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Linear Quantum State Observers

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ABSTRACT This article considers the use of linear state observers to infer the unknown state (density matrix) of a closed quantum system using generalized quantum measurement—positive operator-valued measures (POVMs). An efficient test for observability is described in terms of two quantum observability matrices. The main contribution of this work is the development of a canonical quantum state observer, which may be utilized to estimate the state of any closed quantum system using POVM measurements. The observer ensures that the state estimation error tends to the unobservable space of the system, which is exactly zero when the system is observable. The space of Hermitian matrices is shown to be invariant with respect to the dynamics of the canonical observer, which allows one to project the observer's state onto the space of valid quantum density operators while retaining convergence to the true state.

INDEX TERMS Optimization in control, quantum control, quantum state estimation (QSE), spin systems, state observers.

NOMENCLATURE

Parameter	Description
d	Dimension of quantum system.
$\mathbb{H}$	Hilbert space.
$\lvert\boldsymbol{\psi}\rangle$	Pure quantum state.
$\boldsymbol{\varrho}$	Quantum density operator.
$\hat{\boldsymbol{\varrho}}$	Observer estimate of $\boldsymbol{\varrho}$.
$\boldsymbol{E}$	Error between $\hat{\boldsymbol{\varrho}}$ and $\boldsymbol{\varrho}$.
$\boldsymbol{H}$	System Hamiltonian.
$\boldsymbol{U}(t)$	Unitary dynamics generated by $-\imath\boldsymbol{H}$.
$\mathcal{M}$	Positive operator-valued measure (POVM).
$\boldsymbol{M}_k$	Element of $\mathcal{M}$.
K	Cardinality of $\mathcal{M}$.
p_k	Probability of observing outcome k.
$\mathcal{S}$	Set of all density operators in $\mathbb{H}$.
$\mathcal{P}_{\mathcal{S}}$	Projection onto the set $\mathcal{S}$.
$\mathcal{A}$	Generator of system dynamics.
$\mathcal{C}$	Output map.
$\mathcal{K}$	Observer gain.
$(\lambda_n, \lvert\boldsymbol{\phi}_n\rangle)$	Eigenpair of $\boldsymbol{H}$.
$(\xi_n, \boldsymbol{\Xi}_n)$	Eigenpair of $\mathcal{A}$.
$\mathcal{T}(t)$	C_0-semigroup generated by $\mathcal{A}$.
$\boldsymbol{y}$	System output.
$\hat{\boldsymbol{y}}$	Observer output.
$\boldsymbol{e}$	Error between $\hat{\boldsymbol{y}}$ and $\boldsymbol{y}$.
$\boldsymbol{x}$	Vectorized density operator.
$\boldsymbol{A}$	Generator of vectorized system dynamics.
$\boldsymbol{C}$	Vectorized output map.
$\boldsymbol{O}(\boldsymbol{A}, \boldsymbol{C})$	Observability matrix.
$\mathcal{Q}_{\mathrm{c}}(\mathcal{A}, \mathcal{C})$	Coherent quantum observability matrix.
$\mathcal{Q}_{\mathrm{i}}(\mathcal{A}, \mathcal{C})$	Incoherent quantum observability matrix.
$\mathbb{U}(\mathcal{A}, \mathcal{C})$	Unobservable space of $(\mathcal{A}, \mathcal{C})$.

I. INTRODUCTION

Estimating an unknown quantum state via measurement is a fundamental problem in quantum information science (QIS) [1], [2], [3]. Quantum state estimation (QSE) can be used to calibrate quantum devices and validate quantum state preparation methods. This has played an important role in, e.g., quantum optics [4], [5], [6]. However, estimating a quantum state is considerably more difficult than estimating the state of a classical system—both in terms of the mathematical theory required and the experimental burden. Historically, quantum state tomography (QST) has been the most widely employed estimation method, and introductions to this technique can be found in [7] and [8].

While the name QST has blossomed to include many different techniques, its roots originate in the need to estimate the state of qubit systems [9], [10]. As pointed out in [2, ch. 4], the word tomography originates from the Greek noun "tomos," which translates to "slice" or "section." This corresponds to the fact that QST uses the measurement history (the "slices") of a repeatedly prepared quantum state to reconstruct the entire state. The measurement basis used must be "complete" in that it uniquely determines the quantum state [11]; however, as the dimension of the system grows, the cardinality of a complete measurement basis becomes unruly. An approach proposed to circumvent this issue is "adaptive" or "self-guided" QST, which uses only a handful of measurements but updates them adaptively in order to make up for the lack of informational completeness [12], [13], [14]. This method has proven successful in physical experiments [15], [16]. However, QST is not the only approach to estimating a quantum state.

Classical systems and control theory has permeated QIS since its foundation. Optimal control [17], [18], [19], [20], [21], Lyapunov control [22], [23], [24], [25], [26], [27], adaptive control [28], [29], [30], [31], and, recently, model-predictive control [32], [33] have been applied to solve various problems within QIS. Moreover, classical means for system identification have proven useful in quantum regimes [34], [35], [36], [37]. We are interested in yet another problem deep seated in control literature: state estimation. Classical thinking regarding state estimation could prove quite useful in the quantum regime. Rather than use a quorum of measurements to infer an unknown static state, as is done in QST, systems theorists tend to consider the problem of inferring a dynamic state using fewer measurements. This requires acknowledging the natural dynamics of the underlying quantum system for which the state belongs.

Prior characterizations of *observability*, or the ability to distinguish between any two states of a quantum dynamical system, have been given by Wiseman and Milburn [38] in the Heisenberg picture and by D'Alessandro [39] in the Schrödinger picture of quantum mechanics. However, the scenarios considered by the authors vary in terms of the types of quantum measurement performed. Wiseman and Milburn [38] consider general measurements of a quantum particle's position and momentum, and they define observability in the sense of classical systems theory—that it is possible to exactly reconstruct the initial state in the absence of measurement uncertainty or error. D'Alessandro [39] considers finite-dimensional quantum systems and defines observability as being able to distinguish between the measurement record of two unique quantum states by manipulating a control input provided to the system and the time at which the measurements are performed. In an early paper, he pointed out a connection between observability and informational completeness: the set of measurement operators along with their time evolution due to the dynamics of the system must contain an informationally complete set of measurements in order to be observable [40]. Here, he also considers observability within a finite number of time steps while accounting for the backaction of measurement on the quantum state. Later, he provided an exact algorithm for extracting the maximum amount of information regarding an unknown state given a particular observable [41]. In [42], D'Alessandro addressed observability of quantum systems with selective and nonselective measurements and proposed an asymptotic observer that estimates an unknown state dynamically over time.

Designing asymptotic observers in the Schrödinger picture is the scenario that we are interested; however, our definition of observability is the classical one. This is because classical observability is equivalent to being able to design a linear state observer with arbitrary convergence rate [43, ch. 13], i.e., this cannot be achieved by weakening the definition of observability. The observers studied in this article work as follows. First, a positive operator-valued measure (POVM) is used to measure a repeatedly prepared quantum state at various points in time. This allows one to extract measurement statistics from the state. Then, the observer works offline to infer the system's unknown state from the measurement statistics. Designing these types of quantum state observers has gained attention recently. The work of [44] and [45] proposed vectorizing the dynamics of the quantum density operator in the Schrödinger picture and drew parallels to classical linear systems theory. This approach has much merit due to the control community's collective understanding of linear systems in standard form. For example, the observability of the vectorized dynamics can be tested using the Kalman observability matrix and exponentially stable state observers can be designed using classical techniques. However, the vectorized dynamics lead to a dimensionality curse, and the abstraction away from the natural mathematical form of the dynamics impedes a delicate understanding of observability and the process of designing quantum state observers.

In this work, we venture to peel back the curtain on quantum observability and provide an alternate perspective on designing quantum state observers. The main contributions of this work are as follows.

1) We provide a test for observability of quantum systems in terms of two *quantum observability matrices*. This observability test is shown to be more computationally efficient than the Kalman rank test on the vectorized dynamics.
2) We propose a canonical quantum state observer, which guarantees convergence of the state estimate to the unobservable space of *any* closed quantum system with a POVM output. Of course, when the system is observable, this ensures the state estimation error goes to zero.
3) We prove that the canonical observer preserves the Hermiticity of the state estimate. This allows us to provide an algorithm for projecting the state estimate onto the true set of density operators to ensure a physically meaningful estimate—which is not even done in many QST algorithms.

This article only considers closed quantum systems in order to push the bounds of the theory; however, designing observers for open quantum systems is possible—e.g., see [46]. Potential applications for the proposed work include calibrating quantum information devices and validating quantum state preparation methods in scenarios well within the device's decoherence time.

The rest of this article is organized as follows. Section II presents the notation used in this article. Section III gives a brief introduction to closed quantum systems and POVMs—the class of systems for which this article is concerned. Section IV presents our new test for quantum observability. Section V defines quantum state observers and proposes our canonical state observer. A discussion of projecting the state of a quantum observer onto the set of density matrices is presented in Section VI and several physically motivated examples in Section VII. Finally, Section VIII concludes this article.

II. NOTATION

Let $\mathbb{N}$, $\mathbb{R}$, and $\mathbb{C}$ denote the set of natural, real, and complex numbers, respectively. The set of integers between n and N is denoted $\mathbb{Z}_{n:N}$. Let $\imath \triangleq \sqrt{-1}$. Matrices (and vectors as a special case of matrices) appear in bold font. The d-dimensional identity matrix appears as $\boldsymbol{I}_d$. The notation $\boldsymbol{A} \succcurlyeq \boldsymbol{0}$ means that $\boldsymbol{A}$ is positive semidefinite, and $\boldsymbol{A} \succcurlyeq \boldsymbol{B}$ means that $\boldsymbol{A} - \boldsymbol{B}$ is positive semidefinite. For a vector, $\boldsymbol{x} \succcurlyeq \boldsymbol{0}$ means that each element of $\boldsymbol{x}$ is greater than or equal to zero. Given a square matrix $\boldsymbol{X} \in \mathbb{C}^{d\times d}$, $\operatorname{diag}(\boldsymbol{X})$ represents a column vector in $\mathbb{C}^d$ whose entries are the diagonal elements of $\boldsymbol{X}$; given a vector $\boldsymbol{x} \in \mathbb{C}^d$, $\operatorname{diag}(\boldsymbol{x}) \in \mathbb{C}^{d\times d}$ denotes the diagonal matrix obtained by putting the elements of $\boldsymbol{x}$ along its diagonal. $\operatorname{vec}\{\boldsymbol{X}\} \in \mathbb{C}^{d^2}$ denotes the vectorization of $\boldsymbol{X}$, $\operatorname{tr}\{\boldsymbol{X}\}$ denotes the trace of $\boldsymbol{X}$, and $\|\boldsymbol{X}\|_{\mathrm{F}}$ denotes the Frobenius norm of $\boldsymbol{X}$. $\|\boldsymbol{x}\|$ denotes the Euclidean norm of the vector $\boldsymbol{x}$. The transpose and conjugate transpose of $\boldsymbol{X}$ are written $\boldsymbol{X}^T$ and $\boldsymbol{X}^\dagger$, respectively. The commutator of $\boldsymbol{A}$ and $\boldsymbol{B}$ is written $[\![\boldsymbol{A}, \boldsymbol{B}]\!]$. The symbol $\otimes$ represents the Kronecker product. The set of functions from $[a, b]$ to Hilbert space $\mathbb{H}$ with $n \in \mathbb{N} \cup \{\infty\}$ continuous derivatives is denoted $C^n([a, b];\ \mathbb{H})$.

III. QUANTUM DYNAMICS AND MEASUREMENT

The purpose of a *quantum state observer* is to asymptotically track the state of a quantum dynamical system. The emphasis here being that the state evolves over time, which means we must first investigate the dynamics of the system. If a d-dimensional closed quantum system is initially in a pure state, i.e., $|\boldsymbol{\psi}(0)\rangle \in \mathbb{C}^d$ and $\||\boldsymbol{\psi}(0)\rangle\|_2 = 1$, then it evolves over time according to the Schrödinger equation

$$\imath \frac{d}{dt}|\boldsymbol{\psi}(t)\rangle = \boldsymbol{H}\,|\boldsymbol{\psi}(t)\rangle \tag{1}$$

where the Hermitian matrix $\boldsymbol{H} \in \mathbb{C}^{d\times d}$ is the system Hamiltonian. For well-posedness, we will also assume that $\boldsymbol{H}$ is nondegenerate (its eigenvalues are distinct).[1] Defining $\boldsymbol{U}(t) \triangleq e^{-\imath \boldsymbol{H} t}$, the closed-form solution to the Schrödinger equation is given by

$$|\boldsymbol{\psi}(t)\rangle = \boldsymbol{U}(t)|\boldsymbol{\psi}(0)\rangle. \tag{2}$$

Because $\boldsymbol{U}(t)$ is the exponential of a skew-Hermitian matrix, $\boldsymbol{U}(t)$ is unitary.[2] Since the Euclidean norm is unitarily invariant, it follows that $\||\boldsymbol{\psi}(t)\rangle\| = \||\boldsymbol{\psi}(0)\rangle\| = 1$ for all $t \geq 0$. That is, a closed quantum dynamical system initiating from a pure state remains a pure state for all future time. However, pure states are not the most general form of quantum states.

The most general representation of the state of a finite-dimensional quantum system is the *density matrix* formalization. A density matrix is defined on the Hilbert space $\mathbb{H} \triangleq \mathbb{C}^{d\times d}$ endowed with the trace inner product $\langle \boldsymbol{\varrho}, \boldsymbol{\sigma}\rangle = \operatorname{tr}\{\boldsymbol{\varrho}^\dagger \boldsymbol{\sigma}\}$ and the induced (Frobenius) norm $\|\boldsymbol{\varrho}\|_{\mathrm{F}}^2 \triangleq \operatorname{tr}\{\boldsymbol{\varrho}^\dagger \boldsymbol{\varrho}\}$. A density matrix $\boldsymbol{\varrho} \in \mathbb{H}$ is an ensemble of pure quantum states [47, ch. 2]. Let $\{|\boldsymbol{\psi}_n\rangle\}$ be any finite set of pure quantum states, i.e., $|\boldsymbol{\psi}_n\rangle \in \mathbb{C}^d$ and $\||\boldsymbol{\psi}_n\rangle\| = 1$ for all n. Any density matrix associated with an ensemble of said pure states may be written as

$$\boldsymbol{\varrho} = \sum_n \eta_n \boldsymbol{P}_n \tag{3}$$

where $\boldsymbol{P}_n \triangleq |\boldsymbol{\psi}_n\rangle\langle\boldsymbol{\psi}_n| \in \mathbb{H}$ is the orthogonal projection onto the subspace spanned by the pure state $|\boldsymbol{\psi}_n\rangle$, $\eta_n \geq 0$ for all n, and $\sum_n \eta_n = 1$. A mathematical interpretation of a mixed state is that it is a *convex combination* of projections onto a set of pure quantum states. From the defining equation (3), it immediately follows that $\boldsymbol{\varrho}$ is Hermitian positive semidefinite with unit trace. Note that any pure quantum state can be exactly represented by a density matrix; however, not every mixed state can be represented by a pure state. Hence, it is sufficient to develop the theory in this article using the density-matrix formalism. For convenience, let $\mathcal{S}$ denote the set of all density operators:

$$\mathcal{S} \triangleq \{\boldsymbol{\varrho} \in \mathbb{H} \mid \boldsymbol{\varrho} \succcurlyeq 0,\ \operatorname{tr}\{\boldsymbol{\varrho}\} = 1\}.$$

Using the solution to the Schrödinger equation, which describes the time evolution of each pure state in the ensemble (3), a density matrix initiating from $\boldsymbol{\varrho}(0)$ is in the state

$$\boldsymbol{\varrho}(t) = \boldsymbol{U}(t)\,\boldsymbol{\varrho}(0)\,\boldsymbol{U}^\dagger(t) \tag{4}$$

at time $t \geq 0$. Differentiating (4) with respect to time, the dynamics of the density matrix are found to be

$$\frac{d}{dt}\boldsymbol{\varrho}(t) = -\imath\,[\![\boldsymbol{H},\ \boldsymbol{\varrho}(t)]\!] \tag{5}$$

where $[\![\boldsymbol{H},\ \boldsymbol{\varrho}(t)]\!] \triangleq \boldsymbol{H}\boldsymbol{\varrho}(t) - \boldsymbol{\varrho}(t)\boldsymbol{H}$ is the commutator of $\boldsymbol{H}$ and $\boldsymbol{\varrho}(t)$. Equation (5) is known as the Liouville–von Neumann master equation.

[1] Degenerate Hamiltonians cause a myriad of issues within quantum mechanics. For instance, if a degenerate energy (i.e., eigenvalue) is observed, then the corresponding energy eigenstate (i.e., eigenvector) after measurement is unknown.

[2] A matrix $\boldsymbol{T}$ is unitary if $\boldsymbol{T}^\dagger$ is its inverse.

Remark 1: Despite the abuse of language, we will henceforth refer to the density matrix $\boldsymbol{\varrho}$ describing the mixed state of the quantum system as the system's "state."

Measuring a quantum state is quite different from measuring a classical state, which is often done in real time using appropriate sensors. We will consider generalized quantum measurements known as POVMs.

Definition 1: A *POVM* is a set of Hermitian operators

$$\mathcal{M} = \left\{\boldsymbol{M}_k \in \mathbb{H} : k = 1, 2, \ldots, K\right\}$$

which satisfy

$$\sum_{k=1}^{K} \boldsymbol{M}_k = \boldsymbol{I}_d, \quad \text{and} \quad \boldsymbol{M}_k \succcurlyeq \boldsymbol{0} \tag{6}$$

for $k = 1, 2, \ldots, K$.

Each operator $\boldsymbol{M}_k$ of the POVM corresponds to a potential experimental outcome. When a measurement is made, only one of the K potential outcomes is observed. If the quantum system is in state $\boldsymbol{\varrho}$, the probability of observing outcome k is given by *Born's Rule* [8, p. 99]:

$$p_k = \operatorname{tr}\{\boldsymbol{M}_k \boldsymbol{\varrho}\}, \quad k = 1, 2, \ldots, K. \tag{7}$$

Since $\boldsymbol{\varrho}$ and $\boldsymbol{M}_k$ are both Hermitian, each p_k is a real number. Due to (6), it is clear that each $p_k \geq 0$ and $\sum_{k=1}^{K} p_k = 1$, i.e., the total chance of observing one of the K outcomes is 100%. Exact knowledge of each probability in (7) would require knowledge of $\boldsymbol{\varrho}$. However, the probabilities can be well estimated by repeated measurement of an identically prepared quantum state. For example, see the simple mean-zero estimator used in [11].

As the trace function is utilized repeated throughout this article, recall the following well-known properties.

Lemma 1: Let $\boldsymbol{X}$ and $\boldsymbol{Y}$ be elements of $\mathbb{C}^{d\times d}$. Then, the following properties hold true:

1) *(conjugate property)* $\overline{\operatorname{tr}\{\boldsymbol{X}\}} = \operatorname{tr}\{\boldsymbol{X}^\dagger\}$;
2) *(cyclic property)* $\operatorname{tr}\{\boldsymbol{X}\boldsymbol{Y}\} = \operatorname{tr}\{\boldsymbol{Y}\boldsymbol{X}\}$.

IV. QUANTUM OBSERVABILITY

Prior to defining a *quantum state observer*, which is the focus of this article, we must address *observability*. An observer will attempt to estimate the state $\boldsymbol{\varrho}$ of the closed quantum system (5) using a vector $\boldsymbol{y} \in \mathbb{R}^K$ of quantum measurement statistics defined as

$$\boldsymbol{y} \triangleq \begin{bmatrix} \operatorname{tr}\{\boldsymbol{M}_1 \boldsymbol{\varrho}\} \\ \operatorname{tr}\{\boldsymbol{M}_2 \boldsymbol{\varrho}\} \\ \vdots \\ \operatorname{tr}\{\boldsymbol{M}_K \boldsymbol{\varrho}\} \end{bmatrix}. \tag{8}$$

For notational simplicity, we let $\mathcal{C} : \mathcal{S} \to \mathbb{R}^K$ be the linear operator that maps $\boldsymbol{\varrho}(t)$ to $\boldsymbol{y}(t)$ and $\mathcal{A} : \mathcal{S} \to \mathbb{H}$ be the linear operator defined by

$$\mathcal{A}\boldsymbol{\varrho} = -\imath\,[\![\boldsymbol{H}, \boldsymbol{\varrho}]\!]. \tag{9}$$

Both $\mathcal{C}$ and $\mathcal{A}$ have natural extensions to the whole domain $\mathbb{H}$—simply plug in any element of $\mathbb{H}$ into the formulas given by (8) and (9). We will represent these extensions using the same symbols; however, now $\mathcal{C} : \mathbb{H} \to \mathbb{C}^K$ and $\mathcal{A} : \mathbb{H} \to \mathbb{H}$. Denote the time derivative of $\boldsymbol{\varrho}$ as $\dot{\boldsymbol{\varrho}}$. The full quantum system including state dynamics and output variables is summarized as

$$\begin{cases} \dot{\boldsymbol{\varrho}}(t) = \mathcal{A}\,\boldsymbol{\varrho}(t) \\ \boldsymbol{y}(t) = \mathcal{C}\,\boldsymbol{\varrho}(t). \end{cases} \tag{10}$$

From a classical viewpoint, this is simply a linear dynamical system. However, the reader is cautioned.

Remark 2: Following the discussion of the prior section, note that it would be impossible obtain the output $\boldsymbol{y}(t)$ for more than a finite number of times in any interval $[t_1, t_2]$. This is because at any given time τ, the output $\boldsymbol{y}(\tau)$ may only be obtained by repeatedly preparing the state $\boldsymbol{\varrho}(\tau)$ and measuring it with $\mathcal{M}$. Nevertheless, it is useful to think theoretically about the system (10) in continuous time and then discretize during implementation of a quantum state observer. We are not the first to think (at least theoretically) about observing quantum dynamics in continuous time, e.g., see [39].

The following observability definitions for the pair $(\mathcal{A}, \mathcal{C})$ works for abstract linear systems like (10) on Hilbert space. Our only assumption is that the linear operator $\mathcal{A}$ is the generator of a strongly continuous C_0-semigroup on $\mathbb{H}$, which we will denote $\mathcal{T}(t)$. In the case of our finite dimensional quantum system, this semigroup is exactly the solution (4) to the Liouville–von Neumann equation (5)

$$\mathcal{T}(t)\,\boldsymbol{\sigma} = \boldsymbol{U}(t)\,\boldsymbol{\sigma}\,\boldsymbol{U}^\dagger(t).$$

Definition 2: The *unobservable space* of $(\mathcal{A}, \mathcal{C})$ is the null space of the operator $\mathcal{G} : \mathbb{H} \to C^\infty(\mathbb{R}_{\geq 0}; \mathbb{C}^K)$ defined via

$$\boldsymbol{\sigma} \mapsto \mathcal{C} \circ \mathcal{T}(t)\,\boldsymbol{\sigma}.$$

This space will be denoted via $\mathbb{U}(\mathcal{A}, \mathcal{C})$.

The language used here reflects the fact that any state initiating from the unobservable space cannot be observed using the state's evolution under $\mathcal{T}(t)$ and the output operator $\mathcal{C}$. One may now define observability and detectability.

Definition 3: The pair $(\mathcal{A}, \mathcal{C})$ is said to be *observable* if the unobservable space is a singleton containing only the zero element from $\mathbb{H}$.

Definition 4: The pair $(\mathcal{A}, \mathcal{C})$ is said to be *detectable* if every element of the unobservable space is asymptotically stable. That is, for any $\boldsymbol{\sigma} \in \mathbb{U}(\mathcal{A}, \mathcal{C})$

$$\lim_{t\to\infty} \mathcal{T}(t)\,\boldsymbol{\sigma} = \boldsymbol{0}. \tag{11}$$

A. FIRST-PRINCIPLES APPROACH TO QUANTUM OBSERVABILITY

The linear system $(\mathcal{A}, \mathcal{C})$ is not in standard form. The quantum system's state is a matrix and its dynamics involve operators acting on matrices. In [44] and [45], it has been proposed to vectorize the system (10) in order to obtain a standard linear system. Define $\boldsymbol{x} \in \mathbb{C}^{d^2}$ to be $\boldsymbol{x} \triangleq \operatorname{vec}\{\boldsymbol{\varrho}\}$, which is a natural isometry between $\mathbb{C}^{d^2}$ and $\mathbb{H}$. Moreover, let $\boldsymbol{A} \in \mathbb{C}^{d^2 \times d^2}$ be defined as

$$\boldsymbol{A} \triangleq -\imath\,(\boldsymbol{I}_d \otimes \boldsymbol{H} - \boldsymbol{H} \otimes \boldsymbol{I}_d)$$

and let $\boldsymbol{C} \in \mathbb{C}^{K \times d^2}$ be defined as

$$\boldsymbol{C} \triangleq \begin{bmatrix} \mathrm{vec}\{\boldsymbol{M}_1\}^\dagger \\ \mathrm{vec}\{\boldsymbol{M}_2\}^\dagger \\ \vdots \\ \mathrm{vec}\{\boldsymbol{M}_K\}^\dagger \end{bmatrix}. \tag{12}$$

The dynamics of (10) are then equivalently expressed as

$$\begin{cases} \dot{\boldsymbol{x}}(t) = \boldsymbol{A}\,\boldsymbol{x}(t) \\ \boldsymbol{y}(t) = \boldsymbol{C}\,\boldsymbol{x}(t). \end{cases} \tag{13}$$

Then, the observability of the pair $(\boldsymbol{A}, \boldsymbol{C})$ can be studied using techniques from classical systems theory. In fact, the pair is observable when the "Kalman observability matrix"

$$\boldsymbol{O}(\boldsymbol{A}, \boldsymbol{C}) \triangleq \begin{bmatrix} \boldsymbol{C} \\ \boldsymbol{C}\boldsymbol{A} \\ \boldsymbol{C}\boldsymbol{A}^2 \\ \vdots \\ \boldsymbol{C}\boldsymbol{A}^{(d^2-1)} \end{bmatrix} \tag{14}$$

is full rank [48]. Using this approach will surely allow one to determine the observability of the system. However, there are the following two notable drawbacks of this method.

1) The operators $\boldsymbol{A} \in \mathbb{C}^{d^2 \times d^2}$ and $\boldsymbol{C} \in \mathbb{C}^{K \times d^2}$ are large even for reasonable values of d and K. As a result, the observability matrix $\boldsymbol{O}(\boldsymbol{A}, \boldsymbol{C}) \in \mathbb{C}^{Kd^2 \times d^2}$ becomes cumbersome to deal with.
2) If one determines that the pair $(\boldsymbol{A}, \boldsymbol{C})$ is observable using the observability matrix, they must still go about designing a stable state observer. As we will see, if the system $(\mathcal{A}, \mathcal{C})$ is observable, there exists a universal Hermiticity-preserving quantum state observer that requires no effort to construct. This insight is only available by addressing the system (10) directly.

These drawbacks motivate the investigation pursued in this article.

B. ADDRESSING QUANTUM OBSERVABILITY DIRECTLY

The first goal of this article is to use the structure of closed quantum systems and POVMs to reduce testing observability for quantum systems down to something more manageable than constructing the Kalman observability matrix. The first consequence of addressing observability using Definitions 2–4 is the following theorem, which is nothing more than an observation regarding the unitary dynamics of a closed quantum system.

Theorem 2: The closed quantum system $(\mathcal{A}, \mathcal{C})$ is observable if and only if it is detectable.

Proof: The definition of observability gives the sufficiency. To prove the necessity, note that for any $\boldsymbol{\sigma} \in \mathbb{U}(\mathcal{A}, \mathcal{C})$

$$\|\mathcal{T}(t)\,\boldsymbol{\sigma}\|_{\mathrm{F}} = \|\boldsymbol{U}(t)\,\boldsymbol{\sigma}\,\boldsymbol{U}^\dagger(t)\|_{\mathrm{F}} = \|\boldsymbol{\sigma}\|_{\mathrm{F}} \tag{15}$$

for all t due to the unitary invariance of the Frobenius norm. Hence, by (15), it is impossible for any element of $\mathbb{H}$ to satisfy (11) other than $\boldsymbol{\sigma} = \boldsymbol{0}$. This proves the theorem. ■

Remark 3: In classical systems, detectability is a slightly weakened version of observability. The above theorem shows that it is impossible to weaken the definition of observability for closed quantum systems using the standard classical means.

Since the Hamiltonian $\boldsymbol{H}$ is a Hermitian operator, the spectral theorem states that the eigenvalues of $\boldsymbol{H}$ are real and that it is possible to decompose $\boldsymbol{H}$ into a basis of orthonormal eigenvectors [49]. Denote the nth eigenpair of $\boldsymbol{H}$ by $(\lambda_n, |\boldsymbol{\phi}_n\rangle)$. The eigenvalue λ_n and eigenvector $|\boldsymbol{\phi}_n\rangle$ satisfy the relation

$$\boldsymbol{H}|\boldsymbol{\phi}_n\rangle = \lambda_n\,|\boldsymbol{\phi}_n\rangle$$

and there are d eigenpairs for $\boldsymbol{H} \in \mathbb{H}$. The following lemma relates the eigenvalues and eigenvectors of $\boldsymbol{H}$ to the eigenvalues and *eigenmatrices* of the operator $\mathcal{A}$.

Lemma 3: The d^2 eigenpairs, $(\xi_i, \boldsymbol{\Xi}_i)$, of the operator $\mathcal{A}$ are of the form

$$\xi_i = \imath\,(\lambda_m - \lambda_n) \quad \text{and} \quad \boldsymbol{\Xi}_i = |\boldsymbol{\phi}_n\rangle\langle\boldsymbol{\phi}_m| \tag{16}$$

for $n, m \in \{1, 2, \ldots, d\}$. The eigenmatrices $\{\boldsymbol{\Xi}_i : i = 1, 2, \ldots, d^2\}$ form an orthonormal basis for $\mathbb{H}$.

Proof: For any pair $(\xi_i, \boldsymbol{\Xi}_i)$ defined in (16), it follows that

$$\begin{aligned} -\imath\,[\![\boldsymbol{H}, \boldsymbol{\Xi}_i]\!] &= \imath\,(\boldsymbol{\Xi}_i\boldsymbol{H} - \boldsymbol{H}\boldsymbol{\Xi}_i) \\ &= \imath\,(\,|\boldsymbol{\phi}_n\rangle\langle\boldsymbol{\phi}_m|\boldsymbol{H} - \boldsymbol{H}|\boldsymbol{\phi}_n\rangle\langle\boldsymbol{\phi}_m|\,) \\ &= \imath\,(\,\lambda_m|\boldsymbol{\phi}_n\rangle\langle\boldsymbol{\phi}_m| - \lambda_n|\boldsymbol{\phi}_n\rangle\langle\boldsymbol{\phi}_m|\,) \\ &= \xi_i\,\boldsymbol{\Xi}_i. \end{aligned}$$

Hence, $(\xi_i, \boldsymbol{\Xi}_i)$ is an eigenpair for $\mathcal{A}$. Let $\boldsymbol{\Xi}_i = |\boldsymbol{\phi}_n\rangle\langle\boldsymbol{\phi}_m|$ and $\boldsymbol{\Xi}_j = |\boldsymbol{\phi}_k\rangle\langle\boldsymbol{\phi}_l|$. Using the cyclic property of the trace,

$$\begin{aligned} \mathrm{tr}\left\{\boldsymbol{\Xi}_i\,\boldsymbol{\Xi}_j^\dagger\right\} &= \mathrm{tr}\{|\boldsymbol{\phi}_n\rangle\langle\boldsymbol{\phi}_m|\,|\boldsymbol{\phi}_l\rangle\langle\boldsymbol{\phi}_k|\} \\ &= \mathrm{tr}\{\langle\boldsymbol{\phi}_k|\boldsymbol{\phi}_n\rangle\,\langle\boldsymbol{\phi}_m|\boldsymbol{\phi}_l\rangle\}\,. \end{aligned}$$

If $i \neq j$, then $n \neq k$ or $m \neq l$. By the orthonormality of the eigenvectors of $\mathbb{H}$, it follows that

$$\langle\boldsymbol{\Xi}_i, \boldsymbol{\Xi}_j\rangle = \mathrm{tr}\left\{\boldsymbol{\Xi}_i\,\boldsymbol{\Xi}_j^\dagger\right\} = \begin{cases} 1 & i = j \\ 0 & i \neq j. \end{cases}$$

Hence, the eigenmatrices of $\mathcal{A}$ form an orthonormal basis for $\mathbb{H}$. ■

Since $\mathcal{A}$ admits a set of orthonormal eigenmatrices that form a basis for $\mathbb{H}$, it is possible to expand any density operator $\boldsymbol{\sigma}$ in the $\{\boldsymbol{\Xi}_i \ : \ i = 1, 2, \ldots, d^2\}$ basis

$$\boldsymbol{\sigma} = \sum_{i=1}^{d^2} \underbrace{\mathrm{tr}\left\{\boldsymbol{\Xi}_i^\dagger \boldsymbol{\sigma}\right\}}_{\triangleq \gamma_i} \boldsymbol{\Xi}_i.$$

Moreover, the evolution of any eigenmatrix $\boldsymbol{\Xi}_i$ under the semigroup $\mathcal{T}(t)$ is simple

$$\mathcal{T}(t)\,\boldsymbol{\Xi}_i = e^{\xi_i t}\,\boldsymbol{\Xi}_i \tag{17}$$

where $|e^{\xi_i t}| = 1$ for all $t \geq 0$. Hence

$$\mathcal{T}(t)\,\boldsymbol{\sigma} = \sum_{i=1}^{d^2} \gamma_i\, e^{\xi_i t}\,\boldsymbol{\Xi}_i. \tag{18}$$

As seen in (16), each ξ_i is a purely imaginary number; therefore, each $e^{\xi_i t}$ is a complex sinusoid. We have the following lemma, which is a slight twist on those for linear systems, such as (13), in standard form (e.g., see [50, Th. 6.8]).

Lemma 4: Let ξ be an eigenvalue of $\mathcal{A}$ which is repeated N times, and suppose the eigenmatrices $\{\boldsymbol{\Xi}_i : i \in \mathbb{Z}_{n:n+N}\}$ from (16) all correspond to ξ. The quantum system $(\mathcal{A}, \mathcal{C})$ is observable if and only if for each such eigenvalue ξ the elements of the set

$$\mathcal{Z}_\xi \triangleq \left\{\, \mathcal{C}(\boldsymbol{\Xi}_i) \ : \ i \in \mathbb{Z}_{n:n+N} \,\right\} \tag{19}$$

are linearly independent.

Proof: Suppose for some ξ the elements of $\mathcal{Z}_\xi$ are linearly dependent. Then, there exists a nonzero set of coefficients $\{\alpha_i : i \in \mathbb{Z}_{n:n+N}\}$ such that

$$\sum_{i=n}^{n+N} \alpha_i\, \mathcal{C}(\boldsymbol{\Xi}_i) = \mathbf{0}.$$

Then, $\boldsymbol{\Xi} \triangleq \sum_i \alpha_i\, \boldsymbol{\Xi}_i$ is an eigenmatrix of $\mathcal{A}$ with eigenvalue ξ. The linear independence of the $\boldsymbol{\Xi}_i$'s in Lemma 3 ensures that $\boldsymbol{\Xi}$ is nonzero. However,

$$\mathcal{C} \circ \mathcal{T}(t)\,\boldsymbol{\Xi} = e^{\xi t}\,\mathcal{C}(\boldsymbol{\Xi}) = \mathbf{0}$$

for all $t \geq 0$. Therefore, $\boldsymbol{\Xi}$ is a nonzero element of the unobservable space, and $(\mathcal{A}, \mathcal{C})$ is unobservable.

To prove sufficiency, suppose $(\mathcal{A}, \mathcal{C})$ is unobservable. Then, according to (18), there exists a nonzero set of coefficients $\{\gamma_i' : i = 1, 2, \ldots, d^2\}$ such that

$$\sum_{i=1}^{d^2} \gamma_i'\, e^{\xi_i t}\,\mathcal{C}(\boldsymbol{\Xi}_i) = \mathbf{0} \quad \forall t \geqslant 0. \tag{20}$$

As each $e^{\xi_i t}$ represents a complex sinusoid, we see that for each distinct eigenvalue ξ, which starts at index $i = n$ and is repeated N times

$$\sum_{i=n}^{n+N} \gamma_i'\, e^{\xi t}\,\mathcal{C}(\boldsymbol{\Xi}_i) = \mathbf{0} \quad \forall t \geqslant 0.$$

Therefore

$$\sum_{i=n}^{n+N} \gamma_i'\,\mathcal{C}(\boldsymbol{\Xi}_i) = \mathbf{0}$$

for each distinct ξ. As the set of γ_i's were nonzero, the elements of $\mathcal{Z}_\xi$ are linearly dependent for some ξ. This proves the theorem. ∎

The prior lemma is itself an alternate to constructing the Kalman observability matrix to test observability of the system $(\mathcal{A}, \mathcal{C})$. However, we can harness more of the quantum system's structure to simplify things further.

Lemma 5: Let $\boldsymbol{\Xi}_i = |\boldsymbol{\phi}_n\rangle\langle\boldsymbol{\phi}_m|$ and $\boldsymbol{\Xi}_j = |\boldsymbol{\phi}_m\rangle\langle\boldsymbol{\phi}_n|$ be eigenmatrices of $\mathcal{A}$. Then, $\mathcal{C}(\boldsymbol{\Xi}_i) = \mathbf{0}$ if and only if $\mathcal{C}(\boldsymbol{\Xi}_j) = \mathbf{0}$.

Proof: The kth element of the vector $\mathcal{C}(\boldsymbol{\Xi}_i)$ is given by

$$\mathcal{C}_k(\boldsymbol{\Xi}_i) = \mathrm{tr}\left\{\boldsymbol{M}_k\,\boldsymbol{\Xi}_i\right\}.$$

Moreover, $\mathrm{tr}\{\boldsymbol{M}_k\,\boldsymbol{\Xi}_i\} = 0$ if and only if $\overline{\mathrm{tr}\{\boldsymbol{M}_k\,\boldsymbol{\Xi}_i\}} = 0$. On the other hand

$$\begin{aligned}
\overline{\mathrm{tr}\left\{\boldsymbol{M}_k\,\boldsymbol{\Xi}_i\right\}} &= \overline{\mathrm{tr}\left\{\boldsymbol{M}_k|\boldsymbol{\phi}_n\rangle\langle\boldsymbol{\phi}_m|\right\}} \\
&= \mathrm{tr}\left\{\left(\boldsymbol{M}_k|\boldsymbol{\phi}_n\rangle\langle\boldsymbol{\phi}_m|\right)^\dagger\right\} \\
&= \mathrm{tr}\left\{|\boldsymbol{\phi}_m\rangle\langle\boldsymbol{\phi}_n|\boldsymbol{M}_k\right\} \\
&= \mathrm{tr}\left\{\boldsymbol{M}_k|\boldsymbol{\phi}_m\rangle\langle\boldsymbol{\phi}_n|\right\} \\
&= \mathrm{tr}\left\{\boldsymbol{M}_k\,\boldsymbol{\Xi}_j\right\}
\end{aligned}$$

where the third equality uses the Hermiticity of $\boldsymbol{M}_k$ and the fourth equality uses the cyclic property of the trace. It follows that $\mathcal{C}_k(\boldsymbol{\Xi}_i) = 0$ if and only if $\mathcal{C}_k(\boldsymbol{\Xi}_j) = 0$. This holds for each index k, so $\mathcal{C}(\boldsymbol{\Xi}_i) = \mathbf{0}$ if and only if $\mathcal{C}(\boldsymbol{\Xi}_j) = \mathbf{0}$. ∎

We now produce an observability test on $(\mathcal{A}, \mathcal{C})$ in terms of the system Hamiltonian $\boldsymbol{H}$ and the POVM $\mathcal{M}$, which is the main result of this section. In the process, we introduce the *quantum observability* matrices $\mathcal{Q}_\mathrm{i}(\mathcal{A}, \mathcal{C})$ and $\mathcal{Q}_\mathrm{c}(\mathcal{A}, \mathcal{C})$. The computational complexity of determining whether or not $(\mathcal{A}, \mathcal{C})$ is observable using the quantum observability matrices and the Kalman observability matrix $\boldsymbol{O}(\mathcal{A}, \mathcal{C})$ is studied in the following section. For ease of notation, define the matrix $\boldsymbol{V}_\mathrm{c} \in \mathbb{C}^{d^2\times(d^2-d)/2}$ as in (21) and $\boldsymbol{V}_\mathrm{i} \in \mathbb{C}^{d^2\times d}$ as in (23), which are depicted at the bottom of the next page.

Definition 5: Given $(\mathcal{A}, \mathcal{C})$, the *coherent* and *incoherent quantum observability matrices* are denoted and defined as

$$\mathcal{Q}_\mathrm{c}(\mathcal{A}, \mathcal{C}) \triangleq \boldsymbol{C}\boldsymbol{V}_\mathrm{c} \quad \mathcal{Q}_\mathrm{i}(\mathcal{A}, \mathcal{C}) \triangleq \boldsymbol{C}\boldsymbol{V}_\mathrm{i} \tag{24}$$

respectively. The proof of the following theorem will show that these expressions are equivalent to those in (22), shown at the bottom of this page, and (23). However, (24) will play a useful role in designing an efficient algorithm for testing quantum observability.

Remark 4: We use the term "coherent" because $\mathcal{Q}_\mathrm{c}$ tests the ability to distinguish between coherent quantum states. On the other hand, $\mathcal{Q}_\mathrm{i}$ tests the ability to distinguish between incoherent classical superpositions of energy (Hamiltonian) eigenstates of the form $\boldsymbol{\varrho} = \sum_{n=1}^{d} \eta_n |\boldsymbol{\phi}_n\rangle\langle\boldsymbol{\phi}_n|$.

Theorem 6: Let $\boldsymbol{H}$ be nondegenerate. The closed quantum system $(\mathcal{A}, \mathcal{C})$ is observable if and only if the coherent quantum observability matrix $\mathcal{Q}_\mathrm{c}(\mathcal{A}, \mathcal{C})$ has no zero columns and the incoherent quantum observability matrix $\mathcal{Q}_\mathrm{i}(\mathcal{A}, \mathcal{C})$ has full column rank.

Proof: First, we will show that $\mathcal{Q}_\mathrm{c}(\mathcal{A}, \mathcal{C})$ defined in (24) and (22) are equivalent. Given $\langle \boldsymbol{M}_k\rangle_{|\boldsymbol{\phi}_m\rangle\langle\boldsymbol{\phi}_n|} \triangleq \mathrm{tr}\{\boldsymbol{M}_k|\boldsymbol{\phi}_m\rangle\langle\boldsymbol{\phi}_n|\}$, note that

$$\begin{aligned}\overline{\langle \boldsymbol{M}_k\rangle}_{|\boldsymbol{\phi}_m\rangle\langle\boldsymbol{\phi}_n|} &= \mathrm{vec}\{\boldsymbol{M}_k\}^\dagger\,\mathrm{vec}\{|\boldsymbol{\phi}_n\rangle\langle\boldsymbol{\phi}_m|\}\\ &= \mathrm{vec}\{\boldsymbol{M}_k\}^\dagger\,\overline{|\boldsymbol{\phi}_m\rangle}\otimes|\boldsymbol{\phi}_n\rangle.\end{aligned}$$

The equivalence of (24) and (22), follows from (12) and (21). Similarly, one can show that $\mathcal{Q}_\mathrm{i}(\mathcal{A}, \mathcal{C})$ as defined in (24) and (23), (23) shown at the bottom of next page are equivalent. The alternate descriptions of the quantum observability matrices may be used to prove the theorem.

Since $\boldsymbol{H}$ is nondegenerate, (16) reveals that the only repeated eigenvalue of $\mathcal{A}$ is $\xi = 0$, which is repeated d times and has eigenvectors of the form $\boldsymbol{\Xi}_i = |\boldsymbol{\phi}_n\rangle\langle\boldsymbol{\phi}_n|$. Therefore, for $\xi \neq 0$, Lemma 4 reduces to verifying that $\mathcal{C}(\boldsymbol{\Xi}_i) \neq \boldsymbol{0}$ for each eigenmatrix $\boldsymbol{\Xi}_i = |\boldsymbol{\phi}_m\rangle\langle\boldsymbol{\phi}_n|$ with $m \neq n$. Given two eigenmatrices $\boldsymbol{\Xi}_i = |\boldsymbol{\phi}_m\rangle\langle\boldsymbol{\phi}_n|$ and $\boldsymbol{\Xi}_j = |\boldsymbol{\phi}_n\rangle\langle\boldsymbol{\phi}_m|$ $(m \neq n)$, Lemma 5 states that one need to only verify that $\mathcal{C}(\boldsymbol{\Xi}_i) \neq \boldsymbol{0}$. Given (22), this corresponds to verifying that the coherent quantum observability matrix $\mathcal{Q}_\mathrm{c}(\mathcal{A}, \mathcal{C})$ has no zero columns. Then, according to Lemma 4, we must verify that the elements of $\mathcal{Z}_0$ are linearly independent. Given (23), this is equivalent to the test on $\mathcal{Q}_\mathrm{i}(\mathcal{A}, \mathcal{C})$ stated in the theorem. ■

Theorem 7: Let $\boldsymbol{H}$ be an arbitrary Hamiltonian. If $(\mathcal{A}, \mathcal{C})$ is observable, then the cardinality of the POVM $\mathcal{M}$ is at least d.

Proof: In the case where $\boldsymbol{H}$ is nondegenerate, the result follows from the prior theorem. For $\mathcal{Q}_\mathrm{i}(\mathcal{A}, \mathcal{C})$ to have full column rank, it must have at least d rows. The number of rows of $\mathcal{Q}_\mathrm{i}(\mathcal{A}, \mathcal{C})$ is equal to the cardinality of $\mathcal{M}$.

In the general case, Lemma 3 proves that $\mathcal{A}$ will have at least d zero eigenvalues. Lemma 4 requires that the elements of $\mathcal{Z}_0$, which has cardinality at least d, be linearly independent in order for $(\mathcal{A}, \mathcal{C})$ to be observable. For this to

$$\boldsymbol{V}_\mathrm{c} \triangleq \begin{bmatrix} | & | & & | & | & | & & | & & | \\ \overline{|\boldsymbol{\phi}_1\rangle}\otimes|\boldsymbol{\phi}_2\rangle & \overline{|\boldsymbol{\phi}_1\rangle}\otimes|\boldsymbol{\phi}_3\rangle & \dots & \overline{|\boldsymbol{\phi}_1\rangle}\otimes|\boldsymbol{\phi}_d\rangle & \overline{|\boldsymbol{\phi}_2\rangle}\otimes|\boldsymbol{\phi}_3\rangle & \overline{|\boldsymbol{\phi}_2\rangle}\otimes|\boldsymbol{\phi}_4\rangle & \dots & \overline{|\boldsymbol{\phi}_2\rangle}\otimes|\boldsymbol{\phi}_d\rangle & \dots & \overline{|\boldsymbol{\phi}_{d-1}\rangle}\otimes|\boldsymbol{\phi}_d\rangle \\ | & | & & | & | & | & & | & & | \end{bmatrix} \tag{21}$$

$$\mathcal{Q}_\mathrm{c}(\mathcal{A}, \mathcal{C}) \triangleq \begin{bmatrix} \overline{\langle \boldsymbol{M}_1\rangle}_{|\phi_1\rangle\langle\phi_2|} & \overline{\langle \boldsymbol{M}_1\rangle}_{|\phi_1\rangle\langle\phi_3|} & \dots & \overline{\langle \boldsymbol{M}_1\rangle}_{|\phi_1\rangle\langle\phi_d|} & \overline{\langle \boldsymbol{M}_1\rangle}_{|\phi_2\rangle\langle\phi_3|} & \overline{\langle \boldsymbol{M}_1\rangle}_{|\phi_2\rangle\langle\phi_4|} & \dots & \overline{\langle \boldsymbol{M}_1\rangle}_{|\phi_2\rangle\langle\phi_d|} & \dots & \overline{\langle \boldsymbol{M}_1\rangle}_{|\phi_{d\text{-}1}\rangle\langle\phi_d|} \\ \overline{\langle \boldsymbol{M}_2\rangle}_{|\phi_1\rangle\langle\phi_2|} & \overline{\langle \boldsymbol{M}_2\rangle}_{|\phi_1\rangle\langle\phi_3|} & \dots & \overline{\langle \boldsymbol{M}_2\rangle}_{|\phi_1\rangle\langle\phi_d|} & \overline{\langle \boldsymbol{M}_2\rangle}_{|\phi_2\rangle\langle\phi_3|} & \overline{\langle \boldsymbol{M}_2\rangle}_{|\phi_2\rangle\langle\phi_4|} & \dots & \overline{\langle \boldsymbol{M}_2\rangle}_{|\phi_2\rangle\langle\phi_d|} & \dots & \overline{\langle \boldsymbol{M}_2\rangle}_{|\phi_{d\text{-}1}\rangle\langle\phi_d|} \\ & & & & \vdots & & & & & \\ \overline{\langle \boldsymbol{M}_K\rangle}_{|\phi_1\rangle\langle\phi_2|} & \overline{\langle \boldsymbol{M}_K\rangle}_{|\phi_1\rangle\langle\phi_3|} & \dots & \overline{\langle \boldsymbol{M}_K\rangle}_{|\phi_1\rangle\langle\phi_d|} & \overline{\langle \boldsymbol{M}_K\rangle}_{|\phi_2\rangle\langle\phi_3|} & \overline{\langle \boldsymbol{M}_K\rangle}_{|\phi_2\rangle\langle\phi_4|} & \dots & \overline{\langle \boldsymbol{M}_K\rangle}_{|\phi_2\rangle\langle\phi_d|} & \dots & \overline{\langle \boldsymbol{M}_K\rangle}_{|\phi_{d\text{-}1}\rangle\langle\phi_d|} \end{bmatrix} \tag{22}$$

$$\boldsymbol{V}_\mathrm{i} \triangleq \begin{bmatrix} | & | & & | \\ \overline{|\boldsymbol{\phi}_1\rangle}\otimes|\boldsymbol{\phi}_1\rangle & \overline{|\boldsymbol{\phi}_2\rangle}\otimes|\boldsymbol{\phi}_2\rangle & \dots & \overline{|\boldsymbol{\phi}_d\rangle}\otimes|\boldsymbol{\phi}_d\rangle \\ | & | & & | \end{bmatrix} \qquad \mathcal{Q}_\mathrm{i} \triangleq \begin{bmatrix} \langle \boldsymbol{M}_1\rangle_{|\phi_1\rangle\langle\phi_1|} & \langle \boldsymbol{M}_1\rangle_{|\phi_2\rangle\langle\phi_2|} & & \langle \boldsymbol{M}_1\rangle_{|\phi_d\rangle\langle\phi_d|} \\ \langle \boldsymbol{M}_2\rangle_{|\phi_1\rangle\langle\phi_1|} & \langle \boldsymbol{M}_2\rangle_{|\phi_2\rangle\langle\phi_2|} & & \langle \boldsymbol{M}_2\rangle_{|\phi_d\rangle\langle\phi_d|} \\ \vdots & \vdots & \dots & \vdots \\ \langle \boldsymbol{M}_K\rangle_{|\phi_1\rangle\langle\phi_1|} & \langle \boldsymbol{M}_K\rangle_{|\phi_2\rangle\langle\phi_2|} & & \langle \boldsymbol{M}_K\rangle_{|\phi_d\rangle\langle\phi_d|} \end{bmatrix} \tag{23}$$

Algorithm 1: Observability Test on $\mathcal{Q}_{\mathrm{c}}(\mathcal{A}, \mathcal{C})$ and $\mathcal{Q}_{\mathrm{i}}(\mathcal{A}, \mathcal{C})$.

Input: $\boldsymbol{H}, \boldsymbol{C}$.
Initialize: $\boldsymbol{V}_{\mathrm{c}} = [\ ]$ and $\boldsymbol{V}_{\mathrm{i}} = [\ ]$.
Compute eigenvectors $\{|\boldsymbol{\phi}_k\rangle : k=1, 2, \ldots, d\}$ of $\boldsymbol{H}$.
for $m = 1, 2, \ldots, d$ **do**
  for $n = m+1, m+2, \ldots, d$ **do**
    Set $\boldsymbol{V}_{\mathrm{c}} = \left[\boldsymbol{V}_{\mathrm{c}};\ \overline{|\boldsymbol{\phi}_m\rangle} \otimes |\boldsymbol{\phi}_n\rangle\right]$
  end for
  Set $\boldsymbol{V}_{\mathrm{i}} = \left[\boldsymbol{V}_{\mathrm{i}};\ \overline{|\boldsymbol{\phi}_m\rangle} \otimes |\boldsymbol{\phi}_m\rangle\right]$
end for
Set $\mathcal{Q}_{\mathrm{c}}(\mathcal{A}, \mathcal{C}) = \boldsymbol{C}\boldsymbol{V}_{\mathrm{c}}$
Set $\mathcal{Q}_{\mathrm{i}}(\mathcal{A}, \mathcal{C}) = \boldsymbol{C}\boldsymbol{V}_{\mathrm{i}}$
Search for zero columns of $\mathcal{Q}_{\mathrm{c}}(\mathcal{A}, \mathcal{C})$
Compute rank of $\mathcal{Q}_{\mathrm{i}}(\mathcal{A}, \mathcal{C})$
if zero column found **or** $\mathrm{rank}\{\mathcal{Q}_{\mathrm{i}}(\mathcal{A}, \mathcal{C})\} < d$ **then**
  Return: Unobservable.
else
  Return: Observable.
end if

hold, the codomain of $\mathcal{C}$ must be at least d-dimensional. Since the codomain of $\mathcal{C}$ has dimension equal to the cardinality of $\mathcal{M}$, the theorem is proved. ∎

The results of this section are rooted in the *structure* of the quantum system $(\mathcal{A}, \mathcal{C})$. Theorem 2 and Lemmas 3–5 rest on the structure of $\mathcal{A}$, which generates unitary dynamics, and the structure of quantum measurement via POVMs. Theorem 6 aggregates the prior lemmas into an equivalent test for quantum observability. Theorem 7 provides a fundamental limit on quantum observability. While these results may be seen as elementary, we believe that we are the first to utilize the structure of $(\mathcal{A}, \mathcal{C})$ to deduce these foundational results.

C. COMPUTATIONAL COMPLEXITY OF TESTING OBSERVABILITY VIA THE QUANTUM OBSERVABILITY MATRICES

In addition to providing insight on the detectability and observability of the closed quantum system $(\mathcal{A}, \mathcal{C})$, the work of the prior section provides a computationally efficient technique for testing the system's observability. This section details the complexity of constructing and testing the quantum observability matrices. This procedure is summarized in Algorithm 1 and is comprised of the following seven steps:

1) compute the eigenvectors of $\boldsymbol{H}$;
2) compute the $\frac{1}{2}(d^2 - d)$ columns of $\boldsymbol{V}_{\mathrm{c}}$;
3) compute the d columns of $\boldsymbol{V}_{\mathrm{i}}$;
4) compute $\mathcal{Q}_{\mathrm{c}}(\mathcal{A}, \mathcal{C}) = \boldsymbol{C}\boldsymbol{V}_{\mathrm{c}}$;
5) compute $\mathcal{Q}_{\mathrm{i}}(\mathcal{A}, \mathcal{C}) = \boldsymbol{C}\boldsymbol{V}_{\mathrm{i}}$;
6) search for zero columns of $\mathcal{Q}_{\mathrm{c}}(\mathcal{A}, \mathcal{C})$;
7) compute the rank of $\mathcal{Q}_{\mathrm{i}}(\mathcal{A}, \mathcal{C})$.

The eigendecomposition in step 1 has computational complexity $\mathcal{O}(d^3)$. Computing each of the $\frac{1}{2}(d^2 - d)$ outer products of the form $\overline{|\boldsymbol{\phi}_m\rangle} \otimes |\boldsymbol{\phi}_n\rangle$ in step 2 has complexity $\mathcal{O}(d^2)$. Thus, step 2 has a total complexity of $\mathcal{O}(d^4)$. Similarly, step 3 has complexity $\mathcal{O}(d^3)$. Step 4 requires multiplying $\boldsymbol{C} \in \mathbb{C}^{K\times d^2}$ by $\boldsymbol{V}_{\mathrm{c}} \in \mathbb{C}^{d^2\times\frac{(d^2-d)}{2}}$ for a total complexity of $\mathcal{O}(K\,d^4)$. Similarly, multiplying $\boldsymbol{C}$ by $\boldsymbol{V}_{\mathrm{i}} \in \mathbb{C}^{d^2\times d}$ in step 5 has complexity $\mathcal{O}(K\,d^3)$. The search in step 6 has a maximum of $K\frac{d^2-d}{2}$ logical operations for a complexity upper bound of $\mathcal{O}(K\,d^2)$. Computing the rank of $\mathcal{Q}_{\mathrm{i}}(\mathcal{A}, \mathcal{C}) \in \mathbb{C}^{K\times d}$ may be done to high accuracy with the singular value decomposition (although this is more computationally intense than other methods [51]) with complexity $\mathcal{O}(K\,d^2)$—here, we have assumed $K \geq d$, which is required by Theorem 7. Thus, we have the following.

Theorem 8: The computational complexity of testing the observability of $(\mathcal{A}, \mathcal{C})$ via the quantum observability matrices is upper bounded by $\mathcal{O}(K\,d^4)$.

Our complexity analysis has assumed naive "schoolbook" calculations for all mathematical computations. Let us compare the complexity of Algorithm 1 to that of constructing $\boldsymbol{O}(\boldsymbol{A}, \boldsymbol{C})$, which was defined in (14), and checking its rank. Recall that $\boldsymbol{A} \in \mathbb{C}^{d^2\times d^2}$. Assuming repeated squaring, which is, for example, used by the MATLAB matrix power command [52], the complexity of computing $\boldsymbol{A}^k$ is $\mathcal{O}((k-1)\,(d^2)^3) = \mathcal{O}((k-1)\,d^6)$, and this is done for k up to $d^2 - 1$ for a complexity of $\mathcal{O}(d^8)$. Each of the $d^2 - 2$ terms $\boldsymbol{C}\boldsymbol{A}, \boldsymbol{C}\boldsymbol{A}^2, \ldots, \boldsymbol{C}\boldsymbol{A}^{d^2-1}$ requires a matrix multiplication of complexity $\mathcal{O}(Kd^4)$ for a total complexity of $\mathcal{O}(Kd^6)$. With these pieces in place, one may construct $\boldsymbol{O}(\boldsymbol{A}, \boldsymbol{C})$. Without even considering the complexity of computing the rank of $\boldsymbol{O}(\boldsymbol{A}, \boldsymbol{C}) \in \mathbb{C}^{Kd^2\times d^2}$, we see that the $\mathcal{O}(\max\{d^8, Kd^6\})$ computational complexity of constructing the Kalman observability matrix greatly exceeds the complexity of constructing *and* testing the quantum observability matrices.

V. QUANTUM STATE OBSERVERS

An important object in classical systems is the "state observer," which is a dynamic estimate of a system's true state. It evolves over time by measuring the system's output and updating its estimate of the true state according to a pre-engineered rule. We define a linear quantum state estimator below.

Definition 6: A *linear quantum state observer* is an estimate $\hat{\boldsymbol{\varrho}}(t) \in \mathbb{H}$ of the true quantum state $\boldsymbol{\varrho}(t) \in \mathcal{S}$, which evolves according to a rule

$$\dot{\hat{\boldsymbol{\varrho}}}(t) = \mathcal{A}\,\hat{\boldsymbol{\varrho}}(t) + (\mathcal{K} \circ \mathcal{C})\,\boldsymbol{E}(t) \tag{25}$$

that ensures that the error $\boldsymbol{E}(t) \triangleq \hat{\boldsymbol{\varrho}}(t) - \boldsymbol{\varrho}(t)$ is globally exponentially stable. Here, $\mathcal{K} : \mathbb{C}^K \to \mathbb{H}$ is a linear operator known as the *observer gain*, which is designed by the practitioner.

Remark 5: For the rest of this document, we will simply use "stable" to mean "globally exponentially stable."

A quantum state observer gives rise to the linear error dynamics

$$\dot{\boldsymbol{E}}(t) = (\mathcal{A} + \mathcal{K} \circ \mathcal{C})\boldsymbol{E}(t). \tag{26}$$

The central focus of designing classical observers is to choose an observer gain $\mathcal{K}$ such that the composite operator $\mathcal{A}_o \triangleq \mathcal{A} + \mathcal{K} \circ \mathcal{C}$ has eigenvalues with negative real parts. Clearly, if such a $\mathcal{K}$ exists, then the error dynamics are stable. However, finding the eigenvalues of the abstract operator $\mathcal{A}_o$ would be difficult in general, and designing a gain operator $\mathcal{K}$ that ensures that the stability condition is even more daunting. This section seeks to present three important ideas, given an observable quantum system.

1) It is possible to design a convergent linear quantum state observer.
2) It is possible to construct a linear time-varying observer of the system's initial state.
3) There exists a canonical quantum state observer that requires no analysis to construct.

A. TIME-VARYING OBSERVER FOR THE INITIAL QUANTUM STATE

In classical systems theory, the notion of detectability is a slightly weakened version of observability. Definition 4 states that, if detectable, any unobservable modes of $(\mathcal{A}, \mathcal{C})$ are stable. Then, if there were unobservable modes, it is impossible to know what portion of the state $\boldsymbol{\varrho}(0)$ occupied said modes. We see, however, that in the quantum case

$$\begin{aligned}\|\boldsymbol{E}(t)\|_F &= \|\hat{\boldsymbol{\varrho}}(t) - \boldsymbol{\varrho}(t)\|_F \\ &= \|\boldsymbol{U}^\dagger(t)\,(\hat{\boldsymbol{\varrho}}(t) - \boldsymbol{\varrho}(t))\,\boldsymbol{U}(t)\|_F \\ &= \|\boldsymbol{U}^\dagger(t)\,\hat{\boldsymbol{\varrho}}(t)\,\boldsymbol{U}(t) - \boldsymbol{\varrho}(0)\|_F\end{aligned}$$

due to the unitary invariance of the Frobenius norm and the solution (4) to the Liouville–von Neumann equation. Hence, if $(\mathcal{A}, \mathcal{C})$ is detectable, then it is possible to design a simple stable estimator of the initial state according to the rule

$$\hat{\boldsymbol{\varrho}}_0 \triangleq \mathcal{T}^{-1}(t)\,\hat{\boldsymbol{\varrho}}(t) = \boldsymbol{U}^\dagger(t)\,\hat{\boldsymbol{\varrho}}(t)\,\boldsymbol{U}(t). \tag{27}$$

This indicates the ability to perfectly reconstruct the initial state via a quantum state observer when the pair $(\mathcal{A}, \mathcal{C})$ is detectable. This result is analogous to Theorem 2.

B. CANONICAL QUANTUM STATE OBSERVER

We will now introduce what we believe will be one of the most important linear quantum state observers for the arbitrary closed quantum system $(\mathcal{A}, \mathcal{C})$. Let $\hat{\boldsymbol{\varrho}}(t)$ evolve according to the rule

$$\begin{aligned}\dot{\hat{\boldsymbol{\varrho}}} &= -\imath\,[\![\boldsymbol{H}, \boldsymbol{\varrho}]\!] - \sum_{k=1}^{K}\left(\operatorname{tr}\{\boldsymbol{M}_k\hat{\boldsymbol{\varrho}}(t)\} - \boldsymbol{y}_k(t)\right)\cdot \boldsymbol{M}_k \\ &= -\imath\,[\![\boldsymbol{H}, \boldsymbol{\varrho}]\!] - \sum_{k=1}^{K}\operatorname{tr}\{\boldsymbol{M}_k\boldsymbol{E}(t)\}\cdot \boldsymbol{M}_k.\end{aligned} \tag{28}$$

This estimator has a simple interpretation. Define $\hat{\boldsymbol{y}}(t) \triangleq \mathcal{C}\,\hat{\boldsymbol{\varrho}}(t)$ to be the "output" of the state estimator and $\boldsymbol{e}(t) \triangleq \hat{\boldsymbol{y}}(t) - \boldsymbol{y}(t)$ to be the output error between the observer and the true quantum system. The kth component of $\boldsymbol{e}(t)$ is written $\boldsymbol{e}_k(t)$. Then

$$\frac{\partial\,\boldsymbol{e}_k(t)}{\partial\,\boldsymbol{E}(t)} = \frac{\partial\operatorname{tr}\{\boldsymbol{M}_k\,\boldsymbol{E}(t)\}}{\partial\,\boldsymbol{E}(t)} = \boldsymbol{M}_k^\dagger = \boldsymbol{M}_k$$

for each $k \in \{1, 2, \ldots, K\}$. Thus, the estimator (28) minimizes the output error $\boldsymbol{e}(t)$ by updating $\boldsymbol{E}(t)$ in the direction of steepest descent. In this estimation scheme, the linear operator $\mathcal{K} : \mathbb{C}^K \to \mathbb{H}$ is defined according to the rule

$$\mathcal{K}\,\boldsymbol{e}(t) = -\sum_{k=1}^{K}\boldsymbol{M}_k \cdot \boldsymbol{e}_k(t). \tag{29}$$

It turns out that $(\mathcal{A}, \mathcal{C})$ is observable if and only if (28) is a linear quantum state estimator. In that sense, (28) is a *universal*, or *canonical*, linear quantum state estimator whenever the pair $(\mathcal{A}, \mathcal{C})$ is observable. Hence, one need merely show that $(\mathcal{A}, \mathcal{C})$ is observable, and a linear quantum state estimator has been designed for them.

Theorem 9: The error $\boldsymbol{E}(t)$ of the linear quantum state observer with observer gain (29) tends to the unobservable space $\mathbb{U}(\mathcal{A}, \mathcal{C})$ asymptotically.

Proof: Suppose that observer gain (29) is used in (26), and consider the Lyapunov candidate function $V(t) \triangleq \frac{1}{2}\|\boldsymbol{E}(t)\|_F^2$, which is positive definite and radially unbounded. The candidate function's time derivative is evaluated to be

$$\begin{aligned}\dot{V}(t) &= \frac{1}{2}\left(\operatorname{tr}\left\{\dot{\boldsymbol{E}}^\dagger(t)\boldsymbol{E}(t)\right\} + \operatorname{tr}\left\{\boldsymbol{E}^\dagger(t)\dot{\boldsymbol{E}}(t)\right\}\right) \\ &= \operatorname{Re}\left\{\operatorname{tr}\left\{\boldsymbol{E}^\dagger(t)\dot{\boldsymbol{E}}(t)\right\}\right\} \\ &= \operatorname{Re}\left\{\operatorname{tr}\left\{-\imath\boldsymbol{E}^\dagger(t)[\![\boldsymbol{H}, \boldsymbol{E}(t)]\!]\right\}\right\} \\ &\quad -\operatorname{Re}\left\{\operatorname{tr}\left\{\boldsymbol{E}^\dagger(t)\sum_{k=1}^{K}\operatorname{tr}\{\boldsymbol{M}_k\boldsymbol{E}(t)\}\boldsymbol{M}_k\right\}\right\}.\end{aligned}$$

The second equality follows from the fact that for any $z \in \mathbb{C}$, $z + \bar{z} = 2\operatorname{Re}\{z\}$. The third equality follows from (26) and (29). Using the definition of the commutator and the linearity and cyclic properties of the trace function

$$\begin{aligned}\operatorname{tr}\left\{\boldsymbol{E}^\dagger[\![\boldsymbol{H}, \boldsymbol{E}]\!]\right\} &= \operatorname{tr}\left\{\boldsymbol{E}^\dagger\boldsymbol{H}\boldsymbol{E} - \boldsymbol{E}^\dagger\boldsymbol{E}\boldsymbol{H}\right\} \\ &= \operatorname{tr}\left\{\boldsymbol{E}^\dagger\boldsymbol{H}\boldsymbol{E}\right\} - \operatorname{tr}\left\{\boldsymbol{E}^\dagger\boldsymbol{E}\boldsymbol{H}\right\} \\ &= \operatorname{tr}\left\{\boldsymbol{E}\boldsymbol{E}^\dagger\boldsymbol{H}\right\} - \operatorname{tr}\left\{\boldsymbol{E}^\dagger\boldsymbol{E}\boldsymbol{H}\right\}.\end{aligned}$$

The matrices $\boldsymbol{E}\boldsymbol{E}^\dagger$, $\boldsymbol{E}^\dagger\boldsymbol{E}$, and $\boldsymbol{H}$ are all Hermitian. Hence, $\operatorname{tr}\{\boldsymbol{E}^\dagger(t)[\![\boldsymbol{H}, \boldsymbol{E}(t)]\!]\}$ is a real number and

$$\operatorname{Re}\left\{\operatorname{tr}\left\{-\imath\boldsymbol{E}^\dagger(t)[\![\boldsymbol{H}, \boldsymbol{E}(t)]\!]\right\}\right\} = 0$$

for all t. On the other hand, we have

$$\begin{aligned}\operatorname{tr}\left\{\boldsymbol{E}^{\dagger}\sum_{k=1}^{K}\operatorname{tr}\{\boldsymbol{M}_k\boldsymbol{E}\}\boldsymbol{M}_k\right\} &= \sum_{k=1}^{K}\operatorname{tr}\{\boldsymbol{M}_k\boldsymbol{E}\}\cdot\operatorname{tr}\left\{\boldsymbol{E}^{\dagger}\boldsymbol{M}_k\right\}\\ &= \sum_{k=1}^{K}\operatorname{tr}\{\boldsymbol{M}_k\boldsymbol{E}\}\cdot\overline{\operatorname{tr}\{\boldsymbol{M}_k\boldsymbol{E}\}}\\ &= \sum_{k=1}^{K}|\operatorname{tr}\{\boldsymbol{M}_k\boldsymbol{E}\}|^2.\end{aligned}$$

Thus, the time derivative of $V(t)$ is negative semidefinite

$$\dot{V}(t) = -\sum_{k=1}^{K}|\operatorname{tr}\{\boldsymbol{M}_k\boldsymbol{E}(t)\}|^2 \le 0. \tag{30}$$

Applying LaSalle's invariant set theorem [53, Th. 4.4], $\boldsymbol{E}(t)$ tends to the set

$$\Omega \triangleq \left\{\boldsymbol{E}\in\mathbb{H} \;\middle|\; \dot{V}(t)=0 \text{ and } \dot{\boldsymbol{E}}(t) = -\imath[\![\boldsymbol{H},\boldsymbol{E}]\!] \quad \forall t\right\}.$$

Using (30), we see that Ω is exactly equal to the unobservable space $\mathbb{U}(\mathcal{A},\mathcal{C})$. ■

Theorem 10: The quantum system $(\mathcal{A},\mathcal{C})$ is observable if and only if the observer gain (29) renders the observer error dynamics stable.

Proof: Suppose $(\mathcal{A},\mathcal{C})$ is observable. Then, $\Omega = \mathbb{U}(\mathcal{A},\mathcal{C}) = \{\boldsymbol{0}\}$ and the origin is globally asymptotically stable. However, since the system is linear, it is asymptotically stable if and only if it is exponentially stable. On the other hand, if (29) does not render the origin of the error system stable, then $\Omega = \mathbb{U}(\mathcal{A},\mathcal{C})$ must contain more than the origin. Hence, $(\mathcal{A},\mathcal{C})$ is not observable. This proves the theorem. ■

While these results already emphasize the importance of the observer gain defined in (29), the gain has another property that has practical importance when estimating a quantum density operator. This property will form the basis of the results established in Section VI.

Theorem 11: Let $\hat{\boldsymbol{\varrho}}(0)$ be Hermitian. With observer gain (29), the observer state $\hat{\boldsymbol{\varrho}}(t)$ remains Hermitian for all time $t\ge 0$.

Proof: Define the "Hermitian error" $\boldsymbol{E}_{\rm H}(t)\triangleq\boldsymbol{E}(t)-\boldsymbol{E}^{\dagger}(t)$. When $\boldsymbol{E}_{\rm H}=\boldsymbol{0}$, the matrix $\boldsymbol{E}$ is Hermitian. Since $\boldsymbol{\varrho}\in\mathcal{S}$ is automatically Hermitian, when $\boldsymbol{E}_{\rm H}=\boldsymbol{0}$ one can conclude that $\hat{\boldsymbol{\varrho}}$ is also. According to the statement of the theorem, $\boldsymbol{E}_{\rm H}(0)$ is zero. Applying elementary analysis and Lemma 1, one may deduce the time evolution of $\boldsymbol{E}_{\rm H}(t)$ as follows:

$$\begin{aligned}\dot{\boldsymbol{E}}_{\rm H}(t) &= \dot{\boldsymbol{E}}(t)-\dot{\boldsymbol{E}}^{\dagger}(t)\\ &= -\imath[\![\boldsymbol{H},\boldsymbol{E}_{\rm H}(t)]\!]-\sum_{k=1}^{K}\operatorname{tr}\{\boldsymbol{M}_k\boldsymbol{E}_{\rm H}(t)\}\cdot\boldsymbol{M}_k.\end{aligned}\tag{31}$$

We see that $\boldsymbol{E}_{\rm H}(t)=\boldsymbol{0}$ is an equilibrium of this system. Hence, if $\boldsymbol{E}_{\rm H}(0)=\boldsymbol{0}$ then $\boldsymbol{E}(t)$ will remain Hermitian for all time. ■

Remark 6: The above theorem shows that the set of Hermitian operators is *positively invariant* with respect to the error system (26) when the canonical gain (29) is used.

VI. ENSURING A VALID STATE ESTIMATE

Given the observability of $(\mathcal{A},\mathcal{C})$, we know that it is possible to design a quantum state observer. However, we are not guaranteed that the observer state $\hat{\boldsymbol{\varrho}}(T)$ at any stopping time $T\in(0,\infty)$ is a valid density matrix. We have the following theorem regarding the set $\mathcal{S}$ (the set of all density operators), which proves that there exists a unique projection from $\mathbb{H}$ to the set of density operators $\mathcal{S}$.

Theorem 12: The set $\mathcal{S}$ is a closed convex subset of $\mathbb{H}$. Moreover, for any $\boldsymbol{\rho}\in\mathbb{H}$, there exists a unique density operator $\breve{\boldsymbol{\sigma}}\in\mathcal{S}$ such that $\|\breve{\boldsymbol{\sigma}}-\boldsymbol{\rho}\|_{\rm F}\le\|\boldsymbol{\sigma}-\boldsymbol{\rho}\|_{\rm F}$ for all $\boldsymbol{\sigma}\in\mathcal{S}$ and

$$\|\breve{\boldsymbol{\sigma}}-\boldsymbol{\rho}\|_{\rm F} = \inf_{\boldsymbol{\sigma}\in\mathcal{S}}\|\boldsymbol{\sigma}-\boldsymbol{\rho}\|_{\rm F}.$$

Proof: See [44]. ■

The prior theorem ensures that the projection operator

$$\mathcal{P}_{\mathcal{S}}(\boldsymbol{\rho}) \triangleq \arg\min_{\boldsymbol{\sigma}\in\mathcal{S}}\|\boldsymbol{\sigma}-\boldsymbol{\rho}\|_{\rm F}^2 \tag{32}$$

of $\boldsymbol{\rho}\in\mathbb{H}$ onto the set $\mathcal{S}$ is well defined. Unfortunately, this projection is nonlinear and no closed-form solution is known. However, if observer gain (29) is used and $\hat{\boldsymbol{\varrho}}(t)$ is initiated from a valid density matrix (or any Hermitian matrix for that matter), it is known that $\hat{\boldsymbol{\varrho}}(T)$ is Hermitian for any stopping time $T\ge 0$. This greatly reduces the complexity of the projection onto $\mathcal{S}$. Suppose that $\hat{\boldsymbol{\varrho}}(T)$ is Hermitian. By the spectral theorem, it is possible to write

$$\hat{\boldsymbol{\varrho}}(T) = \boldsymbol{T}\boldsymbol{\Lambda}\boldsymbol{T}^{\dagger}$$

where $\boldsymbol{\Lambda}\in\mathbb{H}$ is the diagonal matrix of real eigenvalues of $\hat{\boldsymbol{\varrho}}(T)$ and $\boldsymbol{T}$ is a unitary eigenvector matrix for $\hat{\boldsymbol{\varrho}}(T)$. Let $\boldsymbol{v}\triangleq\operatorname{diag}(\boldsymbol{\Lambda})\in\mathbb{R}^d$ be the vector of eigenvalues of $\hat{\boldsymbol{\varrho}}(T)$. Let $\boldsymbol{Q}\triangleq\boldsymbol{I}_d$ and $\boldsymbol{c}\triangleq-2\boldsymbol{v}$. Consider the following quadratic program (QP):

$$\begin{aligned}\mathscr{P}_1:\quad \breve{\boldsymbol{x}} \;\triangleq\; &\arg\min_{\boldsymbol{x}\in\mathbb{R}^d} && \boldsymbol{x}^T\boldsymbol{Q}\boldsymbol{x}+\boldsymbol{c}^T\boldsymbol{x}\\ &\text{subject to} && \boldsymbol{x}\succcurlyeq\boldsymbol{0}\\ &&& \langle\boldsymbol{1}_d,\boldsymbol{x}\rangle = 1\end{aligned}$$

where $\boldsymbol{1}_d\in\mathbb{R}^d$ is vector of all ones.

Theorem 13: Let $\hat{\boldsymbol{\varrho}}(T)$ be Hermitian. Then, its projection onto the set $\mathcal{S}$ of valid density matrices is

$$\mathcal{P}_{\mathcal{S}}(\hat{\boldsymbol{\varrho}}(T)) = \boldsymbol{T}\operatorname{diag}(\breve{\boldsymbol{x}})\boldsymbol{T}^{\dagger} \tag{33}$$

where $\breve{\boldsymbol{x}}$ is the solution to Problem 1.

Proof: Let $\boldsymbol{\sigma}\in\mathcal{S}$. Define $\breve{\boldsymbol{\Lambda}}\triangleq\boldsymbol{T}^{\dagger}\boldsymbol{\sigma}\boldsymbol{T}$ and observe that $\breve{\boldsymbol{\Lambda}}\in\mathcal{S}$. By the unitary invariance of the Frobenius norm and the definition (32), it follows that

$$\min_{\boldsymbol{\sigma}\in\mathcal{S}}\|\boldsymbol{\sigma}-\hat{\boldsymbol{\varrho}}\|_{\rm F}^2 = \min_{\breve{\boldsymbol{\Lambda}}\in\mathcal{S}}\|\breve{\boldsymbol{\Lambda}}-\boldsymbol{\Lambda}\|_{\rm F}^2$$

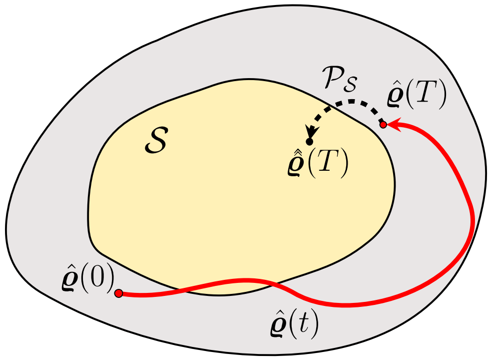

FIGURE 1. **Trajectory of observer state $\hat{\varrho}(t)$ evolving in the positively invariant set of Hermitian matrices (gray) followed by the projection $\mathcal{P}_{\mathcal{S}}$ onto the set $\mathcal{S}$ of density matrices (yellow).**

and

$$\mathcal{P}_{\mathcal{S}}(\hat{\varrho}(T)) = \boldsymbol{T}\,\mathcal{P}_{\mathcal{S}}(\boldsymbol{\Lambda})\,\boldsymbol{T}^{\dagger}.$$

Since $\boldsymbol{\Lambda}$ is a *real* diagonal matrix, we conclude that $\|\breve{\boldsymbol{\Lambda}} - \boldsymbol{\Lambda}\|_{\mathrm{F}}^2$ is only minimized when $\breve{\boldsymbol{\Lambda}}$ is a real diagonal matrix. Let $\boldsymbol{x} \triangleq \mathrm{diag}(\breve{\boldsymbol{\Lambda}})$. The projection $\mathcal{P}_{\mathcal{S}}(\boldsymbol{\Lambda})$ is equal to $\mathrm{diag}(\breve{\boldsymbol{x}})$ where $\breve{\boldsymbol{x}}$ is the solution to

$$\begin{aligned}\mathscr{P}_2: \quad \breve{\boldsymbol{x}} \;=\; &\underset{\boldsymbol{x}\in\mathbb{R}^d}{\arg\min} \quad \|\boldsymbol{x}-\boldsymbol{v}\|^2\\ &\text{subject to} \quad \boldsymbol{x} \succcurlyeq \boldsymbol{0},\\ &\qquad\qquad \langle \boldsymbol{1}_d, \boldsymbol{x}\rangle = 1\end{aligned}$$

Here, the optimization constraints ensure that $\breve{\boldsymbol{\Lambda}}$ is positive semidefinite and has a trace of one—the requirements to be an element of $\mathcal{S}$. Expanding the objective in the last expression,

$$\begin{aligned}\|\boldsymbol{x}-\boldsymbol{v}\|^2 &= (\boldsymbol{x}-\boldsymbol{v})^T(\boldsymbol{x}-\boldsymbol{v})\\ &= \boldsymbol{x}^T\boldsymbol{x} - 2\boldsymbol{v}^T\boldsymbol{x} + \boldsymbol{v}^T\boldsymbol{v}.\end{aligned}$$

As $\boldsymbol{v}$ is not an optimizable parameter, we conclude that Problems 1 and 2 are equivalent. This proves the theorem. ■

The QP in Problem 1 may be solved efficiently by any standard optimization package, such as MATLAB [54]. Then, (33) may be used to project a Hermitian $\hat{\varrho}$ onto $\mathcal{S}$. In prior quantum state estimators, i.e., [44] and [45], there have been no means of projecting $\hat{\varrho}$ onto $\mathcal{S}$ when the dimension d is greater than 2. Using the canonical state estimator proposed in this article, we have overcome this hurdle. Fig. 1 depicts the estimated state $\hat{\varrho}(t)$, when the canonical estimator (28) is used. When $\hat{\varrho}(t)$ is initiated in the set of Hermitian operators, it remains there for all time. Then, (33) may be used to project the observer state onto the set $\mathcal{S}$ of valid density operators. For notation's sake, let

$$\hat{\hat{\varrho}}\,(t) \triangleq \mathcal{P}_{\mathcal{S}}(\hat{\varrho}(t)). \tag{34}$$

As the projection guaranteed by Theorem 12 is *nonexpansive* [55, Th. 5.1], it follows that

$$\begin{aligned}\|\hat{\hat{\varrho}}\,(t) - \varrho(t)\|_{\mathrm{F}} &= \|\mathcal{P}_{\mathcal{S}}(\hat{\varrho}(t)) - \mathcal{P}_{\mathcal{S}}(\varrho(t))\|_{\mathrm{F}}\\ &\le \|\hat{\varrho}(t) - \varrho(t)\|_{\mathrm{F}}.\end{aligned} \tag{35}$$

Hence, if $\hat{\varrho}(t)$ tends to $\varrho(t)$, then so does $\hat{\hat{\varrho}}(t)$. Moreover, the rate of convergence is preserved. We have shown that, if $\hat{\varrho}(t)$ is the state of a convergent linear quantum state observer, then $\hat{\hat{\varrho}}\,(t)$ is a convergent nonlinear estimate of the state $\varrho(t)$, which is also a valid density operator.

VII. EXAMPLES

In this section, we present a few concrete examples for which the theory developed in this article may be applied. All simulations are performed numerically on a classical computer.

A. EXAMPLE 1: THE QUBIT

We first consider an example with the fundamental building block of QIS: the qubit. The system Hamiltonian is given by

$$\boldsymbol{H} \triangleq \boldsymbol{Z}$$

where $\boldsymbol{Z}$ is the Pauli-Z matrix. A two-element POVM $\mathcal{M}$ with measurement operators

$$\boldsymbol{M}_1 \triangleq \frac{1}{4}\begin{bmatrix} 1 & 1-\sqrt{2}\,\imath\\ 1+\sqrt{2}\,\imath & 3\end{bmatrix}$$

$$\boldsymbol{M}_2 \triangleq \frac{1}{4}\begin{bmatrix} 3 & -1+\sqrt{2}\,\imath\\ -1-\sqrt{2}\,\imath & 1\end{bmatrix}$$

is used. The Hamiltonian has eigenvalues $\lambda_1 = 1$ and $\lambda_2 = -1$, which correspond to the eigenvectors

$$|\boldsymbol{\phi}_1\rangle = |\boldsymbol{0}\rangle \triangleq \begin{bmatrix}1\\0\end{bmatrix} \qquad |\boldsymbol{\phi}_2\rangle = |\boldsymbol{1}\rangle \triangleq \begin{bmatrix}0\\1\end{bmatrix}$$

respectively. Here, the standard QIS notation for the zero and one bits, $|\boldsymbol{0}\rangle$ and $|\boldsymbol{1}\rangle$, has been used [8]. The quantum observability matrices are evaluated to be

$$\mathcal{Q}_{\mathrm{c}}(\mathcal{A},\,\mathcal{C}) = \frac{1}{4}\begin{bmatrix}1+\sqrt{2}\,\imath\\ -1-\sqrt{2}\,\imath\end{bmatrix}$$

$$\mathcal{Q}_{\mathrm{i}}(\mathcal{A},\,\mathcal{C}) = \frac{1}{4}\begin{bmatrix}1 & 3\\ 3 & 1\end{bmatrix}.$$

Clearly, the single column of $\mathcal{Q}_{\mathrm{c}}(\mathcal{A},\,\mathcal{C})$ is nonzero, and $\mathcal{Q}_{\mathrm{i}}(\mathcal{A},\,\mathcal{C})$ is full rank. By Theorem 6, this quantum system is observable. As such, the canonical observer developed in Section V-B may be used to estimate the state of this system. Both the system and observer are initiated at pure states denoted $|\boldsymbol{\psi}_0\rangle$ and $|\hat{\boldsymbol{\psi}}_0\rangle$, respectively. The associated density matrices are $\varrho(0) = |\boldsymbol{\psi}_0\rangle\langle\boldsymbol{\psi}_0|$ and $\hat{\varrho}(0) = |\hat{\boldsymbol{\psi}}_0\rangle\langle\hat{\boldsymbol{\psi}}_0|$. The following three scenarios are considered:

1) $|\boldsymbol{\psi}_0\rangle = |\boldsymbol{0}\rangle$ and $|\hat{\boldsymbol{\psi}}_0\rangle = |\boldsymbol{1}\rangle$;
2) $|\boldsymbol{\psi}_0\rangle = \frac{1}{\sqrt{2}}(|\boldsymbol{0}\rangle + |\boldsymbol{1}\rangle)$ and $|\hat{\boldsymbol{\psi}}_0\rangle = \frac{1}{\sqrt{2}}(|\boldsymbol{0}\rangle - |\boldsymbol{1}\rangle)$;
3) $|\boldsymbol{\psi}_0\rangle = \frac{1}{\sqrt{2}}(|\boldsymbol{0}\rangle + \imath|\boldsymbol{1}\rangle)$ and $|\hat{\boldsymbol{\psi}}_0\rangle = \frac{1}{\sqrt{2}}(|\boldsymbol{0}\rangle - \imath|\boldsymbol{1}\rangle)$.

In each scenario, the observer's state is initiated orthogonal to the system's state. The canonical observer is used to

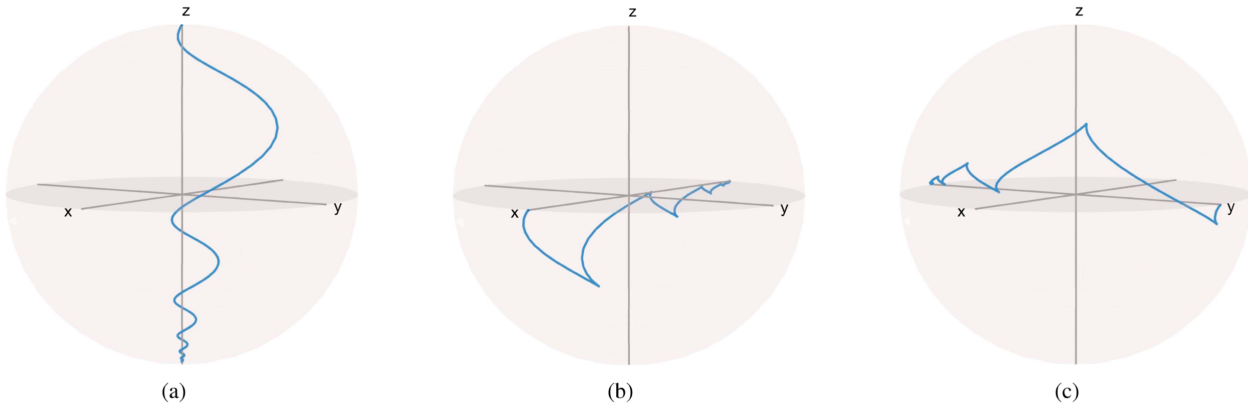

FIGURE 2. **Trajectory (blue) of the observer's estimate of the initial state $\hat{\hat{\varrho}}_0$ plotted on the Bloch sphere. Since the system is observable, the canonical observer gain (29) guarantees convergence of this estimate to the true state.**

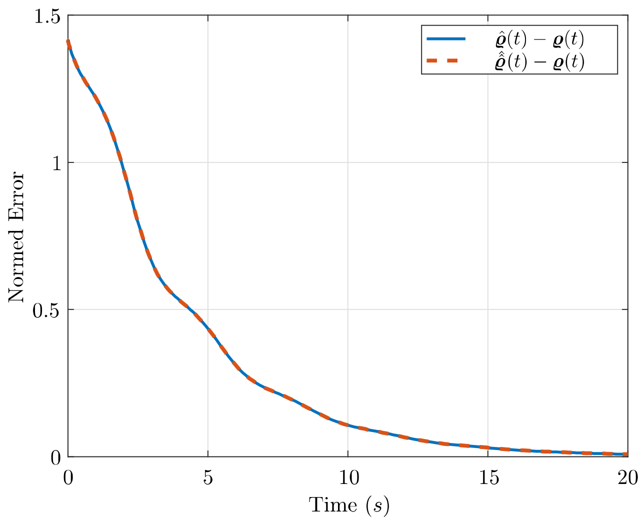

FIGURE 3. **Observer error for scenario 1) of Example 1 plotted over time. Because the system is observable and the canonical observer is used, the error is guaranteed to converge to zero.**

produce an estimate $\hat{\varrho}(t)$. For demonstration, the projection discussed in Section VI is used to compute $\hat{\hat{\varrho}}\ (t)$ at each time step. Then, an estimate $\hat{\hat{\varrho}}_0$ of the true initial state $\varrho(0)$ is obtained via the rule $\hat{\hat{\varrho}}_0 \triangleq \mathcal{T}^{-1}(t)\hat{\hat{\varrho}}\ (t) = \boldsymbol{U}^{\dagger}(t)\hat{\hat{\varrho}}\ (t)\boldsymbol{U}(t)$, as discussed in Section V-A. The trajectory of $\hat{\hat{\varrho}}_0$ for each of the three scenarios is depicted in the Bloch spheres of Fig. 2. For scenario 1, Fig. 3 plots the error of the observer state $\hat{\varrho}(t)$ and its projection, $\hat{\hat{\varrho}}\ (t)$, onto $\mathcal{S}$ with respect to the true quantum state $\varrho(t)$. In this example, we see that $\hat{\varrho}(t)$ remains a valid density matrix for all time, so $\hat{\hat{\varrho}}\ (t) = \mathcal{P}_{\mathcal{S}}(\hat{\varrho}(t)) = \hat{\varrho}(t)$. A QST algorithm with an informationally complete POVM would require $d^2 = 4$ measurement operators. However, with this example, we have shown that it is possible to trade measurement complexity for allowing the system to evolve according to its natural dynamics over time.

B. EXAMPLE 2: A SPIN-2 PARTICLE

We now consider a spin-2 particle, which has dimension $d = 5$. The spin-Z and spin-Y matrices [56] for such a particle are given by

$$\boldsymbol{S}_z \triangleq \begin{bmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{bmatrix}$$

and

$$\boldsymbol{S}_y \triangleq \begin{bmatrix} 0 & -\imath & 0 & 0 & 0 \\ \imath & 0 & -\imath\sqrt{\frac{3}{2}} & 0 & 0 \\ 0 & \imath\sqrt{\frac{3}{2}} & 0 & -\imath\sqrt{\frac{3}{2}} & 0 \\ 0 & 0 & \imath\sqrt{\frac{3}{2}} & 0 & -\imath \\ 0 & 0 & 0 & \imath & 0 \end{bmatrix}.$$

We take the system Hamiltonian be $\boldsymbol{H} \triangleq \boldsymbol{S}_z + \boldsymbol{S}_y$. A 5-element POVM is used, which consists only of rank one projective measurements onto the standard basis:

$$\mathcal{M} \triangleq \left\{ |\boldsymbol{k}\rangle\langle\boldsymbol{k}| \ : \ k = 0, 1, \ldots, 4 \right\}.$$

Rather than construct the large Kalman observability matrix $\boldsymbol{O}(\boldsymbol{A}, \boldsymbol{C}) \in \mathbb{C}^{125\times 25}$, one may opt to work with the quantum observability matrices $\mathcal{Q}_{\mathrm{c}}(\mathcal{A}, \mathcal{C}) \in \mathbb{C}^{5\times 10}$ and $\mathcal{Q}_{\mathrm{i}}(\mathcal{A}, \mathcal{C}) \in \mathbb{C}^{5\times 5}$, which take up less than 1.5% of the space of the Kalman observability matrix. Using Algorithm 1, we conclude that $(\mathcal{A}, \mathcal{C})$ is an observable quantum system. Hence, the canonical observer may be applied to estimate the state of the quantum system, which we take to be $\varrho(0) = |\boldsymbol{0}\rangle\langle\boldsymbol{0}|$ at time $t = 0$ s. For 50 experiments, $\hat{\varrho}(0)$ was randomly generated using QETLAB's random density matrix generator [57] and the canonical observer was used to estimate the state $\varrho(t)$. The results are depicted in Fig. 4(a), which shows the error converging to zero on all 50 runs. Fig. 4(b) shows one of

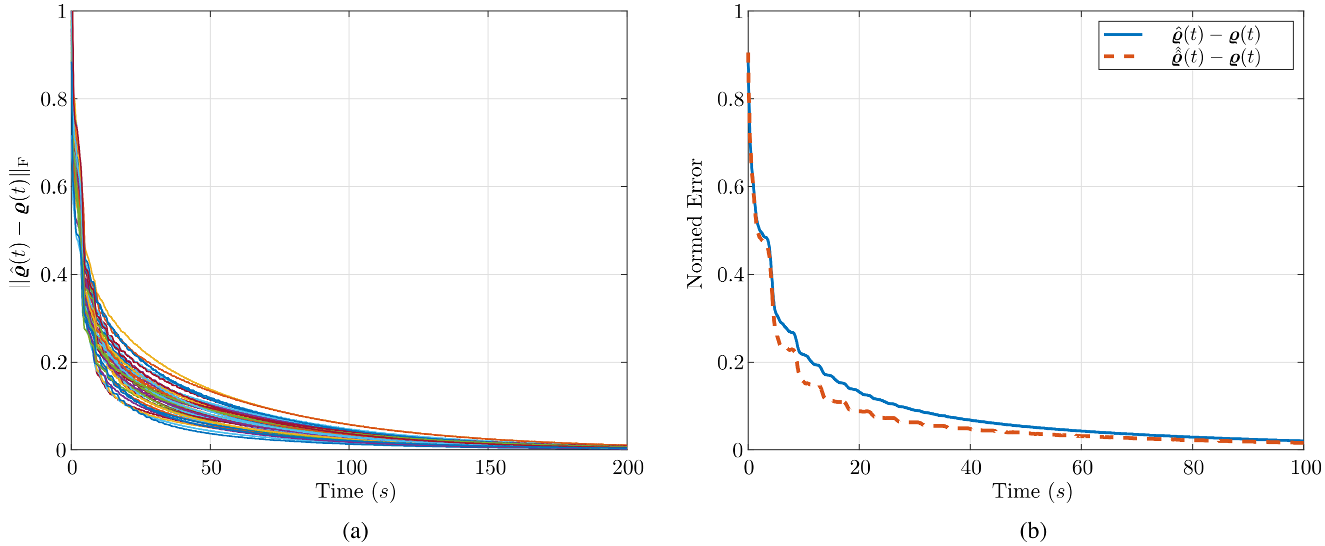

FIGURE 4. For 50 random initial estimates, the canonical observer was used to estimate the unknown state of the spin-2 particle considered in Example 2. (a) Error over time for each of the 50 experiments. (b) Zoomed version of one of the runs to show that the estimate $\hat{\hat{\varrho}}(t)$ left the set of valid density matrices, which is evident by the fact that $\hat{\hat{\varrho}}(t)$ was closer to $\varrho(t)$ than $\hat{\varrho}(t)$.

these runs and demonstrates a time in which $\hat{\varrho}(t)$ did not remain in the set $\mathcal{S}$ of valid density operators for all time. However, as discussed in Section VI, the projection $\hat{\hat{\varrho}}(t)$ of $\hat{\varrho}(t)$ onto $\mathcal{S}$ preserves the convergence rate of $\hat{\varrho}(t)$ to the true state $\varrho(t)$.

VIII. CONCLUSION

This article ventured to use the rich structure of closed quantum dynamical systems to make new conclusions about their observability. The main results of this article may be summarized by the following theorem.

Theorem 14: Let $(\mathcal{A}, \mathcal{C})$ be a closed quantum system. Then, the following are equivalent.

1) $(\mathcal{A}, \mathcal{C})$ is observable.
2) $(\mathcal{A}, \mathcal{C})$ is detectable.
3) (When $\boldsymbol{H}$ is nondegenerate.) The coherent quantum observability matrix $\mathcal{Q}_{\mathrm{c}}(\mathcal{A}, \mathcal{C})$ has no zero columns and the incoherent quantum observability matrix $\mathcal{Q}_{\mathrm{i}}(\mathcal{A}, \mathcal{C})$ has full column rank.
4) The Kalman observability matrix $\boldsymbol{O}(\boldsymbol{A}, \boldsymbol{C})$ has rank d^2.
5) The estimator (28) is a linear quantum state observer for $(\mathcal{A}, \mathcal{C})$.

Prior to this work, only the equivalence between 1 and 4 had been studied [44], [45]. The canonical linear quantum state observer introduced in Section V-B works for *any* observable quantum system and allows one to estimate the state of a quantum dynamical system without having to manually design an observer gain. Moreover, the canonical observer ensures the estimated state remains Hermitian for all time. It was then shown that a Hermitian state estimate can be projected onto the set of valid density matrices, and that this projection preserves convergence of the estimated state to the ground truth. The canonical observer will allow quantum engineers to infer the unknown state of a quantum system without having to manually design an observer.

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