing problems. However, the finite sample properties of ML estimators and test statistics are often less than optimal. Existing literature on quantum ML has not rigorously examined the finite sample performance of the estimators and associated methods of hypothesis testing. To our knowledge, there is only one extant study on the efficiency of frequentist quantum state estimation [5], and robust numerical techniques are lacking. Minimizing finite sample estimation errors is essential for making optimal quantum decisions, which underlie emerging quantum feedback control and computation strategies [6]. Lack of rigorous understanding of the small sample estimation errors has inhibited the application of ML to practical problems in quantum information and control.

We shed light on the following issues:

- How are the small sample biases of the ML estimators affected by the sample size?
- How do the finite-sample standard errors, and hence the associated 95% confidence intervals, compare to the corresponding asymptotic ones and how does the coverage of the intervals change with increase in the sample size?
- How does the small sample behavior of the test statistics for physical quantities of interest in quantum decision theory compare to their known asymptotic behavior for different sample sizes?

We show that the finite sample properties of ML differ significantly from the corresponding asymptotic ones for experimentally realistic sample sizes. In particular, the finite-sample standard errors are orders of magnitude bigger than the corresponding asymptotic ones. This feature holds for sample sizes approaching the limit of experimental feasibility. Consequently, the asymptotic confidence intervals grossly undercover in finite samples and the test statistics exhibit severe size distortions.

In addition, the assessment of the estimation error in QSI is complicated by the existence of multiple measurement strategies due to the noncommutativity of the probability space, and ambiguities regarding the optimal measurement strategy. We compare the relative efficiencies of average-case optimal (MUB) and representative suboptimal measurement strategies. We show that the asymptotically predicted advantages of optimal measurements are diminished in finite samples, to the extent that measurement strategies that are experimentally simpler to implement may perform almost as well as asymptotically optimal measurements.

The paper is organized as follows. Section II discusses the asymptotic properties of the ML and compares it to the alternative estimation approaches. Section III details the properties of ML estimators of the quantum density matrix. Section IV describes the Bloch vector parameterization, mutually unbiased measurement bases (MUB), and representative suboptimal measurement strategies considered in this paper. Section V discusses the details of the globally convergent Newton-Raphson and quasi-Newton algorithms used for constrained parameter optimization, along with methods for kernel density estimation of finite sample distributions. In Section VI, we present the estimation results for general mixed spin-1/2 and spin-1 density matrices, comparing the finite sample versus asymptotic properties of estimators and test statistics for physical quantities of interest in quantum decision theory. Finally, in the concluding Section VII, we draw conclusions regarding the efficiency of frequentist quantum state estimation and discuss Bayesian extensions.

II. PROPERTIES OF FREQUENTIST AND BAYESIAN ESTIMATORS

A. Maximum Likelihood Estimators

Let \( x = (x_1, \ldots, x_m) \) be an i.i.d. sample of size \( m \) from a population with probability density function \( p(x|\theta) \), which depends on the unknown parameter vector \( \theta \) whose true value is \( \theta_0 \). The value of the parameter vector that maximizes the likelihood function - the joint density of the sample defined as a function of the unknown parameter vector \( \theta \) - is called the ML estimator of \( \theta \):

\[
\hat{\theta}_{ML}^m = \arg \max_{\theta \in \Theta} L(\theta|x) = \arg \max_{\theta \in \Theta} \left( \prod_{i=1}^{m} p(x_1|\theta) \cdots p(x_m|\theta) \right),
\]

where \( \Theta \) denotes the admissible parameter space. Typically, the logarithm of the likelihood function, \( \ln L(\theta|x) \), is easier to maximize numerically because of its separability. By maximizing the log likelihood, the ML estimator minimizes the Kullback-Leibler distance between the estimated and true probability distributions.

ML has several properties that make it an attractive frequentist estimation procedure:
1. **Consistency**: An estimator \( \hat{\theta}_m \) is consistent for the parameter \( \theta \) (written as plim \( \hat{\theta}_m = \theta_0 \)) if for every \( \epsilon > 0 \),

\[
\lim_{m \to \infty} P_\theta \left\{ |\hat{\theta}_m - \theta_0| \geq \epsilon \right\} = 0.
\]

The ML estimator is consistent: \( \text{plim} \hat{\theta}_{ML} = \theta_0 \).

2. **Invariance**: The ML estimator of \( c(\theta) \) is \( c(\hat{\theta}_{ML}) \), for a continuous and continuously differentiable function \( c(\cdot) \).

3. **Asymptotic Normality.** For a sequence of estimators \( \hat{\theta}_m \), if \( k_m \left( \hat{\theta}_m - \theta_0 \right) \xrightarrow{d} N(0, \Sigma) \) as \( m \to \infty \), where \( \xrightarrow{d} \) denotes convergence in distribution and \( k_m \) is any function of \( m \), \( \hat{\theta}_m \) is said to be \( \sqrt{k_m} \)-consistent for \( \theta \) and has an asymptotic normal distribution with asymptotic covariance matrix \( \Sigma \).

The ML estimator is asymptotically normally distributed:

\[
\sqrt{m} \left( \hat{\theta}_{ML} - \theta_0 \right) \rightarrow N(0, I^{-1}(\theta_0)),
\]

where \( I(\theta_0) = -\mathbb{E} \left[ \frac{\partial^2 \ln L(\theta_0|x)}{\partial \theta \partial \theta'} \right] \).

\( I(\theta_0) \) is called the expected Fisher information matrix. Note that the asymptotic covariance matrix of the ML estimator is a function of the unknown parameters. Two approaches exist for consistent estimation of the expected Fisher information matrix thereby providing feasible versions of the observed Fisher information matrix. The first estimator replaces the expected second derivatives matrix of the log likelihood function with its sample mean evaluated at the maximum likelihood estimates,

\[
\hat{I}_1(\hat{\theta}_{ML}) = -\left[ \frac{\partial^2 \ln L(\hat{\theta}_{ML}|x)}{\partial \theta \partial \theta'} \right].
\]

The second estimator is based on the result that the expected second derivatives matrix is the covariance matrix of the first derivatives vector,

\[
\hat{I}_2(\hat{\theta}_{ML}) = \left[ \left( \frac{\partial \ln L(\hat{\theta}_{ML}|x)}{\partial \theta} \right) \left( \frac{\partial \ln L(\hat{\theta}_{ML}|x)}{\partial \theta} \right)^T \right].
\]

4. **Asymptotically efficient.** A sequence of consistent estimators \( \hat{\theta}_m \) is asymptotically efficient if

\[
\sqrt{m} \left( \hat{\theta}_m - \theta_0 \right) \xrightarrow{d} N(0, I^{-1}(\theta_0)) \quad \text{where} \quad I(\theta) = -\mathbb{E} \left[ \frac{\partial^2 \ln L(\theta|x)}{\partial \theta \partial \theta'} \right] ; \quad [mI(\theta_0)]^{-1} \quad \text{is called the Cramer-Rao lower bound (CRB) for consistent estimators.}
\]

Property 4 is the subject of the following classic lemma of frequentist inference.

**Lemma 1** The eigenvalues of the covariance matrix of parameter estimates of an asymptotically unbiased frequentist estimator are bounded from below by the eigenvalues of \( (mI(\theta_0))^{-1} \ = \{ -m \mathbb{E} \left[ \frac{\partial^2 \ln L(\theta_0|x)}{\partial \theta \partial \theta'} \right] \}^{-1} \).

The maximum likelihood estimator asymptotically (i.e., in the limit of an infinite number of measurements) achieves this lower bound.

In addition, likelihood based testing approaches are optimal, in the sense of the Neyman-Pearson Fundamental Lemma and the Large Deviation Principle, for a broad class of hypothesis testing problems. A hypothesis test \( T \), based on a test statistic \( W(x) - \) a function of the data - is a rule that specifies for which values of \( x \) (the acceptance region \( A \)) the null hypothesis \( H_0 : \theta \in \Theta_0 \) is accepted, and for which values (the rejection region \( R \)) it is rejected (and the alternative hypothesis \( H_1 : \theta \in \Theta_1 \)) is accepted.

The size \( s(T) \) of a hypothesis test \( T \) is the probability of rejecting the null hypothesis given that it is true. The power \( p(T) \) of a hypothesis test \( T \) is given by the probability of rejecting the null hypothesis given that it is false. Typically, when defining the power of a test, one assigns the test to a class based on its size. For \( 0 \leq \alpha \leq 1 \) a test with power function \( \beta(\theta) \) is a size \( \alpha \) test if \( \sup_{\theta \in \Theta_0} \beta(\theta) = \alpha \).

**Definition 1** Given a class of hypothesis tests for testing \( H_0 : \theta \in \Theta_0 \) versus \( H_1 : \theta \in \Theta_1 \), where \( \Theta_0 \cup \Theta_1 = \Theta \), the admissible parameter space, a test in that class with power function \( \beta(\theta) \) is uniformly most powerful (UMP) if \( \beta(\theta) \geq \beta'(\theta) \) for every \( \beta'(\theta) \) in that class.

An important type of hypothesis test based on ML is the likelihood ratio test. Likelihood ratio test statistics take the form

\[
\lambda(x) = \frac{L(\hat{\theta}_{ML}|x)}{L(\hat{\theta}_{ML}|x)}
\]

where \( \hat{\theta}_{ML} \) is the constrained ML estimator. It can be shown that likelihood ratio tests are UMP in their respective classes. In our simulation analysis, we rely on an alternative testing procedure, namely the Wald test, which inherits the optimality properties of the likelihood ratio test on account of their asymptotic equivalence.

This choice is made primarily on the basis of the ease of computation. The likelihood ratio test requires calculation of both restricted and unrestricted estimators. The Wald test, on the other hand, requires only the unrestricted estimator. Since some of our hypothesis tests involve nonlinear constraints and estimation of the constrained model is cumbersome, we rely on the Wald testing procedure.

Because of properties 1-4 and the fact that likelihood ratio tests are UMP, the maximum likelihood estimation methodology is considered the most desirable among frequentist estimation techniques.
B. Method of Moments Estimators

An alternative method of frequentist inference, which may be used to estimate the parameters of the quantum density matrix, is the Method of Moments approach. Suppose that although the probability density function \( p(x|\theta) \) is unknown, \( n \) moments of the density function have analytical representations in terms of the parameter vector \( \theta \). Let these \( n \) population moments be denoted by \( E[f(x_i)] = \mu(\theta) \), where \( f(x_i) = (f_1(x_i), f_2(x_i), ..., f_n(x_i))^T \) and \( \mu(\theta) = (\mu_1(\theta), \mu_2(\theta), ..., \mu_n(\theta))^T \). The Method of Moments (MM) Estimator of \( \theta \), denoted \( \hat{\theta}_{MM} \), is the value of the parameter vector that equates the population moments with the corresponding sample moments:

\[
\hat{\mu}(\hat{\theta}_{MM}) = \frac{1}{m} \sum_{i=1}^{m} f(x_i)
\]

Note that the Method of Moments approach involves solving a system of \( n \) (possibly nonlinear) equations in \( n \) unknown parameters. Like the ML estimator, the MM estimator is consistent and asymptotically normally distributed. However, while the ML estimator exploits all the information contained in the likelihood of the data, the MM estimator only uses the information in a chosen set of moments of the data. Hence, unlike the ML estimator, the MM estimator is not asymptotically efficient, i.e. its asymptotic variance does not attain the Cramer-Rao lower bound. The asymptotic distribution of the MM estimator is:

\[
\sqrt{m} \left( \hat{\theta}_{MM} - \theta_0 \right) \rightarrow \mathcal{N}[0, V],
\]

where \( V = D^{-1} \Omega (D^{-1})^T \),

\[
D = \mathbb{E} \left[ \frac{\partial (f(x_i) - \mu(\theta_0))}{\partial \theta} \right],
\]

\[
\Omega = \mathbb{E} \left[ (f(x_i) - \mu(\theta_0))(f(x_i) - \mu(\theta_0))^T \right].
\]

C. Bayesian Estimators

In the alternative paradigm of Bayesian estimation, the estimation error that arises is typically lower than that in frequentist estimation. Bayesian estimation differs fundamentally from frequentist methods in that the parameters \( \theta_i \) are treated as random variables. The goal is not to estimate a unique probability distribution, which can only truly be known in the limit of an infinite number of measurements, but to update a so-called prior plausibility distribution to a posterior plausibility distribution based (only) on the observed data. The posterior plausibility distribution is given by

\[
p(\theta \mid x \wedge I) \, d\theta = \frac{L(x \mid \theta) \, p(\theta \mid I) \, d\theta}{\int_{\Theta} L(x \mid \theta) \, p(\theta \mid I) \, d\theta},
\]

where \( p(\theta \mid I) \) denotes the prior plausibility distribution, i.e., the probability of the parameter vector taking on the value \( \theta \) given our prior information \( I \) regarding the parameter space, \( L(x \mid \theta) \) denotes the joint probability density, and \( \Theta \) denotes the space of admissible parameters \( \theta \).

Conditional simulation is required to retrieve quantities of interest, including the parameter estimates, which are given formally by the posterior means

\[
\hat{\theta}_i = \frac{\int_{\Theta} \theta \, p(\theta \mid x \wedge I) \, d\theta}{\int_{\Theta} p(\theta \mid x \wedge I) \, d\theta}.
\]

Unlike frequentist estimators, the notion of a confidence or credible interval can be rigorously defined for finite samples only for Bayesian estimators. This allows one to rigorously report finite sample uncertainties. The 100 \( \ast \ c\% \) Bayesian credible interval for the parameter \( \theta_i \) is the interval \([a, b] \) such that

\[
\int_{-\infty}^{-\infty} \cdots \int_{a}^{b} \cdots \int_{-\infty}^{-\infty} p(\theta \mid x \wedge I) \, d\theta_1, \cdots d\theta_i, \cdots d\theta_n = c.
\]

III. ESTIMATION OF THE DENSITY MATRIX

A. Quantum estimation and the likelihood function for state reconstruction

In this section we apply and extend the classical estimation framework in Section II to estimation of the quantum density matrix. Quantum statistical inference is based on the notion of a quantum probability space.

Definition 2 Consider a measurable space \((\chi, A)\), where \( \chi \) is the set of all possible measurement outcomes and \( A \) is the \( \sigma \)-Algebra of subsets of \( \chi \). An operator-valued probability measure (POVM) is a \((\sigma)\) function \( M : A \rightarrow B(H) \), where \( B(H) \) is the set of bounded positive semidefinite, Hermitian linear operators on a Hilbert space \( H \).

Definition 3 A quantum probability space is a measurable space \((\chi, A)\), together with an operator-valued probability measure \( M \), such that the outcome \( x \in \chi \) has probability density function \( p(x|\theta) = \text{Tr}(\rho(\theta)F(x)) \), where \( F(x) \in H \) and \( \rho(\theta) \) is a positive-semidefinite, unit trace, Hermitian matrix (parametrized by a vector \( \theta \) of parameters) called the density matrix.

Note that \( x \) in this context denotes the outcome of a single measurement. The measure \( M \) is explicitly defined in terms of the operators \( F(x) \), and an associated scalar-valued probability measure \( \mu \) satisfying \( \mu(\chi) = 1 \), through the relation \( M(A) = \int_A F(x) \, \mu(dx) \).

For \( N \)-dimensional (finite) quantum systems, we write \( F(x_i) = F_i \), \( i = 1, \ldots, N^2 - 1 \), and denote the outcome of the \( k \)-th measurement by \( F_{ik} \). \( F_i \) is then a \( N \times N \)
positive-semidefinite Hermitian matrix. The outcomes $x$ are indexed by the set of integers $(1, \cdots, N^2 - 1)$. In this case, we have $\mu(\chi) = \frac{1}{N} \text{Tr}(M(\chi)) = 1$.

For simplicity of exposition, we collect all the distinct parameters of the density matrix, $\rho$, into the $(N^2 - 1)$-dimensional vector, $\theta$. The most convenient parameterization of $\rho(\theta)$ differs based on the state estimation method; various parameterizations are discussed in Section IV. The likelihood function for quantum state estimation is then

$$L(\theta | x) = \prod_{k=1}^{m} \text{Tr}(\rho(\theta)F_{ik})$$

which may be interpreted as the probability of obtaining the set of observed outcomes for a given density matrix $\rho(\theta)$. The ML estimator of the density matrix seeks to identify the admissible parameter vector $\theta$ at which this likelihood is maximal.

### B. Quantum measurement bases

A **resolution of the identity** on a Hilbert space $\mathcal{H}$ of quantum states is a normalized operator-valued measure. Generally, the resolution of the identity satisfies

$$M(\chi) = \int_{\chi} F(x)\mu(dx) = I.$$

For finite-dimensional systems, to which we restrict our attention,

$$\sum_{i} F_{i}\mu(x_{i}) = I_{N},$$

where $I_{N}$ denotes the $N \times N$ identity matrix.

An important feature of quantum probability is that the operators $F_{i}$ do not all mutually commute. The subsets $A \in \mathcal{A}$ of the space of possible measurement outcomes $\chi$ may be chosen to be pairwise disjoint and associated with subsets $M_{A} = \{F_{i_{1}}, \cdots, F_{i_{N-1}}\}$ of commuting observables whose members do not commute with those of any other subset. The $M_{A}$ are then said to constitute distinct measurement “bases”.

Writing each $F_{i}$ as an $N \times N$ Hermitian matrix, it is convenient to represent each basis $M_{A}(\cdot)$ in terms of an $N \times N$ matrix of common eigenvectors $V(\cdot)$, $0 \leq r \leq N$. Given that the density matrix is a function of $N^{2} - 1$ independent parameters, the minimal cardinality resolution of the identity must be composed of $N + 1$ subsets $A \in \mathcal{A}$. We note, however, that many resolutions of the identity are redundant in that they are associated with $n > N + 1$ bases $M_{A}$.

In the current work, the data $x$ consist of $m_{i}$ measurement outcomes in each of $p$ measurement bases with $\sum_{i=1}^{p} m_{i} = m$. The measurement bases used are discussed further in Section IV B.

### C. Quantum maximum likelihood estimation

Among frequentist estimation techniques, ML has been employed most extensively for reconstruction of quantum states. In quantum ML estimation, we aim to identify the maximum of the likelihood function (3) over the set of admissible density matrices. All parameterizations of the density matrix require the imposition of constraints on parameter vector $\theta$ (see Section IV); these constraints are necessary for expression (3) to be a well-defined likelihood. Assuming the constraints on the parameter vector $\theta$ are of the general form $a_{j}(\theta) \geq 0$, $j = 1, \cdots, N$, the problem can be formulated in terms of the Lagrangian function

$$L(\theta, \gamma | x) = \ln \left[ \prod_{k=1}^{m} \text{Tr}(\rho(\theta)F_{ik}) \right] + \sum_{j=1}^{N} \lambda_{j} \left( a_{j}(\theta) - \gamma_{j}^{2} \right),$$

where the first term is $\ln L(\theta | x)$ in the absence of constraints (i.e., $\rho(\theta)$ need not be an admissible density matrix and $L$ need not be a well-defined likelihood), the $\gamma_{j}$ denote slack variables ($\gamma_{j} = 0$ in the case of an equality constraint) and the $\lambda_{j}$ denote Lagrange multipliers. It is convenient to order the $N$ constraints such that the first constraint enforces the unit trace of $\rho$, and the following $N - 1$ constraints enforce its positive semidefiniteness. Note that $L (\theta | x)$ is a well-defined likelihood function only in the presence of these constraints. For parameterizations where positive semidefiniteness is implicit in the parametrization (such as the Cholesky parametrization (2)), $\lambda_{j} = 0$, $j = 2, \cdots, N$, and for parameterizations where the unit trace constraint is implicit in the parametrization (such as the Bloch vector parametrization, Sect. IV), $\lambda_{1} = 0$. We denote the vector of parameters $\theta(\lambda, \gamma) \equiv t$. Finding the optimum corresponding to this Lagrangian entails searching for parameter vector $t$ that renders the gradient vectors $\nabla L(\theta)$ and a linear combination of $\nabla (a_{j}(\theta) - \gamma_{j})$, $j = 1, ..., N$ parallel. There are two common approaches to solving this problem: 1) minimization of the “sum of squares” (of the first-order conditions) function $\sum_{i} \left( \frac{\partial C}{\partial t_{i}} \right)^{2}$; 2) finding the roots of the system of nonlinear equations $\frac{\partial C}{\partial t} = 0$ using the Newton-Raphson (NR) method. In fact, methods 1) and 2) may be combined to produce a globally convergent NR algorithm. Further details on solving the constrained optimization problem are provided in Section IV.

Note that the ML estimator obtained by maximizing the likelihood defined by the Lagrangian (11) is consistent, asymptotically normally distributed, and has an asymptotic covariance matrix equal to the inverse of $m$ times the expected Fisher information matrix, $(mI(\theta_{0}))^{-1}$ (see Section II for details). We estimate the expected Fisher information using equation (11) in Section II.
D. Asymptotic properties of quantum maximum likelihood estimators

In quantum statistics, there are multiple Cramer-Rao type inequalities, each with its own associated (quantum) Fisher information. Some of these correspond to particular measurement strategies, whereas others are in fact unachievable. Work in quantum probability theory [4] has indicated that \( \frac{1}{m} I(\theta_0)^{-1} \) for an arbitrary choice of measurement bases is generally not the tightest asymptotic lower bound achievable in quantum ML estimation. However, the measurements that maximize the Fisher information depend on the true, unknown state of the quantum system, rendering the practical utility of the notion of the tightest possible Cramer-Rao bound questionable.

Although the choice of measurement bases that can achieve the tightest possible Cramer-Rao bound depends on the true \( \rho \), there exists an approach to optimal measurement that is agnostic to the true value of \( \rho \). Wootters [13] proposed a construction of measurement bases that maximizes the average information (over the set of all possible density matrices) obtained via a set of \( m \) measurements. These so-called mutually unbiased measurement bases (MUB) are “maximally noncommutative” in the sense that a measurement in one basis provides no information as to the outcome of a measurement in each basis restricts the variance in the information gained by measurements to the asymptotically normal distribution over the Bloch vector space. The uncertainty distance between the subspaces (and not the parameters) is volume unachievable. Work in quantum probability theory indicates that this condition is equivalent to minimizing the “uncertainty volume” in the parameter space; in the absence of measurements, this is equal to the volume of the Bloch vector space. The uncertainty distance for estimation of a single parameter is the standard deviation of the estimator; the uncertainty volume is the product of the standard deviations of the estimators for each of the parameters. In terms of uncertainty volumes, the information gained by measurements is

\[
D = -\ln \left( \frac{W}{W_0} \right) - \left( \frac{N^2 - 1}{2} \right) \ln(\pi e),
\]

where \( W \) is the uncertainty volume after measurements and estimation and \( W_0 \) is volume of the Bloch vector space.

Denote by \( T_r \) the \((N - 1)\)-dimensional subspace of \( su(N) \) or \( B_{N^2 - 1} \) associated with measurement basis \( V^{(r)} \). The total uncertainty volume is diminished by overlaps between the subspaces \( T_r \). It can be shown that this total volume \( W \) may be written \( W = \frac{1}{\text{vol}(T_1, \cdots, T_{N+1})} \) where \( T_r \) is the \((N - 1)\)-dimensional subspace of \( su(N) \) associated with measurement basis \( V^{(r)} \) and \( (T_1, \cdots, T_{N+1}) \) denotes the \((N^2 - 1)\)-dimensional parallelepiped whose edges are the \( N + 1 \) sets of eigenvectors associated with each of the subspaces \( T_r \). Thus the Kullback-Leibler information gain [11] in updating the flat prior distribution to the asymptotically normal distribution is then

\[
\ln(W_r)), \text{ the log of the average uncertainty volume in subspace } T_r, \text{ does not depend on the choice of measurements since it is the log of the product of standard deviations of multinomial parameters in a single measurement basis, averaged over all possible multinomial parameters } p_1, \cdots, p_N. \text{ Thus the average Kullback-Leibler or Fisher information is a function of only } \text{vol}(T_1, \cdots, T_{N+1}), \text{ which in turn is determined by the relative orientations of the bases (and not the parameters). The total uncertainty volume is minimized when } (T_1, \cdots, T_{N+1}) \text{ is a } \text{rectangular solid with all the unit vectors defining the edges being orthogonal}; \text{ this is equivalent to the condition that the subspaces } T_1, \cdots, T_{N+1} \text{ are mutually orthogonal. Wootters showed [13] that this condition is equivalent to requiring that}

\[
|\langle \mathbf{v}_i^{(r)}, \mathbf{v}_j^{(r')} \rangle| = \frac{1}{\sqrt{N}},
\]

where \( \mathbf{v}_i^{(r)}, \mathbf{v}_j^{(r')} \) are column vectors in the bases \( V^{(r)}, V^{(r')} \) respectively, and \( |\langle \cdot, \cdot \rangle| \) denotes the modulus of the Hermitian inner product. Whereas mutual

\( ^2 \text{In frequentist statistics, the relative entropy is always defined in terms of the passage from the flat plausibility distribution to an asymptotically (multivariate) normal distribution.} \)
nonorthogonality of the edges of the parallelepiped may decrease the asymptotic uncertainty volume in particular subspaces $T_x$, the total asymptotic uncertainty volume is always increased by such nonorthogonality. Explicit formulas for measurement bases that satisfy are known in the cases where the Hilbert space dimension $N$ is the power of a prime, and are discussed in Section IVB.

An unresolved question in the literature is the magnitude of the information loss for finite sample sizes incurred due to not using MUB or other approaches to optimal quantum measurement. In many experimental setups, it is not convenient to use these specialized bases. We aim to clarify the practical utility of optimal quantum measurements in ML estimation, and assess the extent to which frequentist quantum estimation can effectively make use of the associated optimal efficiencies.

E. Estimation of the density matrix by tomographic inversion

An alternative frequentist method of quantum state estimation that is not based on a likelihood function is tomographic inversion [13]. This involves an application of the Method of Moments approach described in Section II. Adopting the notation $x_{ik}$ for the $k$-th observation returning outcome $i$, let the MM estimator functions $f_j(x_{ik})$ be given by $f_j(x_{ik}) = \delta_{ij}$. We then have $E[f_j(x_{ik})] = p_i = \text{Tr}(\theta F(x_{ik}))$, where $p_i$ denotes the probability of observing outcome $F(x_{ik}) = F_{ik}$. The tomographic inversion method estimates the parameters by equating these population moments to the corresponding sample moments: the parameter estimates $\hat{\theta}_{MM,j}$, $1 \leq j \leq N^2 - 1$ are obtained by inverting a system of equations of the form

$$\text{Tr}(\theta F) = c_j, \quad 1 \leq j \leq N^2 - 1,$$

where $c_j$ denotes the frequency with which outcome $F_i$ is observed in the sample. Introducing the notation $A_{ij} = \frac{\partial \text{Tr}(\theta F)}{\partial \theta_j}$, we solve for the estimated parameter vector as $\hat{\theta} = A^{-1}c$ for any parameterization $\rho(\theta)$ that is linear in $\theta$ (see Section IV).

However, this method has two major drawbacks. First, since no parametrization $\rho(\theta)$ guarantees satisfaction of each of the positive-semidefiniteness, unit trace, and Hermiticity constraints on $\rho$ (see Section IV), direct inversion can yield unphysical density matrix estimates. Second, while the ML estimator exploits all the information contained in the likelihood of the data, the MM estimator only uses the information in a chosen set of moments of the data. Hence, unlike the ML estimator, the MM estimator is not asymptotically efficient, i.e. its asymptotic variance does not attain the Cramer-Rao lower bound. For these reasons, we do not consider tomographic inversion in our assessment of the performance of frequentist quantum estimation.

F. Bayesian versus frequentist density matrix estimation

In the alternative, Bayesian approach to quantum state estimation, the posterior distribution $p(\theta | x \land I)$ takes the form:

$$p(\theta | x \land I) d\theta = \frac{L(x | \theta) p(\theta | I) d\theta}{\int_{\Theta} L(x | \theta) p(\theta | I) d\theta}$$

$$= \frac{\prod_k \text{Tr}(F_{ik} \rho(\theta))) p(\theta) d\theta}{\int_{\Theta} \prod_k \text{Tr}(F_{ik} \rho(\theta))) p(\theta) d\theta}.$$  \hspace{1cm} (7)

The density matrix can be estimated by the posterior mean of each of its elements (corresponding to a quadratic “loss function”), namely

$$\rho_{x \land I} \equiv \int_{\Theta} \rho(\theta) p(\theta | x \land I) d\theta$$

$$= \frac{\int_{\Theta} \rho(\theta) \prod_k \text{Tr}(F_{ik} \rho)) p(\theta) d\theta}{\int_{\Theta} \prod_k \text{Tr}(F_{ik} \rho)) p(\theta) d\theta}.$$  \hspace{1cm} (8)

Alternative loss functions can be used to retrieve other estimable quantities of interest.

Bayesian credible intervals can be obtained according to expression (II-C) by sampling from the posterior density [14]. These credible intervals do not rely on asymptotic results / Fisher information. We do not compute Bayesian integrals in this work; our goal is rather to determine whether such a need exists given the finite sample performance of the computationally simpler frequentist estimators.

IV. DENSITY MATRIX PARAMETERIZATION AND CHOICE OF MEASUREMENT BASES

A. Bloch vector parameterization

In maximum likelihood estimation of the quantum density matrix, a constrained optimization must be carried out, where the constraints correspond to preservation of the unit trace and/or positive semidefiniteness properties of the density matrix. The dimension of the parameter space increases quadratically with the Hilbert space dimension, necessitating the use of efficient parameterizations of the density matrix. The three most commonly used parameterizations are the Bloch vector [15], Euler angle [16] and the Cholesky [2] parameterizations. Within the last few years, considerable advancements have been made in extending the Bloch and Euler parameterizations to arbitrary $N$-dimensional Hilbert spaces. The Euler angle parameterization of the density matrix, which is based on the Euler angle parameterization of the special unitary group $SU(N)$, employs the generators in the Lie algebra $su(N)$ to parameterize $\rho$ in terms of the Lie algebra exponential map.
constraint equations are linear in the parameters, but because the parameters appear as exponents, the likelihood takes on a complicated form. In the Cholesky parameterization, \( \rho = A^\dagger A \) with \( A \) upper triangular has real elements on the diagonal. \( \rho \) is then automatically positive-semidefinite, but is associated with a nonlinear expression for the likelihood, and is not standard in other applications. Here, we employ the so-called Bloch vector parameterization, where the probability of an observable outcome according to the Born rule, \( \text{Tr}(\rho(\theta)F_i) \), is a simple linear function of the parameter vector \( \theta \). Moreover, the Bloch vector parameterization is perhaps the most commonly used in the statistical physics of finite-dimensional quantum systems (especially in quantum information applications). Most importantly, asymptotic standard errors in the Bloch vector parameterization can be computed using the standard methods described in Section II because the positive-semidefinite constraints are inequality restrictions that are nonbinding at the optimum.

In the Bloch vector parameterization \(^[15]\), the Hermitian operator \( \rho \) is parameterized in terms of an orthogonal basis \( \{ \lambda_j \} \), \( 1 \leq j \leq N^2 - 1 \) for the vector space of traceless Hermitian operators on an \( N \)-dimensional Hilbert space. In two dimensions, these are the familiar Pauli spin matrices, whereas in three dimensions they are the so-called Gell-Mann matrices. \( \rho \) can then be written

\[
\rho \equiv \rho(\theta) = \frac{1}{N} I_N + \frac{1}{2} \sum_{j=1}^{N^2-1} \theta_j \lambda_j,
\]

\( (\theta_1, ..., \theta_{N^2-1}) \equiv \theta \in B_{N^2-1} \subset R^{N^2-1}, \)

where the \( N^2 - 1 \) matrices \( \lambda_j \) satisfy the conditions a) \( \lambda_j = \lambda_j^\dagger \), b) \( \text{Tr}(\lambda_j) = 0 \), c) \( \text{Tr}(\lambda_i \lambda_j) = 2\delta_{ij} \). These are the defining conditions of the generators of the Lie group \( SU(N) \) that generalize the Pauli spin matrices. The \( \theta_j \) are given by \( \theta_j(\rho) = \text{Tr}(\lambda_j \rho) \) (i.e., are expectation values of the observable generators). The vector \( \theta_j \lambda_j \) is called the Bloch vector.

\( B_{N^2-1} \) is a compact convex subset of \( R^{N^2-1} \). Let \( a_i(\lambda) \) denote the coefficients of the characteristic polynomial of \( \rho \), \( \det(gI_N - \rho) \), where \( \rho \) takes the form \(^3\). In the alternative Euler angle parameterization, neither the unit trace nor the positive semidefinite constraints are automatically satisfied. The unit trace constraint is automatically satisfied in the Bloch vector parameterization \(^3\). It can be shown that the conditions of Hermiticity and positive-semidefiniteness of \( \rho \) correspond to the following definition of the “Bloch vector set” \( B_{N^2-1} \) of admissible values of \( \theta \)

\[
B_{N^2-1} \equiv \{ \theta \in R^{N^2-1} \mid a_i(\theta) \geq 0, \quad i = 1, ..., N \}.
\]

(11)

This follows from the standard result that the roots of a characteristic polynomial are positive semidefinite iff the coefficients of the polynomial are positive semidefinite \(^[15] \). The \( a_i \) in the above definition of \( B \) are themselves polynomials in \( \theta \) whose coefficients can be expressed in terms of the structure constants of the Lie algebra \( su(N) \) of traceless Hermitian matrices, and will be written explicitly below for \( N = 2, 3, 4 \). The structure constants, which characterize the generators of \( su(N) \), are the elements of the completely antisymmetric and completely symmetric tensors \( f \) and \( g \), respectively defined by the relations:

\[
[\lambda_i, \lambda_j] = 2f_{ijk}\lambda_k
\]

\[
[\lambda_i, \lambda_j]^+ = \frac{4}{N} \delta_{ij} I_N + 2g_{ijk}\lambda_k,
\]

which can be solved \(^[16] \) for \( f_{ijk}, g_{ijk} \):

\[
f_{ijk} = \frac{1}{4i} \text{Tr}\{[\lambda_i, \lambda_j]\lambda_k\}
\]

\[
g_{ijk} = \frac{1}{4} \text{Tr}\{([\lambda_i, \lambda_j]^+, - \frac{4}{N} \delta_{ij})\lambda_k\},
\]

where \([,]\) denotes the antisymmetric commutator and \([,]^+\) denotes the symmetric commutator, and where we have used the Einstein (implicit) summation convention for repeated indices. It can be shown \(^[15] \) that the \( \lambda_i \) that satisfy these conditions can be expressed:

\[
\{\lambda_i\}_{i=1}^{N^2-1} = \{\{u_{jk}\}, \{v_{jk}\}, \{w_l\}\}
\]

where

\[
2l_2 = \frac{N - 1}{N} - \frac{1}{2} |\theta|^2 \geq 0.
\]

(12)

1. Spin-1/2 systems

When \( N = 2 \), the conditions \( a_i \geq 0 \) (equation (11)) correspond to \( 1l_2 = 1 \) and
The latter condition defines the familiar Bloch sphere for spin-$\frac{1}{2}$ systems. The Lagrangian \( \mathcal{L} \) in this case becomes

\[
\mathcal{L}(\theta, \lambda) = \ln \left[ \prod_{k=1}^{m} \text{Tr} \left( \rho(\theta) F_{ik} \right) \right] + \lambda_2 \left( \frac{N-1}{N} - \frac{1}{2} |\theta|^2 - \gamma_2 \right),
\]

where we have omitted the constant term originating from \( a_1 \) since it is independent of \( \theta \).

2. Spin-1 systems

For \( N = 3 \), in addition to the constraint \( \text{Eq. 12} \), we have

\[
\sum_{i=0}^{3} \theta i \geq N \]

where the structure constants \( g_{ijk} \) are components of the completely symmetric tensor of the Lie algebra \( \text{su}(N) \) (Eq. 12). The Lagrangian \( \mathcal{L} \) for spin-1 systems then becomes

\[
\mathcal{L}(\theta, \lambda) = \ln \left[ \prod_{k=1}^{m} \text{Tr} \left( \rho(\theta) F_{ik} \right) \right] + \\
\frac{N-1}{N} - \frac{1}{2} |\theta|^2 - \gamma_2 \]

\[
+ \lambda_3 \left[ \frac{(N-1)(N-2)}{N^2} \sum_{i=0}^{3} \sum_{j=0}^{3} \sum_{k=0}^{3} g_{ijk} \theta_i \theta_j \theta_k \geq 0, \right)
\]

where we have (again) used the Einstein summation convention for repeated indices, i.e., \( g_{ijk} \theta_i \theta_j \theta_k = \sum_{i=0}^{3} g_{ijk} \theta_i \theta_j \theta_k \).

Note that while for \( N = 2 \), the Bloch vector space is exactly a ball, the additional constraints starting with \( a_3 \geq 0 \) restrict the Bloch vector space for \( N = 3 \) and higher dimensions to a proper subset of a ball. Since the structure constants of \( \text{su}(N) \) for \( N \geq 3 \) have no rotational invariance, neither do these conditions. The Bloch vector space has an asymmetric structure in \( \mathbb{R}^{N^2-1} \) for \( N \geq 3 \).

In the Bloch vector parameterization, the Fisher information takes on a particularly simple analytical form. For \( N = 2 \), we have for the score vectors

\[
\begin{align*}
\frac{\partial \ln L(\theta|x)}{\partial \theta_1} &= \frac{1}{2} \sum_{k=1}^{m} \frac{1}{\text{Tr}(\rho F_{ik})} [F_{ik}(2,1) + F_{ik}(1,2)] \\
\frac{\partial \ln L(\theta|x)}{\partial \theta_2} &= \frac{1}{2} \sum_{k=1}^{m} \frac{k}{\text{Tr}(\rho F_{ik})} [F_{ik}(1,2) + F_{ik}(2,1)] \\
\frac{\partial \ln L(\theta|x)}{\partial \theta_3} &= \frac{1}{2} \sum_{k=1}^{m} \frac{1}{\text{Tr}(\rho F_{ik})} [F_{ik}(1,1) + F_{ik}(2,2)]
\end{align*}
\]

with \( \mathcal{J}_2(\theta) \) \( i,j \). The Fisher information decomposes similarly to \( N = 2 \) for \( N = 3 \) due to the linearity of the Born probability in \( \theta \).

B. Mutually unbiased (average case optimal) measurements

As discussed in section IIIB, quantum measurement strategies capable of fully reconstructing the density matrix can be characterized by a set of \( N+1 \) measurement bases (matrices of eigenvectors) \( V(r) \), \( 0 \leq r \leq N \). Each such choice yields a different asymptotic variance for the ML estimator, i.e., a different Fisher information matrix.

In the present work, we focus on the use of mutually unbiased measurement bases. For 1-qubit systems \( (N = 2) \), MUB bases \( V(r) \), \( 0 \leq r \leq N \) can be written

\[
V^{(0)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad V^{(1)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad V^{(2)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}.
\]

The observables are then simply the standard Pauli spin operators.

For \( N = 3 \), or more generally when \( N \) is the power of an odd prime, these bases \( V^{(r)} \) are given by \( \text{Eq. 13} \)

\[
V^{(r)} = \left\{ \begin{array}{ll}
\delta_{pq}, & r = 0 \\
\frac{1}{\sqrt{N}} \exp\left(\frac{2\pi i}{N}(rp^2 + pq)\right), & 1 \leq r \leq N.
\end{array} \right.
\]

The orthonormal observables can then be taken to be

\[
F_{r(N-1)+i} = V^{(r)} \tilde{F}_i (V^{(r)})^\dagger,
\]

\[
\tilde{F}_i = |i\rangle\langle i| = \text{diag}(0, \ldots, 1, \ldots),
\]

\[
1 \leq i \leq N - 1.
\]

Recall that the MUB measurements maximize the average Fisher information over the set of all true density matrices \( \rho_0 \), and hence are “average-case optimal” as discussed in Section IIID.

C. Complete, average case suboptimal measurements

In order to interrogate the asymptotic and finite sample losses induced by using biased or suboptimal measurement bases, the MUB bases are rotated, causing the associated parallelepipeds \( (T_{1}, \ldots, T_{N+1}) \) in Section III D to no longer be a rectangular solid and the average Fisher information to decrease. After rotation, the new bases can be written

\[
\tilde{V}^{(r)} = U(s)V^{(r)}U^\dagger(s)
\]

where \( U(s) = e^{iA^{(r)}s} \), \( A \) being a random Hermitian matrix specifying a random axis of rotation in the \( N \)-dimensional Hilbert space; \( s \) is a scalar parameter specifying the extent of rotation (magnitude of the solid angle). To generate a set of measurement bases that is sufficiently different from the MUB, \( N \) measurement bases
were rotated according to the above formula; for basis \( r \), the parameter \( s \) was incrementally increased until
\[
|\langle v_i^{(r)}, v_j^{(r')} \rangle| \geq \alpha \frac{1}{\sqrt{N}}.
\]
where \( r' \) runs over all the other bases and \( \alpha > 1 \) is a chosen scalar, for at least one pair of eigenvectors \( i, j \) from bases \( r \) and \( r' \), respectively. If necessary, this procedure was iterated self-consistently. We refer to the resulting bases as mutually biased measurement bases (MBB).

V. NUMERICAL IMPLEMENTATION

In the Bloch vector parametrization, the maximum of the likelihood corresponding to Lagrangian function \( \mathcal{L} \) can be found by solving for roots of the nonlinear system of \( N^2 + 2N - 3 \) equations \( \frac{\partial \mathcal{L}}{\partial t} \) in \( N^2 + 2N - 3 \) unknowns \( \theta_i, \gamma_j, \lambda_k \). The number of constraints and hence unknowns will differ in other parametrizations; for example, for parameterizations where positive semidefiniteness is implicit in the parametrization (such as the Cholesky parametrization), \( \lambda_j = 0, \ j = 1, \cdots, N - 1 \) in equation (11). The Newton-Raphson algorithm can be used to find the roots of this nonlinear system. Writing \( \frac{\partial \mathcal{L}}{\partial t} = H(t) \), the Newton step for
\[
H(t) = 0
\]
is
\[
t_{\text{new}} = t_{\text{old}} + \delta t,
\]
with \( \delta t = -J^{-1}H \), where \( J_{ij} = \frac{\partial H}{\partial t_i} \) is the Jacobian matrix. Denoting the rows of \( H \) by \( H_i \), we have

\[
H_i(\theta) = \frac{\partial \mathcal{L}(\theta, \lambda, \gamma | x)}{\partial \theta_i} = \frac{\partial \ln L(\theta | x)}{\partial \theta_i} = 0, \quad 1 \leq i \leq N^2 - 1,
\]
\[
H_{N^2+j-1}(\theta) = \frac{\partial \mathcal{L}(\theta, \lambda, \gamma | x)}{\partial \lambda_j} = a_j(\theta) = 0, \quad 1 < j < N - 1,
\]
\[
H_{N^2+N+j-2}(\lambda, \gamma) = \frac{\partial \mathcal{L}(\theta, \lambda, \gamma | x)}{\partial \gamma_j} = 2\lambda_j \gamma_j = 0, \quad 1 < j < N - 1.
\]

In order to facilitate global convergence of the Newton-Raphson algorithm, the “sum-of-squares” function \( h = H \cdot H \) is evaluated after each iteration, and the step length progressively shortened until the value of this function is found to decrease (the existence of such a step length is guaranteed [17]).

Alternatively, the “sum-of-squares” function \( h(t) \) may be minimized directly to locate the constrained maximum of the likelihood. In general, direct minimization of this function may be prone to encountering local traps. In the present case, minimization using an optimization algorithm capable of escaping from traps was employed. The quasi-Newton algorithm, in which the algorithmic step \( k + 1 \) is given by \( t^{(k+1)} = t^{(k)} - A^{-1} \nabla h(t^{(k)}) \), where \( A^{-1} \) denotes the approximate inverse Hessian computed with the Broyden-Fletcher-Goldfarb-Shanno (BFGS) update, was first used to search for a zero of \( \nabla h(t) \) until convergence slowed "below a specified stepwise tolerance", again using an adaptive line search strategy to identify the optimal step size. Traps were often encountered that could not be escaped from using the above technique. To surmount them, a fixed number of stochastic simulated annealing steps were applied.

In order to have a scalar measure of the accuracy of the entire density matrix estimate, the Josza fidelity (generalized overlap) \( \mathcal{F} = \text{Tr}^2 \{ \sqrt{\rho \rho' \sqrt{\rho'}} \} \), which is related to the statistical distance on the space of density matrices, was used. The convergence tolerance (i.e., objective function value below which the optimized parameter estimate was accepted as an estimator) for each \( \rho \) was chosen by running a set of ML optimizations with a very large sample size (\( m = 10000 \) observations), and determining the objective function value below which \( \mathcal{F} \geq 0.999 \) for all cases. In order to make the convergence tolerance compatible across difference sample sizes, the log of the unconstrained likelihood function was scaled as \( \frac{1}{m} \ln L(\theta | x) \).

Kernel density estimators (KDEs), nonparametric density estimators that avoid some of the deficiencies of histograms, were used to estimate finite sample probability density functions. Unlike histograms, they are smooth. KDEs center a kernel function at each data point; the contribution of data point \( x(i) \) to the estimate at \( x^* \) depends on \( x^* - x(i) \). The estimated density takes the form
\[
\hat{f}(x) = \frac{1}{n} \sum_{i=1}^{n} K \left( \frac{x - x(i)}{h} \right)
\]
with \( \int K(t) dt = 1 \). Bandwidth \( h \) optimization, which avoids values of \( h \) that lead to spiky estimates (under-smoothing) or oversmoothing, was based on minimization of the asymptotic mean integrated squared error (AMISE) [13], i.e., \( h_{\text{opt}} = \arg \min \text{AMISE} \). A Gaussian
The primary goal in this subsection is to determine whether the limiting asymptotic normal distribution of the parameter estimates provides a good approximation to the finite-sample distribution when MUB’s are used to generate quantum observations, and how the approximation improves with increase in the sample size.

Note that frequentist inferential methods are based on the notion of hypothetical repeated samples. Hence, an important practical consideration when assessing the finite-sample performance of these methods is the choice of the number of simulated samples. In particular, the number of samples should be large enough such that the finite-sample statistics adequately characterize the corresponding population quantities and the finite-sample distributions are sufficiently smooth. To obtain such a choice, Figure 1 compares the finite-sample distributions for the ML estimator of $\theta_1$ for the mixed spin-1/2 system for 100, 500, 1000, and 1500 simulated samples. Figure 1 reveals that the finite-sample performance of the ML estimator is quite insensitive to the choice of the number of simulated samples. Note that the finite-sample pdf’s for different numbers $q$ of simulated samples are barely distinguishable. Therefore, in all subsequent analysis, we set the number of hypothetical samples to 1000.

We next turn our attention to mixed spin-1/2 systems ($N = 2$). Table II reports statistics from the asymptotic and finite-sample distributions of the ML estimators of the parameters and diagonal elements of the density matrix. Panels A, B, and C report results for $m = 100, 400,$ and 1000, respectively. In particular, we report the following statistics from the finite-sample distribution: Bias, Standard Deviation (std), Root Mean Square Errors (RMSE), and 95% confidence intervals. These statistics broadly summarize a probability distribution and are defined as follows. Let $\{\hat{\theta}_j^{(i)}\}_{i=1,j=1}^{N^2-1,q}$ denote the estimator of $\theta_i$ in sample $j$. We have

$\text{Bias}(\hat{\theta}_i) = \frac{1}{q} \sum_{j=1}^{q} \hat{\theta}_j^{(i)} - \theta_{i,0}$,

$\text{std}(\hat{\theta}_i) = \left( \frac{1}{q} \sum_{j=1}^{q} \left( \hat{\theta}_j^{(i)} - \bar{\theta}_i \right)^2 \right)^{1/2}$

$\bar{\theta}_i = \frac{1}{q} \sum_{j=1}^{q} \hat{\theta}_j^{(i)}$

$\text{RMSE}(\hat{\theta}_i) = \left( \frac{1}{q} \sum_{j=1}^{q} \left( \hat{\theta}_j^{(i)} - \theta_{i,0} \right)^2 \right)^{1/2}$

$\text{Bias}(\hat{\theta}_i)$

$\text{std}(\hat{\theta}_i)$

$\bar{\theta}_i$

$\text{RMSE}(\hat{\theta}_i)$

These choices of sample sizes enable us to assess the impact of the sample size on the properties of the parameter estimates for experimentally realistic scenarios.
\[ \left\{ \text{std}(\hat{\theta}_i) \right\}^2 + \left[ \text{Bias}(\hat{\theta}_i) \right]^2 \right\}^{1/2}, \] and the 95% confidence interval is the region bounded by the 2.5% and 97.5% quantiles of the finite-sample distribution of \( \hat{\theta}_i \).

Note that the diagonal elements of the density matrix \( \rho \) are smooth real functions of the parameter vector \( \theta \). Let \( \rho_{ij}(\theta) \) denote the \( ij \)-th element of the density matrix. Given the Invariance property of the ML estimator (see Section II), the maximum likelihood estimator of \( \rho_{ij}(\theta) \) is \( \rho_{ij}(\hat{\theta}) \). Also, the asymptotic distribution of the estimators of the diagonal elements of \( \rho \) can be obtained using the Continuous Mapping Theorem: \( \sqrt{m}(\rho_{ij}(\hat{\theta}) - \rho_{ij}(\theta_0)) \) has an asymptotic normal distribution with asymptotic variance given by

\[ \text{var} (\rho_{ij}(\hat{\theta})) = \left( \frac{\partial \rho_{ij}(\theta_0)}{\partial \theta_0} \right)^T \Sigma \left( \frac{\partial \rho_{ij}(\theta_0)}{\partial \theta_0} \right), \quad (18) \]

where \( \Sigma \) is the asymptotic variance of \( \hat{\theta} \).

Row 1 of Panel A reports the true values of the parameters and the diagonal elements of the density matrix. The row labeled "Asymptotic" in each panel reports the point estimates of the parameters and diagonal elements, along with the asymptotic standard errors in parentheses and asymptotic 95% confidence intervals in square brackets. We estimate the asymptotic covariance matrix consistently using the observed Fisher information given by equation (1). As mentioned above, the asymptotic distribution of the estimators of the diagonal elements of \( \rho \) are obtained using the Continuous Mapping Theorem. For the computation of the asymptotic distribution, 1 out of the 1000 hypothetical samples was selected randomly.

Note that the asymptotic standard errors are very small, ranging from 0.004 for \( \theta_1 \) to 0.02 for \( \theta_2 \) and \( \theta_3 \) in Panel A. Consequently, the asymptotic 95% confidence intervals are tightly centered around the point estimates. The asymptotic standard errors decrease with the increase in sample size to \( m = 400 \) and \( m = 1000 \) in Panels B and C, respectively. Consequently, as predicted by asymptotic theory, the distributions get narrower with increase in the sample size. However, note that, with the exceptions of \( \theta_2 \) in Panel A, none of the asymptotic confidence intervals contain the true value of the parameter.

The subsequent rows of each Panel report statistics from the finite-sample distribution of the parameter estimates. The Table reveals that the finite-sample biases are negligible, even for small sample sizes, ranging from \(-0.0055\) for \( \theta_2 \) to 0.0027 for \( \rho_{22} \) for \( m = 100 \) in Panel A. However, the finite-sample standard errors reveals that the asymptotic standard errors grossly underestimate the estimation error in finite samples. The finite-sample standard errors vary from 0.09 for \( \rho_{11} \) to 0.19 for \( \theta_2 \) for \( m = 100 \). These are about an order of magnitude bigger than the corresponding asymptotic estimates. Consequently, the finite-sample confidence intervals are substantially wider than the asymptotic ones and do contain the true value of the parameter. Thus, the asymptotic confidence intervals grossly undercover in finite samples, thereby rendering any inference based on the asymptotic distribution of the parameters unreliable. While increase in the sample size to 400 and 1000 in Panels B and C, respectively, reduces the finite sample standard errors, the rate of convergence is much slower than the theoretically predicted \( \sqrt{m} \).

To further illustrate the discrepancy between the asymptotic and the finite-sample properties of the parameter estimates and how the asymptotic approximation improves with increase in the sample size, Figure 2 plots the finite sample distributions of the parameter estimates for sample sizes \( m = 100, 400, \) and 1000 in the same graph. We also include in the graph the corresponding asymptotic distributions which are degenerate at the true values of the parameters. As expected, the finite-sample distributions get narrower and more concentrated around the true value with increase in the sample size.

While Figure 2 focuses on the consistency property of the ML estimators, the quality of the asymptotic normal
finite-sample performance of the estimators is more pro-
standard errors decrease at a rate slower than
In fact, the finite sample distributions get wider with in-
corresponding asymptotic ones for all three sample sizes.
Table II, Panels A, B, and C report results for
quantum systems. Most proposed applications of state
estimation, including quantum information processing
approximation is considered in Figures 3 and 4. Figure
the finite-sample and asymptotic distributions of
Panels A-C plot the distributions for $\theta_1$
for $m = 100, 400, 1000$, respectively, while Panels D-F
do the same for $\theta_2$.
Panels A-C in Figure 4 plot asymptotic and finite-
sample distributions of $\sqrt{m}(\hat{\theta}_1 - \theta_{1,0})$ for the upper
diagonal element of the density matrix, for $m = 100, 400$, and 1000, respectively. Note that the finite
sample distributions are substantially wider than the
asymptotic ones for all three sample sizes. In fact, the finite sample distributions get wider with in-
crease in sample size, indicating that the finite sample
standard errors decrease at a rate slower than $\sqrt{m}$.
The analysis so far has been restricted to spin-1/2
quantum systems. Most proposed applications of state
estimation, including quantum information processing
models, generally involve higher dimensional systems. In
order to assess the impact of Hilbert space dimension on
the performance of frequentist inference, we investigated
the state estimation of spin-1 systems. Table III reports
the asymptotic and finite-sample behavior of the ML
estimators of the parameters and diagonal elements of
the density matrix for a spin-1 quantum system. As in
Table II, Panels A, B, and C report results for $m = 100,
400$, and 1000, respectively.
Note that the divergence between the asymptotic and
finite-sample performance of the estimators is more pro-

| Panel A: Sample size 100 |
|-------------------------|
| $\theta_1$ | $\theta_2$ | $\theta_3$ | $\rho_{11}$ | $\rho_{22}$ |
| True Value | -0.44 | -0.02 | 0.19 | 0.59 | 0.41 |
| Asymptotic | -0.45 | 0.03 | 0.00 | 0.55 | 0.45 |
| [0.004] | [0.02] | [0.01] | [0.01] | [0.01] |
| Bias ($\times 10^2$) | -0.40 | -0.14 | -0.55 | -0.27 | 0.27 |
| Standard error | 0.16 | 0.19 | 0.17 | 0.09 | 0.09 |
| RMSE | 0.16 | 0.19 | 0.17 | 0.09 | 0.09 |
| 95% CE | [-0.76, -0.09] | [-0.39, 0.33] | [-0.15, 0.52] | [0.42, 0.77] | [0.23, 0.58] |

| Panel B: Sample size 400 |
|-------------------------|
| $\theta_1$ | $\theta_2$ | $\theta_3$ | $\rho_{11}$ | $\rho_{22}$ |
| Asymptotic | -0.49 | -0.14 | 0.31 | 0.65 | 0.35 |
| [0.004] | [0.004] | [0.002] | [0.002] | [0.002] |
| Bias ($\times 10^2$) | -0.33 | -0.17 | 0.24 | 0.12 | -0.12 |
| Standard error | 0.08 | 0.09 | 0.09 | 0.05 | 0.05 |
| RMSE | 0.08 | 0.09 | 0.09 | 0.05 | 0.05 |
| 95% CE | [-0.61, -0.26] | [-0.19, 0.16] | [0.02, 0.37] | [0.51, 0.76] | [0.24, 0.49] |

| Panel C: Sample size 1000 |
|--------------------------|
| $\theta_1$ | $\theta_2$ | $\theta_3$ | $\rho_{11}$ | $\rho_{22}$ |
| Asymptotic | -0.48 | -0.03 | 0.22 | 0.61 | 0.39 |
| [0.002] | [0.002] | [0.001] | [0.001] | [0.001] |
| Bias ($\times 10^2$) | -0.46 | 0.00 | 0.36 | 0.18 | -0.18 |
| Standard error | 0.06 | 0.07 | 0.07 | 0.04 | 0.04 |
| RMSE | 0.06 | 0.07 | 0.07 | 0.04 | 0.04 |
| 95% CE | [-0.56, -0.35] | [-0.14, 0.09] | [0.09, 0.32] | [0.54, 0.77] | [0.22, 0.46] |

Table I: Finite sample distribution statistics (1000 repeated samples) for state estimation of spin-1/2 quantum systems:
MUB measurement bases.

![Figure 3](image-url)

FIG. 3: Finite sample distributions of $\sqrt{m}(\hat{\theta}_1 - \theta_{1,0})$, mixed spin-1/2 state, MUB bases. Panels A-C: $\theta_1$. (A) $m = 100$;
(B) $m = 400$; (C) $m = 1000$. Panels D-F: $\theta_2$. (D) $m = 100$;
(E) $m = 400$; (F) $m = 1000$. In each panel, the finite sample
distributions (1000 simulations) are shown alongside the c or-
describing asymptotic ones. Asymptotic variances
are estimated from one of the 1000 repeated samples (chosen
at random).
for mixed spin-1/2 state, MUB bases. (A)

of the parameters including 0 increase in the number of parameters and nonlinearity corresponding asymptotic distribution. (B) \( \mu = 100 \); (C) \( \mu = 1000 \). In each panel, finite sample distributions (1000 simulations) are shown alongside the corresponding asymptotic distribution.

FIG. 4: Finite sample distributions of \( \sqrt{m}(\hat{\rho}_{11} - \rho_{11}(\theta_0)) \), for mixed spin-1/2 state. MUB bases. (A) \( \mu = 100 \); (B) \( \mu = 400 \); (C) \( \mu = 1000 \). In each panel, finite sample distributions (1000 simulations) are shown alongside the corresponding asymptotic distribution.

The finite-sample standard errors are also substantial for \( \mu = 100 \), ranging from 0.15 for \( \theta_1 \) to 0.17 for \( \theta_8 \). Moreover, these vary from being about 8 to 9 times bigger than the corresponding asymptotic standard errors. The small sample standard errors decrease with increase in the sample size - the standard errors in Panel B are about 1/2 and those in Panel C about 1/3 of those in Panel A. This is also shown in Figure 5, where each panel plots the finite sample distribution of the ML estimator of one parameter for sample sizes \( \mu = 100, 400, \) and 1000 in the same graph.

However, as in the case of spin-1/2 systems, the discrepancy between the asymptotic and finite-sample standard errors does not diminish with sample size. Although the finite-sample standard errors decrease with sample size and, consequently, the confidence intervals get shorter, the rate of convergence is much slower than the theoretically predicted rate \( \sqrt{m} \). This is also revealed in Figures 6 and 7, which plot, respectively, the finite-sample and asymptotic distributions of \( \sqrt{m}(\hat{\theta}_i - \theta_{i,0}) \) and \( \sqrt{m}(\rho_{ii}(\hat{\theta}) - \rho_{ii}(\theta_0)) \). Panels A-C in Figure 6 (7) plot the distributions for \( \theta_7 \) (\( \rho_{11} \)) for \( \mu = 100, 400, \) and 1000, respectively, while Panels D-F report the same for \( \theta_8 \) (\( \rho_{22} \)). Note that the finite-sample distribution gets wider with increase in the sample size. This trend continues even for very large sample sizes. For example, for sample sizes 10000 and 20000 in the spin-1/2 system under consideration, the finite sample standard errors for \( \theta_1 \) were 0.017 and 0.0092, respectively, whereas representative asymptotic standard errors were \( 1.5 \times 10^{-4} \) and \( 7.8 \times 10^{-5} \) - two orders of magnitude smaller. For very large sample sizes, computational likelihood maximization can become prohibitively expensive even if experimental data collection is not.

Another serious shortcoming of frequentist methods, which unlike Bayesian methods are based on constrained optimization, is that local traps in the likelihood landscape can result in the optimization algorithm converging to points in the parameter space where all the constraints on the density matrix are not precisely satisfied; in the Bloch vector parametrization, this phenomenon can result in negative eigenvalues. Parameterizations that automatically satisfy the positive semidefiniteness constraints (such as the Cholesky parametrization) do not have this problem, but may not satisfy the unit trace condition. In the likelihood optimizations carried out here, because of the nonlinear nature of the constraints, the parameter estimates did produce negative eigenvalues; the problem was most pronounced for \( \rho \)'s with eigenvalues near 0 or 1 and small sample sizes. Because the local minima can be far from the global optimum, this can result in multimodality of the estimate distributions in addition to unphysical parameter estimates. This is shown in Figure 8, which plots the raw distributional results obtained from the optimization procedure, without elimination of unphysical \( \rho \) estimates that have negative eigenvalues. The Figure also shows how the standard errors of the raw estimate distributions are increased by the presence of unphysical estimates. In certain cases, restarting the optimization from a different initial guess can circumvent local optima, but this method is not always successful. In the present work, we filtered the estimate distributions to exclude estimations producing negative eigenvalues originating from the optimization algorithm being trapped, since the resulting multimodality masks the true performance of the estimator. Note that Bayesian methods, which depend on conditional simulation, do not produce unphysical parameter estimates.

C. Effect of measurement bases

The above results were all obtained for simulated samples employing MUB. As noted in Section III D, the MUB set maximizes the average Fisher information, or,
FIG. 5: Finite sample distributions of parameter estimates, spin-1 system, MUB bases. Each Panel reports results for one parameter of the density matrix and superimposes results from estimations using sample sizes 100, 400, and 1000. The finite sample distributions were computed from 1000 simulations.

FIG. 6: Finite sample distributions of $\sqrt{m}(\hat{\theta}_i - \theta_{0,i})$, mixed spin-1 state, MUB bases. Panels A-C: $\theta_1$. (A) $m = 100$; (B) $m = 400$; (C) $m = 1000$. Panels D-F: $\theta_2$. (D) $m = 100$; (E) $m = 400$; (F) $m = 1000$. In each panel, the finite sample distributions (1000 simulations) are shown alongside the corresponding asymptotic distributions. Asymptotic variances are estimated from one of the 1000 repeated samples (chosen at random).

FIG. 7: Finite sample distributions of $\sqrt{m}(\rho_{ii}(\hat{\theta}) - \rho_{ii}(\theta_0))$, for mixed spin-1 state, MUB bases. Panels A-C, $\rho_{11}$. (A) $m = 100$; (B) $m = 400$; (C) $m = 1000$. Panels D-F, $\rho_{22}$. (D) $m = 100$; (E) $m = 400$; (F) $m = 1000$. In each panel, finite sample distributions (1000 simulations) are shown alongside the corresponding asymptotic distribution.
FIG. 8: Unfiltered finite sample distributions of parameter estimates, spin-1 system, MUB bases. Each Panel reports results for one parameter of the density matrix and superimposes results from estimations using sample sizes 100, 400, and 1000. The finite sample distributions were computed from 1000 simulations. Unlike the other Figures, physically inadmissible $\rho$ estimates with negative eigenvalues were not removed from the finite sample distributions.

equivalently, minimizes the asymptotic covariance matrix of the estimators, over the set of all possible density matrices. However, implementing MUB measurements in the laboratory is quite difficult for $N > 2$.

In order for all the parameters of the density matrix to be identifiable by frequentist inference, measurements in at least $N + 1$ bases are required. Most laboratory setups use $> N + 1$ redundant bases and are suboptimal from the standpoint of average-case Fisher information. Hence, it is crucial to determine whether suboptimal measurement bases achieve similar estimation accuracies in finite samples. In this work, suboptimal measurement bases were generated according to the method described in Section IV C, and are reported in the Appendix: $\alpha$ in equation 14 was set to 1.2. The primary goal of this subsection is to compare the asymptotic and finite sample relative efficiencies across optimal and suboptimal measurement strategies.

Table III reports the asymptotic and finite-sample performance of the ML estimators using the suboptimal bases for $N = 3$. Panels A, B, and C report results for $m = 100$, 400, and 1000, respectively. We begin with a comparison of the asymptotic relative efficiencies of MUB and MBB bases. The asymptotic standard errors vary from 0.01 for $\rho_{22}$ and $\rho_{33}$ to 0.04 for $\theta_3$ in Panel A. Comparing with the results obtained with MUB in Table II reveals that the asymptotic standard errors for the suboptimal measurement strategy are bigger for most parameters than those for the MUB, as expected based on the asymptotic theory. The asymptotic standard errors decrease and, hence, the confidence intervals become shorter, with the increase in sample size. We next turn to a comparison of the relative finite-sample efficiencies of frequentist estimators using these measurement strategies. Table III reveals that the finite-sample standard errors for the parameters and diagonal elements of the density matrix are generally bigger for the suboptimal measurement strategy relative to the MUB, especially for larger sample sizes. The finite-sample standard errors range from 0.07 for $\rho_{22}$ to 0.26 for $\theta_3$ for the suboptimal strategy, compared to the variation from 0.08 for $\rho_{11}$ to 0.17 for $\theta_3$ for the MUB for $m = 100$. While increase in the sample size reduces the finite sample standard errors, they still remain large, ranging from 0.04 to 0.31 for $m = 400$ and from 0.03 to 0.29 for $m = 1000 -$ bigger than the corresponding values obtained with the MUB. Consequently, the finite-sample confidence intervals are wider for the suboptimal bases relative to the MUB for all three sample sizes. Thus, the ML estimators using MUB also have superior finite-samples properties than those using suboptimal bases, although the difference can be marginal for small sample sizes. Note that while the rate of convergence to the asymptotic limit is smaller than the theoretically
predicted $\sqrt{m}$ in both cases, it is somewhat greater for MUB than for the suboptimal bases.

Comparing the relative asymptotic efficiencies of the MUB versus suboptimal measurement strategies (RE$_{1:2} = \frac{\sigma_1^2}{\sigma_2^2}$) with the corresponding relative finite-sample efficiencies, we find that for small sample sizes, the former are larger for most of the parameters and diagonal elements of the density matrix. For bigger sample sizes, due to the greater rate of convergence of the efficiency of MUB bases to the asymptotic limit, the finite sample RE’s are sometimes slightly larger than the asymptotic RE’s. These results suggest that although frequentist inferential methods using MUB have theoretically predicted superior performance compared to suboptimal measurement strategies, the relative improvement is strongly dependent on the sample size and is much less pronounced in finite-samples. This feature was also observed for measurement bases that differed more substantially from MUB, such as randomly generated bases (data not shown). The theoretically predicted advantages of the optimal measurement strategy can be dramatically diminished for experimentally realistic sample sizes - raising doubts about the practical utility of these types of measurements, which are difficult to implement experimentally for Hilbert space dimensions $N > 2$, in frequentist inference.

Figures 11 and 12 compare asymptotic and finite-sample properties of the optimal MUB and the suboptimal bases.

**D. Hypothesis Testing**

An important application of quantum state estimation is optimal decision making and control, and by extension, quantum information processing. Control logic is often Boolean, in that decisions are made based on whether a hypothesis is true or false, rather than the precise state of the system. Therefore, in this subsection, we examine the finite-sample performance of maximum likelihood-based hypothesis testing procedures that aid in making decisions.

Hypothesis testing problems may involve a single restriction or multiple restrictions on the parameters. We consider first the case of single restrictions. The appropriate hypothesis test for testing a single restriction is the $t$-test. The $t$-test statistic for the null hypothesis $H_0 : f(\theta) = c$ against the alternative hypothesis $H_1 : f(\theta) \neq c$, where $c$ is a known constant, is

$$ t = \frac{1}{\hat{\sigma}(f(\hat{\theta}))} (f(\hat{\theta}) - c), \quad (19) $$

where $\hat{\sigma}(f(\hat{\theta}))$ is a consistent estimate of the asymptotic standard error of $f(\hat{\theta})$. Asymptotically, under the null hypothesis, the $t$-statistic converges in distribution to the standard normal distribution; thus, for a two-sided size $\alpha = 0.05$ test, the null hypothesis is rejected if $|t| > 1.96$. 

![](image)

**FIG. 9:** Distributions of $\sqrt{m}(\hat{\theta}_1 - \theta_{1,0})$ for a spin-1 system, sample size 100: comparison of MUB and MBB bases. (A) $\sqrt{m}(\theta_2 - \theta_{1,0})$; (B) $\sqrt{m}(\theta_8 - \theta_{8,0})$. Panels C and D: magnified comparison of asymptotic variances obtained for MUB and MBB bases in A and B, respectively. MBB bases used are listed in Appendix A.

**FIG. 10:** Distributions of $\sqrt{m}(\hat{\theta}_1 - \theta_{1,0})$ for a spin-1 system, sample size 1000: comparison of MUB and MBB bases. (A) $\sqrt{m}(\theta_2 - \theta_{1,0})$; (B) $\sqrt{m}(\theta_8 - \theta_{8,0})$. Panels C and D: magnified comparison of asymptotic variances obtained for MUB and MBB bases in A and B, respectively. MBB bases used are listed in Appendix A.
Panel A: Sample size 100

|                | $\theta_1$ | $\theta_2$ | $\theta_3$ | $\theta_4$ | $\theta_5$ | $\theta_6$ | $\theta_7$ | $\theta_8$ | $\rho_{11}$ | $\rho_{22}$ | $\rho_{33}$ |
|----------------|------------|------------|------------|------------|------------|------------|------------|------------|-------------|-------------|-------------|
| True Value     | 0.15       | -0.14      | -0.07      | -0.04      | -0.15      | -0.01      | -0.17      | -0.23      | 0.23        | 0.30        | 0.46        |
| Asymptotic     | 0.24       | -0.05      | -0.44      | -0.04      | -0.02      | -0.12      | -0.25      | -0.25      | 0.04        | 0.48        | 0.48        |
| [9.28 0.02]    | [-0.08 0.01] | [-0.46 0.01] | [-0.07 0.01] | [-0.05 0.01] | [-0.15 0.09] | [-0.29 0.22] | [-0.29 0.22] | [0.03 0.05] | [0.48 0.50] | [0.46 0.50] | [$0.30 0.09$] |
| Bias ($\times 10^2$) | -0.55     | 2.20       | 1.90       | 0.89       | -0.22      | -0.69      | 1.43       | 5.35       | 2.50        | 0.59        | -3.09       |
| Standard error | 0.15       | 0.15       | 0.14       | 0.15       | 0.15       | 0.16       | 0.16       | 0.17       | 0.08        | 0.09        | 0.10        |
| RMSE           | 0.15       | 0.15       | 0.14       | 0.15       | 0.15       | 0.16       | 0.16       | 0.17       | 0.09        | 0.09        | 0.10        |
| 95% CE         | [-0.19 0.44] | [-0.39 0.18] | [-0.36 0.20] | [-0.31 0.29] | [-0.46 0.12] | [-0.33 0.28] | [-0.46 0.16] | [-0.47 0.16] | [-0.14 0.51] | [0.08 0.82] | [0.17 0.96] |

Panel B: Sample size 400

|                | $\theta_1$ | $\theta_2$ | $\theta_3$ | $\theta_4$ | $\theta_5$ | $\theta_6$ | $\theta_7$ | $\theta_8$ | $\rho_{11}$ | $\rho_{22}$ | $\rho_{33}$ |
|----------------|------------|------------|------------|------------|------------|------------|------------|------------|-------------|-------------|-------------|
| Asymptotic     | 0.17       | -0.22      | -0.10      | 0.11       | -0.07      | -0.08      | -0.14      | -0.27      | 0.21        | 0.31        | 0.49        |
| [0.16 0.04]    | [-0.22 0.04] | [-0.10 0.04] | [0.03 0.04] | [0.04 0.04] | [-0.08 0.07] | [-0.09 0.08] | [-0.16 0.14] | [-0.28 0.26] | [0.00 0.02] | [0.00 0.02] | [0.00 0.03] |
| Bias ($\times 10^2$) | -0.09     | 0.32       | -0.31      | -0.32      | 0.47       | 0.00       | 0.26       | 0.35       | -0.05       | 0.26        | -0.20       |
| Standard error | 0.08       | 0.08       | 0.08       | 0.08       | 0.08       | 0.08       | 0.09       | 0.09       | 0.04        | 0.05        | 0.05        |
| RMSE           | 0.08       | 0.08       | 0.08       | 0.08       | 0.08       | 0.08       | 0.09       | 0.09       | 0.04        | 0.05        | 0.05        |
| 95% CE         | [-0.02 0.32] | [-0.30 0.03] | [-0.23 0.07] | [-0.21 0.13] | [-0.30 0.01] | [-0.16 0.14] | [-0.34 0.00] | [-0.43 0.05] | [0.07 0.31] | [0.11 0.44] | [0.34 0.79] |

Panel C: Sample size 1000

|                | $\theta_1$ | $\theta_2$ | $\theta_3$ | $\theta_4$ | $\theta_5$ | $\theta_6$ | $\theta_7$ | $\theta_8$ | $\rho_{11}$ | $\rho_{22}$ | $\rho_{33}$ |
|----------------|------------|------------|------------|------------|------------|------------|------------|------------|-------------|-------------|-------------|
| Asymptotic     | 0.17       | -0.13      | -0.18      | -0.04      | -0.23      | -0.05      | -0.19      | -0.21      | 0.18        | 0.36        | 0.46        |
| [0.16 0.02]    | [-0.13 -0.12] | [-0.19 -0.18] | [-0.04 -0.03] | [-0.23 -0.226] | [-0.05 -0.047] | [-0.20 -0.19] | [-0.22 -0.21] | [0.178 0.181] | [0.36 0.37] | [0.45 0.46] | [0.45 0.46] |
| Bias ($\times 10^2$) | 0.04     | -0.31      | -0.01      | -0.16      | -0.32      | 0.07       | -0.25      | -0.21      | -0.06       | -0.06       | 0.12        |
| Standard error | 0.06       | 0.06       | 0.05       | 0.05       | 0.06       | 0.05       | 0.06       | 0.06       | 0.03        | 0.03        | 0.04        |
| RMSE           | 0.06       | 0.06       | 0.05       | 0.05       | 0.06       | 0.05       | 0.06       | 0.06       | 0.03        | 0.03        | 0.04        |
| 95% CE         | [0.04 0.27] | [-0.25 -0.03] | [-0.16 0.02] | [-0.15 0.06] | [-0.27 -0.05] | [-0.11 0.10] | [-0.29 -0.07] | [-0.36 -0.12] | [0.11 0.29] | [0.16 0.36] | [0.39 0.70] |

TABLE II: Finite sample distribution statistics (1000 repeated samples) for state estimation of spin-1 quantum systems: MUB measurement bases.
### Panel A: Sample size 100

|                | $\theta_1$ | $\theta_2$ | $\theta_3$ | $\theta_4$ | $\theta_5$ | $\theta_6$ | $\theta_7$ | $\theta_8$ | $\rho_{11}$ | $\rho_{22}$ | $\rho_{33}$ |
|----------------|------------|------------|------------|------------|------------|------------|------------|------------|-------------|-------------|-------------|
| **True Value** | 0.15       | -0.14      | -0.07      | -0.04      | -0.15      | -0.01      | -0.17      | -0.23      | 0.23        | 0.30        | 0.46        |
| **Asymptotic** | 0.11       | 0.28       | 0.15       | -0.10      | 0.21       | 0.15       | -0.21      | -0.46      | 0.27        | 0.13        | 0.60        |
| Bias ($\times 10^3$) | -13.5      | 23.9       | 6.41       | 3.31       | 11.6       | 23.9       | 4.98       | 8.27       | 5.59        | -0.82       | -4.77       |
| Standard error | 0.19       | 0.24       | 0.13       | 0.16       | 0.22       | 0.26       | 0.20       | 0.19       | 0.10        | 0.07        | 0.11        |
| RMSE           | 0.23       | 0.34       | 0.14       | 0.16       | 0.25       | 0.35       | 0.20       | 0.20       | 0.11        | 0.07        | 0.12        |
| 95% CE         | [-0.37, 0.35] | [-0.42, 0.49] | [-0.24, 0.25] | [-0.39, 0.27] | [-0.55, 0.37] | [-0.25, 0.66] | [-0.48, 0.24] | [-0.52, 0.21] | [-0.62, 0.59] | [0.05, 0.54] | [0.09, 0.74] |

### Panel B: Sample size 400

|                | $\theta_1$ | $\theta_2$ | $\theta_3$ | $\theta_4$ | $\theta_5$ | $\theta_6$ | $\theta_7$ | $\theta_8$ | $\rho_{11}$ | $\rho_{22}$ | $\rho_{33}$ |
|----------------|------------|------------|------------|------------|------------|------------|------------|------------|-------------|-------------|-------------|
| **Asymptotic** | -0.03      | 0.37       | -0.02      | 0.11       | 0.001      | 0.58       | -0.18      | -0.12      | 0.29        | 0.31        | 0.41        |
| Bias ($\times 10^3$) | -12.1      | 20.2       | 3.31       | -0.37      | 10.3       | 23.9       | 0.35       | 4.22       | 2.87        | -0.43       | -2.44       |
| Standard error | 0.16       | 0.24       | 0.09       | 0.11       | 0.11       | 0.31       | 0.13       | 0.11       | 0.07        | 0.04        | 0.07        |
| RMSE           | 0.20       | 0.32       | 0.10       | 0.11       | 0.22       | 0.39       | 0.13       | 0.12       | 0.07        | 0.04        | 0.07        |
| 95% CE         | [-0.28, 0.34] | [-0.38, 0.43] | [-0.20, 0.14] | [-0.24, 0.16] | [-0.46, 0.29] | [-0.36, 0.65] | [-0.43, 0.05] | [-0.43, 0.03] | [0.06, 0.43] | [0.17, 0.39] | [0.32, 0.65] |

### Panel C: Sample size 1000

|                | $\theta_1$ | $\theta_2$ | $\theta_3$ | $\theta_4$ | $\theta_5$ | $\theta_6$ | $\theta_7$ | $\theta_8$ | $\rho_{11}$ | $\rho_{22}$ | $\rho_{33}$ |
|----------------|------------|------------|------------|------------|------------|------------|------------|------------|-------------|-------------|-------------|
| **Asymptotic** | 0.09       | -0.26      | -0.09      | -0.10      | -0.13      | 0.08       | -0.21      | -0.26      | 0.21        | 0.30        | 0.48        |
| Bias ($\times 10^3$) | -7.87      | 14.7       | 1.48       | -1.58      | 8.48       | 19.2       | -1.32      | 2.56       | 1.48        | -0.00       | -1.48       |
| Standard error | 0.13       | 0.21       | 0.06       | 0.07       | 0.16       | 0.29       | 0.09       | 0.08       | 0.05        | 0.03        | 0.04        |
| RMSE           | 0.15       | 0.26       | 0.06       | 0.07       | 0.18       | 0.35       | 0.09       | 0.08       | 0.05        | 0.03        | 0.05        |
| 95% CE         | [-0.19, 0.31] | [-0.35, 0.39] | [-0.16, 0.05] | [-0.19, 0.10] | [-0.37, 0.24] | [-0.33, 0.63] | [-0.37, 0.01] | [-0.36, 0.06] | [0.11, 0.34] | [0.26, 0.36] | [0.36, 0.58] |

**TABLE III:** Finite sample distribution statistics (1000 repeated samples) for state estimation of spin-1 quantum systems: MBB measurement bases. See Appendix A for measurement bases.
### TABLE IV: Finite sample test statistic size, power, and critical values for state estimation of spin-1/2 quantum systems (1000 repeated samples).

| Hypothesis | size | power | crit val | size | power | crit val |
|------------|------|-------|----------|------|-------|----------|
| \( \theta_2 = \theta_{2,0} \) | 0.93 | 1.0 | [−50.2 34.7] | 0.96 | 1.0 | [−66.1 66.4] |
| \( \theta_2 = 0.5 \) | 0.99 | 1.0 | [−363.6 − 229.6] | 0.98 | 1.0 | [−19.5 7.0] |
| \( \delta_1 = \delta_{1,0} \) | 0.95 | 0.98 | [−1.5 14.5] | \( \delta_1 = 0.5 \) | \( \delta_1 = 0.5 \) | \( \delta_1 = 0.5 \) |
| \( \theta_i = \theta_{i,0}, \ i = 1, 2, 3 \) | \( \theta_i = \theta_{i,0}, \ i = 1, 2, 3 \) | \( \theta_i = \theta_{i,0}, \ i = 1, 2, 3 \) | \( \theta_i = \theta_{i,0}, \ i = 1, 2, 3 \) |

| Hypothesis | size | power | crit val | size | power | crit val |
|------------|------|-------|----------|------|-------|----------|
| \( \delta_1 = \delta_{1,0} \) | 0.92 | 1.0 | [−21.5 35.6] | \( \delta_1 = 0.5 \) | \( \delta_1 = 0.5 \) | [−21.5 35.6] |
| \( \theta_i = \theta_{i,0}, \ i = 1, 2, 3 \) | \( \theta_i = \theta_{i,0}, \ i = 1, 2, 3 \) | \( \theta_i = \theta_{i,0}, \ i = 1, 2, 3 \) | \( \theta_i = \theta_{i,0}, \ i = 1, 2, 3 \) |

### TABLE V: Finite sample test statistic size, power for state estimation of spin-1 quantum systems (1000 repeated samples).

| Hypothesis | size | power | crit val | size | power | crit val |
|------------|------|-------|----------|------|-------|----------|
| \( \delta_1 \) denotes the first eigenvalue of \( \rho(\theta) \). The true eigenvalues of \( \rho \) were \( \delta_{1,0} = 0.55, \delta_{2,0} = 0.30, \delta_{3,0} = 0.15 \). |
The finite-sample size and power of the t-test vis-a-vis their corresponding asymptotic values provide a means of interrogating the finite sample performance of quantum state ML inferential methods. Recall from Section II A that the size of a hypothesis test is the probability of rejecting the null hypothesis given that it is true. Therefore, the finite sample size of the two-sided t-test for the hypothesis testing problem - $H_0 : f(\theta) = c$ against the alternative hypothesis $H_1 : f(\theta) \neq c$, is given by the fraction of times $t = \frac{\hat{\theta}}{\sigma(f(\theta))}(f(\theta) - c)$ is greater than 1.96 in absolute value; the t-test has an asymptotic size of 0.05.

Similarly, as defined in Section II A, the power of a hypothesis test is the probability of rejecting the null hypothesis given that it is false. Hence, the finite-sample power for the hypothesis testing problem - $H_0 : f(\theta) = c$ against the alternative hypothesis $H_1 : f(\theta) \neq c$, with $c \neq f(\theta_0)$ - is given by the fraction of times $t = \frac{\hat{\theta}}{\sigma(f(\theta_0))}(f(\hat{\theta}) - c)$ is greater than 1.96 in absolute value; the t-test has an asymptotic power of 1. It can be shown [14] that the t-test based on ML estimates is UMP; it is therefore ideal for interrogating finite sample performance of frequentist hypothesis testing.

We consider single hypothesis testing problems involving restrictions on the parameters $\theta$ of the density matrix. In particular, for the spin-1/2 system, we test the hypothesis $H_0 : \theta_2 = \theta_{2,0}$ against the alternative $H_1 : \theta_2 \neq \theta_{2,0}$. For the spin-1 system, the hypothesis tested is $H_0 : \theta_6 = \theta_{6,0}$ against the alternative $H_1 : \theta_6 \neq \theta_{6,0}$. These hypotheses provide information about the finite-sample size of the testing procedure. For the finite-sample power, we test the hypothesis $H_0 : \theta_2 = 0.5$ against the alternative $H_1 : \theta_2 \neq 0.5$ for the spin-1/2 system and the hypothesis $H_0 : \theta_6 = 0.5$ against the alternative $H_1 : \theta_6 \neq 0.5$ for the spin-1 system. Note that the true values of both $\theta_2$ for the spin-1/2 system and $\theta_6$ for the spin-1 system are sufficiently different from 0.5 to ensure a proper size and power comparison of the tests.

Tables IV and V report the finite-sample size and power of the t-tests for the above hypotheses for the mixed spin-1/2 and spin-1 systems, respectively. Panels A, B, and C in each Table report results for $m = 100$, 400, and 1000, respectively. Consider first Table IV. The finite-sample size of the t-test is 0.87 for $m = 100$, i.e. the probability of rejecting the null, $H_0 : \theta_2 = \theta_{2,0}$, given that it is true is 87%. This is more than 17 times bigger than the theoretically predicted asymptotic value of 0.05. This is a reflection of the fact that the asymptotic standard errors grossly underestimate the estimation error in finite-samples. The asymptotic standard error for $\theta_2$ is about 0.02 - an order of magnitude smaller than the finite-sample value 0.19 (see Table II, Panel A). Consequently, the 2.5% and 97.5% quantiles from the finite-sample distribution of the t-statistic are -37.8 and 27.7, respectively, whereas the corresponding asymptotic values are only -1.96 and 1.96, respectively.

The increase in sample size to 400 and 1000 does not improve the size of the test. In fact, the finite-sample distribution of the t-statistic widens relative to the asymptotic standard normal distribution. The 2.5% and 97.5% quantiles from the finite-sample distribution of the t-statistic are -50.2 and 34.7, respectively, for $m = 400$ and -66.1 and 66.4, respectively, for $m = 1000$. This is because, although the finite-sample standard errors decrease with the increase in the sample size, the rate of convergence is much slower than the theoretically predicted rate $\sqrt{m}$. The asymptotic standard errors for $\theta_2$ for $m = 400$ and $m = 1000$ relative to $m = 100$ are 0.2 and 0.1, respectively. However, the finite-sample standard errors for $\theta_2$ for $m = 400$ and $m = 1000$ relative to $m = 100$ are much higher at 0.5 and 0.4, respectively (see Table II). This is also shown in Panel A of Figure 11 that plots the finite sample t-statistic distribution for different sample sizes, along with the asymptotic standard normal distribution. Similar results are obtained for the spin-1 system in Table V and Panel A of Figure 12.

The power of the t-test is 0.98 for $m = 100$, close to the asymptotic value of 1. For higher sample sizes, both the finite sample and asymptotic powers coincide at 1. However, note that the finite sample size (above) is also 1 in spite of 0.5 being substantially different from $\theta_{2,0} = 0.02$, indicating that the testing procedure is incapable of distinguishing between the two hypotheses. Similar results are obtained for the spin-1 system (Table V).

In certain applications, such as quantum information processing, it is important to simultaneously test whether several elements or parameters of the density matrix have prescribed values. For these testing problems involving multiple parameter restrictions, we rely on the Wald test. As an example, for the spin-1/2 system, we test the hypothesis that each of the parameters $\theta_i, \quad 1 \leq i \leq 3$ is equal to its true known value: $H_0 : \theta = \theta_0$ against the alternative $H_1 : \theta \neq \theta_0$. The Wald statistic is given by

$$W = \mathbf{v}^T \hat{\Sigma}^{-1} \mathbf{v},$$

where $\mathbf{v} = (\hat{\theta}_1 - \theta_{1,0}, \cdots, \hat{\theta}_3 - \theta_{3,0})$ and $\hat{\Sigma}$ is the estimated asymptotic covariance matrix of the parameter estimates. Asymptotically, under the null, the Wald statistic converges in distribution to a chi-squared random variable $\chi^2_k$, with the number of degrees of freedom $k$ equal to the number of parameter restrictions (in this case 3). A size $\alpha = 0.05$ Wald test has a rejection region corresponding to the tail of the $\chi^2_k$ distribution beyond which the cumulative probability density is 0.05. For $k = 3$, the null hypothesis is rejected if $W > 7.81$.

The Wald test at significance level $\alpha = 0.05$ has asymptotic size 0.05 and power 1. The finite sample size of the test for the hypothesis testing problem - $H_0 : \theta_i = \theta_{i,0}, \quad i = 1, \cdots, 3$ against the alternative hypothesis $H_1 : \theta_i \neq \theta_{i,0}, \quad i = 1, \cdots, 3$ - is given by the fraction of times $W = \mathbf{v}^T \hat{\Sigma}^{-1} \mathbf{v}$ where
\( \mathbf{v} = (\hat{\theta}_1 - \theta_{1,0}, \ldots, \hat{\theta}_4 - \theta_{3,0}) \), is greater than 7.81. The finite-sample power for the hypothesis testing problem - \( H_0 : \theta = c \) against the alternative hypothesis \( H_1 : \theta \neq c \), where \( c \neq \theta_0 \) - is given by the fraction of times \( W = \mathbf{v}^\dagger \hat{\Sigma}^{-1} \mathbf{v} \), where \( \mathbf{v} = (\hat{\theta}_1 - c_1, \ldots, \hat{\theta}_4 - c_4) \), is greater than 7.81. The Wald test based on ML estimates is asymptotically equivalent to a likelihood ratio test, and hence is UMP (see Section II for details).

The finite-sample size and power of the Wald test for the above hypothesis for different sample sizes is reported in Table IV, for the spin-1/2 system. The finite-sample size of the Wald test for \( m = 100 \) is 0.98, almost 20 times bigger than the asymptotic value of 0.05. The 95\% quantile from the finite-sample distribution of the Wald-statistic is 47.5, whereas the corresponding asymptotic value is only 7.81. However, it is difficult and chi-squared, as would be expected from asymptotic theory. In finite samples of practical size, hypothesis testing performs rather poorly for parameters, \( \rho \) elements or eigenvalues, underscoring the inadequacy of the frequentist quantum state estimation approach for such sample sizes.

Finally, another important conjecture to test regarding the density matrix is whether an eigenvalue of \( \rho \) has a given value. Hence, we also test the hypothesis \( H_0 \) that an eigenvalue of \( \rho \) equals its true (known) value. We denote the \( i \)-th eigenvalue of the estimated density matrix \( \hat{\rho}(\hat{\theta}) \) by \( \delta_i(\hat{\theta}) \). The Hellmann-Feynman theorem can be used to compute \( \frac{\partial \delta_i(\theta)}{\partial \theta} \). Denoting the eigenvectors of \( \rho \) by \( x_i \), we have:

\[
\frac{\partial \delta_i}{\partial \theta} = \frac{\partial x_i^\dagger}{\partial \theta} \rho x_i + x_i^\dagger \frac{\partial \rho}{\partial \theta} x_i = \delta_i \frac{\partial x_i^\dagger}{\partial \theta} x_i + x_i^\dagger \frac{\partial \rho}{\partial \theta} x_i = x_i^\dagger \frac{\partial \rho}{\partial \theta} x_i,
\]

since \( (x_i | x_i) = 1, \frac{\partial}{\partial \theta} (x_i | x_i) = \frac{\partial}{\partial \theta} (1) = 0 \).

For spin-1/2 systems, the exact analytical solution for the eigenvalue derivatives is available directly since the characteristic polynomial is a quadratic:

\[
\delta_1 = r_{22} + r_{11} + \frac{1}{2} \sqrt{r_{22}^2 - 2r_{11}r_{22} + 4r_{12}^2 + r_{11}^2 + r_{12}^2} \\
\delta_2 = r_{22} + r_{11} - \frac{1}{2} \sqrt{r_{22}^2 - 2r_{11}r_{22} + 4r_{12}^2 + r_{11}^2 + r_{12}^2}
\]

where \( r_{ij} \equiv \text{Re}(\rho_{ij}), \quad i_{ij} \equiv \text{Im}(\rho_{ij}) \). However, it is difficult to analytically compute asymptotic standard errors for the estimated eigenvalues of higher-dimensional quantum states by using the Hellmann-Feynman theorem since the characteristic polynomial is of higher order. Here, eigenvalue test statistics, along with the size and power of the associated tests, were computed for the spin-1 system under consideration (Table V), because they are representative of the higher-order non-linearity common in applied problems. Note that hypothesis tests involving a single eigenvalue are t-tests.

A hypothesis of practical interest is the purity of the state. In this case, parameter values in the null hypothesis lie on the boundary of the maintained hypothesis. Hence, standard regularity conditions (the parameter value in the null should be an interior point of a compact set) that ensure asymptotic convergence of the null distributions of the t-statistic and the Wald statistic to standard normal and chi-squared distributions, respectively, fail to hold. Andrews provides general asymptotic results for testing problems of this sort. He derives the asymptotic null and local alternative distributions of the test statistics under a set of high level conditions. Although the distributions are non-standard, the critical values can be obtained by simulation.

The salient conclusion from the above examples is that the size and power of hypothesis tests fall substantially far from the asymptotically predicted values, and that the finite sample test statistic distributions are not normal and chi-squared, as would be expected from asymptotic theory. In finite samples of practical size, hypothesis testing performs rather poorly for parameters, \( \rho \) elements or eigenvalues, underscoring the inadequacy of the frequentist quantum state estimation approach for such sample sizes.

VII. DISCUSSION AND EXTENSIONS

In this paper we have examined the performance of frequentist estimators of the density matrix of a quantum system using quantum observations simulated using different measurement strategies. We provided numerical techniques for likelihood optimization under multiple constraints that are robust across arbitrary spin-1/2 and spin-1 system density matrices. In addition, we have presented methodologies and prescriptions for hypothesis testing in the frequentist quantum framework, an essential requirement for optimal decision making and control.

Performing inference in the frequentist framework, we find that the finite sample variances are significantly larger than the asymptotic bounds (predicted by the
Cramer-Rao theorem) for typical experimental sample sizes, and that these bounds are not approached at the rate predicted by asymptotic theory. This finding is robust to the choice of the density matrix and is more pronounced for small datasets. A prior study [8] showed close correspondence between asymptotic and finite sample performance in a single example, but did not consider the rate of convergence to the CRB, or higher-dimensional systems.

A unique feature of quantum statistics is the quantum Cramer-Rao bound, a generalization of the classical Cramer-Rao bound that originates due to the dependence of the quantum Fisher information on the mode of measurement. In prior work, considerable attention has been devoted to understanding the asymptotic relative efficiencies of different quantum measurement strategies. Our results warrant a careful re-examination of the relative efficiencies of these measurement strategies in finite samples. Recent studies [14] have aimed to assess the resource requirements of various quantum tomography implementations employing different measurement strategies; future efforts along these lines would benefit from attention to finite sample losses and the rate at which asymptotic predictions are approached.

Given that the finite sample variances are order(s) of magnitude bigger than the corresponding asymptotic ones, we conclude that in order to improve parameter estimates in finite samples, it is important to incorporate additional information that exploits the information geometry of quantum states into the estimation procedure. An ideal approach in this regard is Bayesian estimation. Since it is based on updating a prior plausibility distribution about the parameters based on observed data, Bayesian methods are generally more reliable than standard frequentist methods away from the asymptotic limit. The prior plausibility distribution permits the introduction of auxiliary information about the parameter space that is not contained within the likelihood. By contrast, such information is impossible to incorporate in frequentist estimation techniques. Consequently, due to the incorporation of prior knowledge, the credible intervals produced by Bayesian inference are generally shorter than their asymptotic frequentist counterparts. Moreover, as we have seen, Bayesian credible intervals do not refer to the asymptotic limit of an infinite number of measurements.

FIG. 11: Finite sample test statistic distributions, spin-1/2 quantum system. (A) t-statistic distribution for null hypothesis $H_0 : \bar{\theta}_2 = \theta_{2,0}$. The asymptotic t-statistic distribution is standard normal (superimposed). (B) Wald-statistic distribution for null hypothesis $H_0 : \bar{\theta}_1 = \theta_{i,0}, i = 1, 2, 3$. The asymptotic Wald statistic distribution is chi-squared with degrees of freedom equal to 3, the number of restrictions (superimposed).

FIG. 12: Finite sample test statistic distributions, spin-1 quantum systems. (A) t-statistic distribution for null hypothesis $H_0 : \bar{\theta}_6 = \theta_{6,0}$. The asymptotic t-statistic distribution is standard normal (superimposed). (B) Wald-statistic distribution for null hypothesis $H_0 : \bar{\theta}_i = \theta_{i,0}, i = 3, 4, 6$. The asymptotic Wald statistic distribution is chi-squared with degrees of freedom equal to 3, the number of restrictions (superimposed).
APPENDIX A: AVERAGE-CASE SUBOPTIMAL MEASUREMENT BASES

The following complete, nonoptimal measurement bases were used in Section IV C in order to assess the finite sample losses incurred due to not using mutually unbiased measurements for spin-1 systems:

\[ V^{(1)} = \begin{pmatrix} 0.732 + 0.350i & -0.078 - 0.223i & -0.163 - 0.507i \\ -0.078 - 0.223i & 0.705 - 0.649i & -0.152 - 0.036i \\ -0.163 - 0.507i & -0.152 - 0.036i & 0.460 - 0.693i \end{pmatrix} \]

\[ V^{(2)} = \begin{pmatrix} 0.571 + 0.016i & -0.738 - 0.337i & -0.122 - 0.024i \\ 0.074 + 0.144i & 0.089 - 0.001i & 0.790 + 0.584i \\ 0.796 - 0.115i & 0.563 + 0.130i & -0.075 + 0.114i \end{pmatrix} \]

\[ V^{(3)} = \begin{pmatrix} 0.301 + 0.387i & -0.095 - 0.697i & -0.168 - 0.487i \\ 0.538 + 0.003i & 0.281 - 0.336i & 0.197 + 0.693i \\ 0.674 + 0.124i & 0.119 + 0.545i & 0.264 - 0.382i \end{pmatrix} \]

\[ V^{(4)} = \begin{pmatrix} -0.115 + 0.952i & 0.009 + 0.214i & -0.129 - 0.132i \\ 0.009 + 0.214i & 0.290 - 0.391i & 0.841 + 0.097i \\ -0.129 - 0.132i & 0.841 + 0.097i & -0.156 - 0.474i \end{pmatrix} \]

These bases were generated through rotation of MUB measurement bases according to the method described in Section IV C, with \( \alpha = 1.2 \) in equation (17).

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