Admissible Optimal Control for Parameter Estimation in Quantum Systems

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***Abstract*—This letter investigates parameter estimation in quantum systems that undergo dynamical evolution. Optimal control problems are formulated to maximize the information, about an unknown parameter, extracted by a given quantum measurement apparatus. This letter introduces the concept of "admissible controls"—control laws that do not depend on the unknown parameter they elicit. For scalar parameter estimation in unital quantum systems interrogated by binary measurements, this letter derives a necessary and sufficient condition on quantum measurement operators so that an information maximizing control law is admissible. When the admissibility condition is satisfied, it is shown that the resulting optimal control problem may be solved using well-established techniques.**

***Index Terms*—Quantum parameter estimation, Fisher information, quantum control, statistical inference, control-enhanced parameter estimation.**

I. Introduction

INFERRING a parameterized quantum state by optimally controlling its dynamical evolution, a new problem at the intersection of statistical inference and control, is investigated in this letter. At a prescribed time instant, the quantum state is measured using the physical apparatus that is available to the experimenter. The goal is to extract as much information about the unknown parameter as possible from the measurement outcomes. To this aim, optimal control theory is used to maximize the information extraction at the time of measurement. In general, information maximizing control laws may depend on the particular parameter that they elicit. However, such a control law would be like a point estimator (in statistical inference) that depends on the parameter it aims to infer, which is absurd [1, pp. 211, 311]. Motivated by this observation, we introduce the concept of "admissible" control laws that do not depend on the unknown parameter. This letter establishes a foundation for optimally controlling the dynamical evolution of a quantum state to maximize the information extracted by a given quantum measurement apparatus.

Inference and control play a central role in quantum engineering and enable many beyond-classical capabilities in sensing, communications, localization, and synchronization [2], [3], [4], [5], [6]. Prior works have studied the problem of controlling information extraction in both classical [7], [8] and quantum systems [9], [10], [11], [12], [13]. In particular, [9], [10], [11], [12], [13] considered scenarios where the parameter dependence of a quantum state arises from its dynamical evolution, and control laws for information extraction were numerically generated using Pontryagin's maximum principle [10], [11] or gradient ascent pulse engineering (GRAPE) [12], [13]. While parameter dependence of a quantum state is a recurring theme, a characterization of the parameter dependence of information maximizing control laws is missing in the literature.

This letter puts forth a scenario where a quantum state is initially dependent on an unknown parameter and then evolves under known dynamics. The foundation established here can address a broad class of control-enhanced quantum parameter estimation problems. For scalar parameter estimation in unital quantum systems interrogated by binary measurements,[1] we:

- develop time-dependent Fisher information analysis for density operators that are characterized by an unknown parameter;
- derive a necessary and sufficient condition on the measurement operators so that information maximizing control laws are admissible; and
- show that, when the admissibility condition is met, information maximizing control laws can be designed using well-established techniques.

Our analysis allows for general time-local non-Markovian quantum dynamics [16].

Notation: Random variables are displayed in sans serif, upright fonts; their realizations in serif, italic fonts. For example, a random variable and its realization are denoted by x and x. The probability mass function (PMF) or probability density function (PDF) of a random variable x is denoted $p_{\mathsf{x}}(x)$. The symbol $\mathbb{E}_{\mathsf{x}}\{\cdot\}$ denotes the expectation with respect to the random variable x. The set of linear operators and

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[1] Binary quantum measurements are relevant, among others, for qubit-based systems [14, p. 15] and for quantum communication systems [15, p. 316].

density operators on a Hilbert space $\mathcal{H}$ are denoted $\mathcal{L}(\mathcal{H})$ and $\mathcal{D}(\mathcal{H})$, respectively. Operators are denoted using bold uppercase letters. The adjoint of a linear operator $\boldsymbol{A} \in \mathcal{L}(\mathcal{H})$ is denoted $\boldsymbol{A}^\dagger$. The anti-commutator and commutator of $\boldsymbol{A}$ and $\boldsymbol{B} \in \mathcal{L}(\mathcal{H})$ are denoted $[\![\boldsymbol{A}, \boldsymbol{B}]\!]_\pm = \boldsymbol{A}\boldsymbol{B} \pm \boldsymbol{B}\boldsymbol{A}$ with $+$ or $-$, respectively. The Hilbert-Schmidt inner product on $\mathcal{L}(\mathcal{H})$ is denoted $\langle \boldsymbol{A}, \boldsymbol{B} \rangle = \mathrm{tr}\{\boldsymbol{A}^\dagger \boldsymbol{B}\}$. The adjoint of a linear operator $\boldsymbol{O} : \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{H})$ with respect to the Hilbert-Schmidt inner product is denoted $\boldsymbol{O}^\ddagger$.[2] The notation $\boldsymbol{A} \succcurlyeq \boldsymbol{B}$ means that $\boldsymbol{A} - \boldsymbol{B}$ is positive semidefinite. The imaginary unit $\sqrt{-1}$ is denoted $\imath$. The symbol $\overset{\forall}{}$ means "for almost all." A dot, as in $\dot{\boldsymbol{\Xi}}_\theta(t)$, denotes the derivative with respect to time t.

II. Fisher Information Analysis

The state of a finite d-dimensional quantum system may be represented by a density operator, which is a positive semidefinite, unit-trace linear operator on a complex Hilbert space $\mathcal{H}$ of dimension $d < \infty$. To begin, consider a *time-independent* state[3] which is parameterized by an unknown scalar $\theta \in \mathbb{R}$ written as

$$\boldsymbol{\Xi}_\theta = \tfrac{1}{d}\,\boldsymbol{I} + \theta\,\boldsymbol{Z} \in \mathcal{D}(\mathcal{H}) \tag{1}$$

where $\boldsymbol{I} \in \mathcal{L}(\mathcal{H})$ is the identity operator, $\boldsymbol{I}/d$ is the maximally mixed state, and $\boldsymbol{Z} \in \mathcal{L}(\mathcal{H})$ is an arbitrary non-zero, traceless, self-adjoint operator. Note that, like the density in (1), *all* density operators on $\mathcal{H}$ may be written as the sum of the maximally mixed state and a traceless operator. Parameterized states of the form (1) appear in many applications [17], [18] and include depolarized states as well as two-qubit Werner states. For $\boldsymbol{\Xi}_\theta$ to be a valid density operator it must be positive semidefinite; hence, there is only a finite range of values that the parameter θ may take.

Lemma 1: The operator $\boldsymbol{\Xi}_\theta$ is positive semidefinite if and only if

$$\theta \in \left[\frac{-1}{d\,\lambda_d}, \frac{1}{d\,|\lambda_1|}\right] \tag{2}$$

where λ_d and λ_1 are the largest and smallest eigenvalues of $\boldsymbol{Z}$, respectively. □

Proof: Since $\boldsymbol{Z}$ is non-zero, self-adjoint, and traceless, its smallest and largest eigenvalues satisfy $\lambda_1 < 0 < \lambda_d$.[4] Given (1), the eigenvalues of $\boldsymbol{\Xi}_\theta$ are exactly of the form $\frac{1}{d} + \theta\,\lambda_i$ where λ_i is the i-th eigenvalue of $\boldsymbol{Z}$ [19, p. 55]. The statement of the lemma follows. ⊠

Henceforth the parameter space, denoted Θ, is allowed to be a subinterval of that in (2). This letter considers quantum measurement systems represented by binary positive operator-valued measures (POVMs) [20]. In contrast to classical measurement, a quantum measurement will generally alter the state such that successive measurements using the same POVM system provide no additional information regarding the state prior to measurement. Thus, once the state $\boldsymbol{\Xi}_\theta$ is measured, one must prepare an identical state before another measurement containing information about θ can be made.

Definition 1 (Binary POVM): A binary POVM system is a set of non-zero, self-adjoint linear operators $\{\boldsymbol{M}, \boldsymbol{I} - \boldsymbol{M}\}$ on $\mathcal{H}$ with $\boldsymbol{0} \preccurlyeq \boldsymbol{M} \preccurlyeq \boldsymbol{I}$. The result of measuring the state $\boldsymbol{\Xi}_\theta$ using this system is a random variable $\mathsf{y} = \pm 1$ where

$$\mathbb{P}\{\,\mathsf{y} = +1 \,|\, \boldsymbol{\Xi}_\theta\} = \mathrm{tr}\{\,\boldsymbol{M}\,\boldsymbol{\Xi}_\theta\}, \text{ and} \tag{3a}$$

$$\mathbb{P}\{\,\mathsf{y} = -1 \,|\, \boldsymbol{\Xi}_\theta\} = \mathrm{tr}\{\,(\boldsymbol{I} - \boldsymbol{M})\,\boldsymbol{\Xi}_\theta\} \tag{3b}$$

according to Born's rule. □

A. Analysis for Time-Independent Quantum States

The *Fisher information*—a key quantity in statistical inference that is used to determine the fundamental limits of point estimators—is defined below.

Definition 2 (Fisher Information): The Fisher infrmation about ϑ contained in a random variable x with PMF or PDF $p_\mathsf{x}(x;\vartheta)$ is

$$J_\vartheta = \mathbb{E}_\mathsf{x}\{\jmath(\mathsf{x};\vartheta)\} \tag{4}$$

where $\jmath(x;\vartheta) = [\frac{\partial}{\partial\vartheta} \ln p_\mathsf{x}(x;\vartheta)]^2$ for each x in the support of $p_\mathsf{x}(\,\cdot\,;\vartheta)$. □

The Fisher information about θ contained in y (obtained via measuring $\boldsymbol{\Xi}_\theta$ with the POVM system $\{\boldsymbol{M}, \boldsymbol{I} - \boldsymbol{M}\}$) is given by (5), which is presented at the bottom of the page. Employing the Hilbert-Schmidt inner product of two operators and the fact that $\mathrm{tr}\{\boldsymbol{Z}\} = 0$, the Fisher information in (5) can be rewritten as

$$J_\theta = \frac{\langle \boldsymbol{M}, \boldsymbol{Z} \rangle^2}{a_\mathrm{m} + \theta\, b_\mathrm{m} \langle \boldsymbol{M}, \boldsymbol{Z} \rangle - \theta^2 \langle \boldsymbol{M}, \boldsymbol{Z} \rangle^2} \tag{6}$$

where

$$a_\mathrm{m} \triangleq \tfrac{1}{d}\,\mathrm{tr}\{\boldsymbol{M}\}\,(1 - \tfrac{1}{d}\,\mathrm{tr}\{\boldsymbol{M}\}) \in (0, 1/4) \tag{7a}$$

$$b_\mathrm{m} \triangleq 1 - \tfrac{2}{d}\,\mathrm{tr}\{\boldsymbol{M}\} \in (-1, 1)\,. \tag{7b}$$

The information inequality [1] states that, under appropriate regularity conditions, the mean-square error of any unbiased estimator $\hat{\theta}(\mathsf{y})$ of θ satisfies

$$\mathbb{E}_\mathsf{y}\{(\hat{\theta}(\mathsf{y}) - \theta)^2\} \geqslant \frac{1}{J_\theta}\,. \tag{8}$$

The importance of having a large Fisher information J_θ is evident from (8). Optimal control offers a way to systematically increase the information and hence reduce the lower bound on the estimation error.

B. Analysis for Time-Dependent Quantum States

In general, the state $\boldsymbol{\Xi}_\theta(t)$ of the quantum system is a function of time. Our goal in this section is to extend the prior Fisher information analysis to the time-dependent setting. At the initial time $t = t_0$, the state is written as before

$$\boldsymbol{\Xi}_\theta(t_0) = \tfrac{1}{d}\,\boldsymbol{I} + \theta\,\boldsymbol{Z} \tag{9}$$

and the evolution of the state is described by the Gorini–Kossakowski–Sudarshan–Lindblad (GKSL) equation [21]

$$J_\theta = \frac{\mathrm{tr}^2\{\boldsymbol{M}\boldsymbol{Z}\}}{\frac{1}{d}\,\mathrm{tr}\{\boldsymbol{M}\} + \theta\,\mathrm{tr}\{\boldsymbol{M}\boldsymbol{Z}\}} + \frac{\mathrm{tr}^2\{(\boldsymbol{I} - \boldsymbol{M})\boldsymbol{Z}\}}{\frac{1}{d}\,\mathrm{tr}\{\boldsymbol{I} - \boldsymbol{M}\} + \theta\,\mathrm{tr}\{(\boldsymbol{I} - \boldsymbol{M})\boldsymbol{Z}\}} \tag{5}$$

[2]The Hilbert space of the operators $\boldsymbol{O} : \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{H})$ equipped with the Hilbert-Schmidt inner product is known as a Liouville space.

[3]In the following, the term "quantum state" and corresponding "density operator" will be used interchangeably.

[4]This can be proved using the spectral theorem and the fact that the trace of an operator is the sum of its eigenvalues.

$$\begin{aligned}\dot{\boldsymbol{\Xi}}_\theta(t) &= -\imath[\![\boldsymbol{H}(u(t),t),\boldsymbol{\Xi}_\theta(t)]\!]_- \\ &\quad + \sum_{k=1}^{N_l} \boldsymbol{L}_k(t)\boldsymbol{\Xi}_\theta(t)\boldsymbol{L}_k^\dagger(t) - \tfrac{1}{2}[\![\boldsymbol{L}_k^\dagger(t)\boldsymbol{L}_k t),\boldsymbol{\Xi}_\theta(t)]\!]_+ \\ &\triangleq F(\boldsymbol{\Xi}_\theta(t),u(t),t) \end{aligned} \tag{10}$$

for all $t \geqslant t_0$. At any point in time, $\boldsymbol{H}(u(t),t) \in \mathcal{L}(\mathcal{H})$ denotes the system's Hamiltonian (which is self-adjoint) and $\boldsymbol{L}_k(t) \in \mathcal{L}(\mathcal{H})$ for $k \in \{1,2,\ldots,N_l\}$ denote noise operators, where $N_l \in \mathbb{N}$. While the time-independent GKSL equation is generally used to model Markovian noise, the time-dependent form shown in (10) can be used to model non-Markovian noise [16].[5] The time-varying Hamiltonian is

$$\boldsymbol{H}(u(t),t) = \boldsymbol{H}_{\mathrm{f}}(t) + u(t)\boldsymbol{H}_{\mathrm{c}}(t) \tag{11}$$

where $\boldsymbol{H}_{\mathrm{f}}(t) \in \mathcal{L}(\mathcal{H})$ is the *free* Hamiltonian, $\boldsymbol{H}_{\mathrm{c}}(t) \in \mathcal{L}(\mathcal{H})$ is the *control* Hamiltonian, and $u(t) \in \mathbb{R}$ is a control input. The set of allowable controls $\mathcal{U}$ is an arbitrary open subset of the space of all regulated functions[6] from the time interval $[t_0,t_{\mathrm{f}}]$ into $\mathbb{R}$, with $t_{\mathrm{f}} > t_0$. The free Hamiltonian describes unitary evolution over which one has no control, whereas the control Hamiltonian describes unitary evolution which can be actively adjusted to alter the behavior of the system. The Hamiltonian and noise operators are well-behaving functions of time so as to ensure existence and uniqueness of solutions to (10).

Denote the solution to the GKSL equation as $\boldsymbol{\Xi}_\theta(t) \triangleq \Phi(t;t_0,\boldsymbol{\Xi}_\theta(t_0),u(\cdot))$ for $t \geqslant t_0$, where $\Phi(t;t_0,\cdot,u(\cdot))$ is known as the state transition map. Note that (10) is linear in the state; therefore, the state transition map is linear and

$$\boldsymbol{\Xi}_\theta(t) = \tfrac{1}{d}\,\Phi(t;t_0,\boldsymbol{I},u(\cdot)) + \theta\,\Phi(t;t_0,\boldsymbol{Z},u(\cdot))\,. \tag{12}$$

The GKSL equation preserves the trace, therefore $\mathrm{tr}\{\Phi(t;t_0,\boldsymbol{Z},u(\cdot))\} = \mathrm{tr}\{\boldsymbol{Z}\} = 0$ for all $t \geqslant t_0$ [21, p. 121]. Using this fact, Fisher information analysis may be conducted as before, which results in the time-dependent Fisher information (13) at the bottom of the page.

Let us turn our attention to the class of unital quantum systems. Recall, a map $\Psi : \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{H})$ is unital if it maps the identity to itself, i.e., $\Psi(\boldsymbol{I}) = \boldsymbol{I}$.

Definition 3: The quantum system described by (10) is said to be unital if the state transition map $\Phi(t;t_0,\cdot,u(\cdot))$ is a unital map at *all* times $t \geqslant t_0$. □

Lemma 2: The quantum system (10) is unital if and only if one of the following equivalent statements hold:

1) The maximally mixed state $\frac{1}{d}\boldsymbol{I}$ is a steady state of the GKSL equation (10).
2) The following equality holds for almost all $t \geqslant t_0$:

$$\sum_{k=1}^{N_l} \boldsymbol{L}_k(t)\boldsymbol{L}_k^\dagger(t) = \sum_{k=1}^{N_l} \boldsymbol{L}_k^\dagger(t)\boldsymbol{L}_k(t)\,. \tag{14}$$

□

[5]The presentation in [16] has additional terms known as "decoherence rates" in the GKSL equation. These may be absorbed by the noise operators $\{\boldsymbol{L}_k(\cdot) : k = 1,2,\ldots,N_l\}$ for notational simplicity.

[6]A function $u : [t_0,t_{\mathrm{f}}] \to \mathbb{R}$ is regulated if it has (i) left and right limits at each point $t \in (t_0,t_{\mathrm{f}})$ and (ii) one-sided limits at end points t_0 and t_{f}.

Proof: Unitality is equivalent to the identity $\boldsymbol{I}$ being a steady state of (10); however, since (10) is linear in the state, this is equivalent to the maximally mixed state $\frac{1}{d}\boldsymbol{I}$ being a steady state. This proves that the first statement is equivalent to (10) being unital. Let us now prove equivalence of the second statement. The solution to the GKSL equation is

$$\begin{aligned}\boldsymbol{\Xi}_\theta(t) &= \boldsymbol{\Xi}_\theta(t_0) + \int_{t_0}^{t} \Big[-\imath[\![\boldsymbol{H}(u(s),s),\boldsymbol{\Xi}_\theta(s)]\!]_- \\ &\quad + \sum_{k=1}^{N_l} \boldsymbol{L}_k(s)\boldsymbol{\Xi}_\theta(s)\boldsymbol{L}_k^\dagger(s) - \tfrac{1}{2}[\![\boldsymbol{L}_k^\dagger(s)\boldsymbol{L}_k(s),\boldsymbol{\Xi}_\theta(s)]\!]_+ \Big]\mathrm{d}s \end{aligned} \tag{15}$$

for $t \geqslant t_0$. Under the hypothesis that $\boldsymbol{I}/d$ is a steady state, the integral solution starting from the initial condition $\boldsymbol{\Xi}_\theta(t_0) = \boldsymbol{I}/d$ yields

$$\boldsymbol{0} = \int_{t_0}^{t} \sum_{k=1}^{N_l} \Big[\boldsymbol{L}_k(s)\boldsymbol{L}_k^\dagger(s) - \boldsymbol{L}_k^\dagger(s)\boldsymbol{L}_k(s)\Big]\,\mathrm{d}s \tag{16}$$

for any $t \geqslant t_0$. This proves that (14) holds for almost all $t \geqslant t_0$. The reverse direction follows similarly. ⊠

Remark 1: Closed quantum systems are unital. In this case $\boldsymbol{L}_k(t) = \boldsymbol{0}$ for all $k \in \{1,2,\ldots,N_l\}$ and $t \geqslant t_0$; the corresponding GKSL equation is known as a Liouville–von Neumann equation [21, pp. 110–111]. □

In unital quantum systems a major simplification of the time-dependent Fisher information (13) occurs. Defining $\boldsymbol{Z}(t) \triangleq \Phi(t;t_0,\boldsymbol{Z},u(\cdot))$,

$$J_\theta(t) = \frac{\langle \boldsymbol{M},\boldsymbol{Z}(t)\rangle^2}{a_{\mathrm{m}} + \theta\,b_{\mathrm{m}}\langle \boldsymbol{M},\boldsymbol{Z}(t)\rangle - \theta^2\langle \boldsymbol{M},\boldsymbol{Z}(t)\rangle^2} \tag{17}$$

where a_{m} and b_{m} are given in (7a) and (7b), respectively.

The Fisher information can be increased if one is allowed to alter the POVM [22, p. 234]. However, in many experimental setups the physical apparatus that implements the POVM is fixed, making information extraction challenging. We propose alleviating this problem by controlling the time evolution of the system to effectively alter the measurement performed by the fixed physical apparatus. The extent to which control can increase the information extraction is determined by the controllability of the system.

III. Information Maximizing Control

Suppose that the state $\boldsymbol{\Xi}_\theta(t)$ is measured using the binary POVM $\{\boldsymbol{M},\boldsymbol{I}-\boldsymbol{M}\}$ at some predetermined measurement time $t_{\mathrm{f}} > t_0$. One may seek to determine a control law which maximizes the Fisher information, or equivalently minimizes

$$J_\theta^{-1}(t_{\mathrm{f}}) = \frac{a_{\mathrm{m}}}{\langle \boldsymbol{M},\boldsymbol{Z}(t_{\mathrm{f}})\rangle^2} + \frac{\theta\,b_{\mathrm{m}}}{\langle \boldsymbol{M},\boldsymbol{Z}(t_{\mathrm{f}})\rangle} - \theta^2\,. \tag{18}$$

This task may be written as the following optimal control problem

$$\mathscr{P}_1(\theta) : \underset{u(\cdot)\in\mathcal{U}}{\text{minimize}} \quad J_\theta^{-1}(t_{\mathrm{f}}) + \int_{t_0}^{t_{\mathrm{f}}} K_1(u(t),t)\,\mathrm{d}t \tag{19a}$$

$$\text{subject to} \quad \dot{\boldsymbol{Z}}(t) = F(\boldsymbol{Z}(t),u(t),t), \tag{19b}$$

$$\boldsymbol{Z}(t_0) = \boldsymbol{Z}, \qquad t \in [t_0,t_{\mathrm{f}}] \tag{19c}$$

$$J_\theta(t) = \frac{\langle \boldsymbol{M},\Phi(t;t_0,\boldsymbol{Z},u(\cdot))\rangle^2}{\frac{1}{d}\langle \boldsymbol{M},\Phi(t;t_0,\boldsymbol{I},u(\cdot))\rangle + \theta\,\langle \boldsymbol{M},\Phi(t;t_0,\boldsymbol{Z},u(\cdot))\rangle} + \frac{\langle \boldsymbol{M},\Phi(t;t_0,\boldsymbol{Z},u(\cdot))\rangle^2}{\frac{1}{d}\langle \boldsymbol{I}-\boldsymbol{M},\Phi(t;t_0,\boldsymbol{I},u(\cdot))\rangle - \theta\,\langle \boldsymbol{M},\Phi(t;t_0,\boldsymbol{Z},u(\cdot))\rangle} \tag{13}$$

where $K_1(\cdot,\cdot) : \mathbb{R}\times[t_0,t_\mathrm{f}]\to\mathbb{R}$ characterizes the control cost. This cost is allowed to be quite general but will adhere to the following regularity conditions:

1) $K_1(\cdot,\cdot)$ is continuously differentiable with respect to its first argument;
2) for any $u(\cdot)\in\mathcal{U}$ the function $K_1(u(\cdot),\cdot)$ is integrable on the time interval $[t_0,t_\mathrm{f}]$; and,
3) for all fixed $t\in[t_0,t_\mathrm{f}]$, $g_t(\mu)\triangleq\partial K_1(\mu,t)/\partial\mu : \mathbb{R}\to\mathbb{R}$ is invertible and $g_t(0)=0$.

The first two conditions are standard in optimal control literature [23, pp. 73, 113] whereas the third condition is used in the proof of the next result. Note in $\mathscr{P}_1(\theta)$ that the inverse of the Fisher information represents a *terminal cost* whereas the control cost is a *running cost*. One possible choice is to consider $K_1(u(t),t)=\frac{\kappa}{2}|u(t)|^2$ where $\kappa>0$ may be tuned to balance the terminal and running costs. Then, the integral of $K_1(u(\cdot),\cdot)$ over the domain $[t_0,t_\mathrm{f}]$ is proportional to the squared norm

$$\|u(t)\|^2\triangleq\int_{t_0}^{t_\mathrm{f}}|u(t)|^2\,\mathrm{d}t \tag{20}$$

on $\mathcal{U}$, which is the energy of the control signal. A control law $u(\cdot)\in\mathcal{U}$ is said to be *non-zero energy (NZE)* if $\|u(\cdot)\|>0$.

A. Admissibility of Optimal Controls

In general an optimal control law which solves $\mathscr{P}_1(\theta)$, denoted by $u(t)=\mu_\theta^\star(t)$, will depend on the unknown parameter θ since $J_\theta^{-1}(t_\mathrm{f})$ is parameter-dependent. However, a control law that depends on the parameter it elicits would be like a point estimator that depends on the parameter it aims to infer, which is absurd [1, pp. 211, 311].[7] Motivated by this observation, we define admissible control laws below.

Definition 4: A control law $\mu_\theta : [t_0,t_\mathrm{f}]\to\mathbb{R}$ for regulating $J_\theta(\cdot)$ is said to be *admissible* if it does not depend on θ. □

The following theorem provides a necessary and sufficient condition for information maximizing controls, i.e., controls which solve $\mathscr{P}_1(\theta)$, to be admissible.

Theorem 1: Any NZE optimal control law $\mu_\theta^\star(\cdot)\in\mathcal{U}$ which solves $\mathscr{P}_1(\theta)$ is admissible if and only if $b_\mathrm{m}=0$, i.e.,

$$\mathrm{tr}\{\boldsymbol{M}\}=\frac{d}{2}\,. \tag{21}$$

□

Proof: If $b_\mathrm{m}=0$, then the admissibility of $\mu_\theta^\star(\cdot)$ follows immediately from (18) and (19a) with $b_\mathrm{m}=0$. This proves the sufficiency of the condition (21). Proving the necessity of (21) involves two steps: (i) constructing the necessary conditions for optimal control in a Hilbert space, see, e.g., [23, pp. 112–117][8]; and (ii) showing that $b_\mathrm{m}=0$ if the necessary conditions for optimal control hold simultaneously for any two different values $\theta=\theta_1$ and $\theta=\theta_2$ in Θ. The Hamiltonian functional $h_\mathrm{c} : \mathcal{L}(\mathcal{H})\times\mathcal{L}(\mathcal{H})\times\mathbb{R}\times[t_0,t_\mathrm{f}]\to\mathbb{R}$ corresponding to the optimal control problem $\mathscr{P}_1(\theta)$ is[9]

$$\begin{aligned}h_\mathrm{c}(\boldsymbol{Z}(t),\boldsymbol{\Lambda}(t),u(t),t)\\ =K_1(u(t),t)+\langle\boldsymbol{\Lambda}(t),F(\boldsymbol{Z}(t),u(t),t)\rangle\,.\end{aligned} \tag{22}$$

[7]A point estimator is first and foremost a statistic, and the analytical expression of a statistic cannot be a function of an unknown parameter.

[8]The presentation in [23] is a more general treatment in Banach spaces; however, quantum mechanical problems are always formulated in Hilbert spaces. For a tutorial on necessary conditions for optimal control of quantum systems in finite dimensions see [24].

[9]This is not to be confused with the Hamiltonians of the quantum system.

The operator $\boldsymbol{\Lambda}(t)$ is known as the costate. Suppose that a NZE optimal control $\mu_\theta^\star(t)$ and optimal state trajectory $\boldsymbol{Z}^\star(t)$ exist which solve $\mathscr{P}_1(\theta)$. Then, the objective (19a) evaluated along the optimal control and state trajectory is finite, implying via (18) that $\langle\boldsymbol{M},\boldsymbol{Z}^\star(t_\mathrm{f})\rangle\neq 0$. By continuity there exists a neighborhood of $\mu_\theta^\star(t)$ in $\mathcal{U}$ such that $\langle\boldsymbol{M},\boldsymbol{Z}(t_\mathrm{f})\rangle\neq 0$ for any control law in this neighborhood. Let us apply the necessary conditions for optimal control within this neighborhood where $J_\theta^{-1}(t_\mathrm{f})$ is continuously differentiable with respect to $\boldsymbol{Z}(t_\mathrm{f})$. The necessary conditions involve the costate variable $\boldsymbol{\Lambda}^\star(t)$ which solves the following final value problem:

$$\begin{cases}\dot{\boldsymbol{\Lambda}}^\star(t) &= -F^\ddagger(\boldsymbol{\Lambda}^\star(t),\mu_\theta^\star(t),t)\\ \boldsymbol{\Lambda}^\star(t_\mathrm{f}) &= \nabla_{\boldsymbol{Z}^\star(t_\mathrm{f})}J_\theta^{-1}(t_\mathrm{f})\end{cases} \tag{23}$$

where $\nabla_{\boldsymbol{Z}^\star(t_\mathrm{f})}J_\theta^{-1}(t_\mathrm{f})$ denotes the gradient of $J_\theta^{-1}(t_\mathrm{f})$ with respect to $\boldsymbol{Z}^\star(t_\mathrm{f})$. Supplemental calculations for (23) are given in the Appendix. It can be shown that

$$\nabla_{\boldsymbol{Z}(t_\mathrm{f})}J_\theta^{-1}(t_\mathrm{f})=\Big[\frac{-2a_\mathrm{m}}{\langle\boldsymbol{M},\boldsymbol{Z}(t_\mathrm{f})\rangle}-b_\mathrm{m}\theta\Big]\frac{1}{\langle\boldsymbol{M},\boldsymbol{Z}(t_\mathrm{f})\rangle^2}\,\boldsymbol{M}\,. \tag{24}$$

The necessary conditions state that the optimal control law satisfies $\partial h_\mathrm{c}(\boldsymbol{Z}^\star(t),\boldsymbol{\Lambda}^\star(t),\mu_\theta^\star(t),t)/\partial\mu_\theta^\star(t)=0$ for almost all $t\in[t_0,t_\mathrm{f}]$. Using the regularity conditions on $K_1(\cdot,\cdot)$, this means that the optimal control is

$$\mu_\theta^\star(t)=g_t^{-1}\big(\langle\boldsymbol{\Lambda}^\star(t),\imath[\![\boldsymbol{H}_\mathrm{c}(t),\boldsymbol{Z}^\star(t)]\!]_-\rangle\big) \tag{25}$$

for almost all $t\in[t_0,t_\mathrm{f}]$, where $g_t(\mu)=\partial K_1(\mu,t)/\partial\mu$.

Suppose that the optimal control law (25) is admissible, which completely determines $\boldsymbol{Z}^\star(t)$, irrespective of θ, via the GKSL equation and the initial condition $\boldsymbol{Z}^\star(t_0)=\boldsymbol{Z}$. Consider any two different values $\theta=\theta_1$ and $\theta=\theta_2$ in Θ. With the control and state fixed, existence and uniqueness of solutions to (23) determines the costate $\boldsymbol{\Lambda}_1^\star(t)$ when $\theta=\theta_1$ and $\boldsymbol{\Lambda}_2^\star(t)$ when $\theta=\theta_2$. These costates satisfy the following boundary conditions:

$$\boldsymbol{\Lambda}_1^\star(t_\mathrm{f})=\Big[\frac{-2a_\mathrm{m}}{\langle\boldsymbol{M},\boldsymbol{Z}^\star(t_\mathrm{f})\rangle}-b_\mathrm{m}\theta_1\Big]\frac{1}{\langle\boldsymbol{M},\boldsymbol{Z}^\star(t_\mathrm{f})\rangle^2}\,\boldsymbol{M} \tag{26a}$$

$$\boldsymbol{\Lambda}_2^\star(t_\mathrm{f})=\Big[\frac{-2a_\mathrm{m}}{\langle\boldsymbol{M},\boldsymbol{Z}^\star(t_\mathrm{f})\rangle}-b_\mathrm{m}\theta_2\Big]\frac{1}{\langle\boldsymbol{M},\boldsymbol{Z}^\star(t_\mathrm{f})\rangle^2}\,\boldsymbol{M}\,. \tag{26b}$$

The terms in brackets must be non-zero. To prove this, suppose the contrary. Then $\boldsymbol{\Lambda}_1^\star(t)$ or $\boldsymbol{\Lambda}_2^\star(t)$ (or both) is zero for all time since the dynamics (23) are linear in the costate. Consequently, using the regularity conditions on $K_1(\cdot,\cdot)$, the optimal control (25) is zero for almost all $t\in[t_0,t_\mathrm{f}]$ and thus $\|\mu_\theta^\star(\cdot)\|=0$. However, this is a contradiction since the control law $\mu_\theta^\star(\cdot)$ is NZE. This proves that the terms in brackets in (26a) and (26b) are non-zero.

To prove that $b_\mathrm{m}=0$ is necessary for the same control law $\mu_\theta^\star(\cdot)$ to be optimal for both cases $\theta=\theta_1$ and $\theta=\theta_2$, suppose the contrary: $b_\mathrm{m}\neq 0$. Defining $\boldsymbol{\Lambda}_{1-2}^\star(t)\triangleq\boldsymbol{\Lambda}_1^\star(t)-\boldsymbol{\Lambda}_2^\star(t)$,

$$\boldsymbol{\Lambda}_{1-2}^\star(t_\mathrm{f})=\frac{b_\mathrm{m}(\theta_2-\theta_1)}{\langle\boldsymbol{M},\boldsymbol{Z}^\star(t_\mathrm{f})\rangle^2}\boldsymbol{M} \tag{27}$$

which is non-zero since the parameters were assumed distinct. Applying the linearity of the dynamics (23) in the costate, it follows that

$$\boldsymbol{\Lambda}_{1-2}^\star(t)=b_\mathrm{m}(\theta_2-\theta_1)\Big[\frac{-2a_\mathrm{m}}{\langle\boldsymbol{M},\boldsymbol{Z}^\star(t_\mathrm{f})\rangle}-b_\mathrm{m}\theta_1\Big]^{-1}\boldsymbol{\Lambda}_1^\star(t) \tag{28}$$

for all $t\in[t_0,t_\mathrm{f}]$. On the other hand, recalling (25) and the fact that $\mu_\theta^\star(\cdot)$ is optimal for both θ_1 and θ_2, it follows that

$$\langle \boldsymbol{\Lambda}_1^\star(t), [\![\boldsymbol{H}_{\mathrm{c}}(t), \boldsymbol{Z}^\star(t)]\!]_- \rangle = \langle \boldsymbol{\Lambda}_2^\star(t), [\![\boldsymbol{H}_{\mathrm{c}}(t), \boldsymbol{Z}^\star(t)]\!]_- \rangle, \quad \forall t \in [t_0, t_{\mathrm{f}}] \tag{29}$$

and subsequently that

$$\langle \boldsymbol{\Lambda}_{1-2}^\star(t), [\![\boldsymbol{H}_{\mathrm{c}}(t), \boldsymbol{Z}^\star(t)]\!]_- \rangle = 0, \quad \forall t \in [t_0, t_{\mathrm{f}}]. \tag{30}$$

Combining this with (28) proves that $\langle \boldsymbol{\Lambda}_1^\star(t), [\![\boldsymbol{H}_{\mathrm{c}}(t), \boldsymbol{Z}^\star(t)]\!]_- \rangle = 0$ for almost all $t \in [t_0, t_{\mathrm{f}}]$. However, using (25) and the regularity conditions on $K_1(\cdot,\cdot)$ this means that the control is zero for almost all $t \in [t_0, t_{\mathrm{f}}]$ and consequently $\|\mu_\theta^\star(\cdot)\| = 0$. This is a contradiction since $\mu_\theta^\star(\cdot)$ is NZE. It is therefore necessary that $b_{\mathrm{m}} = 0$, and the theorem is proven. ⊠

A few remarks are in order regarding Theorem 1.

1) Though the optimal control is admissible if $b_{\mathrm{m}} = 0$, the Fisher information $J_\theta(t_{\mathrm{f}})$ still depends on θ as seen in (17). Therefore the performance of an estimator of θ may well depend on the unknown parameter.
2) The theorem also applies to control laws corresponding to local optima of problem $\mathscr{P}_1(\theta)$ since the proof relies only on necessary conditions for locally optimal control [25]. This is relevant for computing control laws.
3) The theorem does not specify the sensitivity of optimal control laws to changes in θ when $b_{\mathrm{m}} \neq 0$. Such sensitivity would depend on the dynamics F, parameter space Θ, control cost K_1, and constants a_{m} and b_{m}.

Suppose that $\boldsymbol{M}$ is a projection (implying that $\boldsymbol{I} - \boldsymbol{M}$ is a projection), which is frequently the case in quantum systems. Then, the spectrum of $\boldsymbol{M}$ contains only ones and zeros, thus the trace of $\boldsymbol{M}$ equals the rank of $\boldsymbol{M}$. We have the following corollary to the admissibility condition of Theorem 1.

Corollary 1: Let $\boldsymbol{M}$ be a projection. Any NZE optimal control law $\mu_\theta^\star(\cdot) \in \mathcal{U}$ which solves $\mathscr{P}_1(\theta)$ is admissible if and only if

$$\operatorname{rank} \boldsymbol{M} = \frac{d}{2}. \tag{31}$$

□

Notably the condition in this corollary cannot occur in systems of odd dimension, but there is still hope of satisfying the more general condition (21). On the other hand, many systems arising in quantum information applications are of even dimension: e.g., any system comprised of n qubits is of dimension 2^n.

B. Design of Admissible Optimal Control

The prior section proved that an information maximizing control law is admissible if and only if $b_{\mathrm{m}} = 0$. If $b_{\mathrm{m}} = 0$ then the expression for the inverse of the Fisher information (18) is significantly simpler, and minimizing $J_\theta^{-1}(t_{\mathrm{f}})$ is equivalent to making $\langle \boldsymbol{M}, \boldsymbol{Z}(t_{\mathrm{f}}) \rangle^2$ as large as possible. This corresponds to concentrating the probability mass on one of the outcomes $\mathrm{y} = +1$ or $\mathrm{y} = -1$. Minimizing $J_\theta^{-1}(t_{\mathrm{f}})$ can be formulated as the optimal control problem

$$\mathscr{P}_2: \underset{u(\cdot) \in \mathcal{U}}{\text{minimize}} \quad -\langle \boldsymbol{M}, \boldsymbol{Z}(t_{\mathrm{f}}) \rangle^2 + \int_{t_0}^{t_{\mathrm{f}}} K_2(u(t), t)\, \mathrm{d}t \tag{32a}$$

$$\text{subject to} \quad \dot{\boldsymbol{Z}}(t) = F(\boldsymbol{Z}(t), u(t), t), \tag{32b}$$

$$\boldsymbol{Z}(t_0) = \boldsymbol{Z}, \qquad t \in [t_0, t_{\mathrm{f}}] \tag{32c}$$

where $K_2(\cdot,\cdot) : \mathbb{R} \times [t_0, t_{\mathrm{f}}] \to \mathbb{R}$ characterizes the control cost and is potentially different than $K_1(\cdot,\cdot)$ in problem $\mathscr{P}_1(\theta)$.

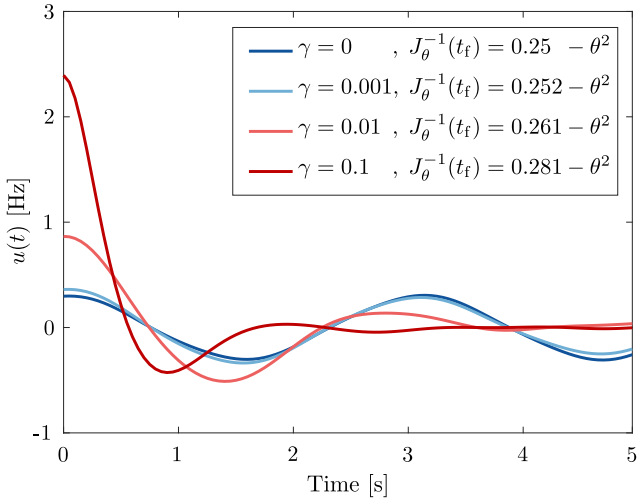

Fig. 1. Control laws solving $\mathscr{P}_2$ for varying levels γ of dephasing noise.

This control problem is well-posed: control laws which solve the problem are admissible by construction. Techniques to solve $\mathscr{P}_2$ are well-known [26].

C. Case Study: Qubit Subject to Dephasing Noise

Consider a parameter estimation problem involving a qubit ($d = 2$) subject to dephasing noise, as appears in many practical scenarios [27]. The free Hamiltonian, control Hamiltonian, and noise operator can be modeled respectively by

$$\boldsymbol{H}_{\mathrm{f}} = \tfrac{\omega_{\mathrm{q}}}{2} \boldsymbol{P}_z, \quad \boldsymbol{H}_{\mathrm{c}} = \boldsymbol{P}_x \quad \text{and} \quad \boldsymbol{L} = \sqrt{\gamma}\, \boldsymbol{P}_z. \tag{33}$$

In (33), $\omega_{\mathrm{q}} > 0$ is the qubit frequency and $\gamma \geqslant 0$ is the strength of the dephasing noise. The Pauli operators are denoted $\boldsymbol{P}_x$, $\boldsymbol{P}_y$, and $\boldsymbol{P}_z$. Using the fact that $\boldsymbol{P}_z = \boldsymbol{P}_z^\dagger$, Lemma 2 shows that the quantum system described by (33) is unital. For $d = 2$, any projective measurement system satisfies $\operatorname{tr}\{\boldsymbol{M}\} = d/2 = 1$. Then, Theorem 1 or Corollary 1 shows that optimal control laws which solve $\mathscr{P}_1(\theta)$ are admissible. Consider the particular projective measurement system

$$\boldsymbol{M} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad \boldsymbol{I} - \boldsymbol{M} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}. \tag{34}$$

Suppose that the initial state of the qubit is $\boldsymbol{\Xi}_\theta(t_0) = \boldsymbol{I}/2 + \theta \boldsymbol{P}_y$ (the only requirement is that $\boldsymbol{Z}$ in (9) is traceless). According to Lemma 1, the range of possible θ values is $[-1/2, 1/2]$. Take the parameter space Θ to be this entire interval. For any $\theta \in \Theta$, the Fisher information (6) at time t_0 is zero. That is, no information regarding θ may be obtained by measuring $\boldsymbol{\Xi}_\theta(t_0)$ with the projective measurement system (34). Moreover, it can be shown that $J_\theta(t_{\mathrm{f}}) = 0$ for any $t_{\mathrm{f}} \geqslant t_0$ if no control is applied. Thus, if there is any hope of inferring $\theta \in \Theta$, *control is essential*.

Since the admissibility condition (21) or (31) is satisfied, maximization of $J_\theta(t_{\mathrm{f}})$ at some time $t_{\mathrm{f}} > t_0$ translates to solving problem $\mathscr{P}_2$. As an example, suppose that $t_0 = 0$ s, $t_{\mathrm{f}} = 5$ s, $\omega_{\mathrm{q}} = 2$ Hz, and $K_2(u(t), t) = \frac{\kappa}{2} |u(t)|^2$ with $\kappa = 0.01$. The optimization problem is solved computationally by employing the gradient method [23, p. 147].[10] Control laws generated for four different values of dephasing

[10] The gradient method uses the same ideas as the necessary conditions for optimal control employed in the proof of Theorem 1, which makes it a natural computational method to use in this context.

noise strength γ are displayed in Figure 1. In all cases the Fisher information $J_\theta(t_\mathrm{f})$ is non-zero, which demonstrates the efficacy of control-enhanced quantum parameter estimation. Notice that as the dephasing noise strength γ increases, the maximized Fisher information $J_\theta(t_\mathrm{f})$ decreases and the control transforms from an almost-periodic signal to a damped oscillation. For large noise levels, we find that the control exerts high-energy upfront and quickly moves $\boldsymbol{Z}(t)$ to the null-space of the noise contribution in (10), i.e., the space of $\boldsymbol{A} \in \mathcal{L}(\mathcal{H})$ such that $\boldsymbol{L}\boldsymbol{A}\boldsymbol{L}^\dagger - \frac{1}{2}[\![\boldsymbol{L}^\dagger\boldsymbol{L}, \boldsymbol{A}]\!]_+ = \boldsymbol{0}$.

IV. Conclusion

This letter established a foundation for optimally controlling the dynamical evolution of a quantum state to maximize the information, about an unknown parameter, extracted by a given quantum measurement apparatus. Inspired by notions from statistical inference, the concept of admissible control laws was introduced. For the class of unital quantum systems interrogated by binary measurements, we derived a necessary and sufficient condition on the POVM operators such that information maximizing control laws are admissible. This condition concerns the trace of the POVM operators. When such condition is satisfied, it was shown that information maximizing control laws can be designed using well-established techniques. The utility of this methodology was demonstrated on a dephasing qubit system.

Appendix

Theorem 1 Supplementary Calculations

Following [23, p. 115], the costate associated with an optimal state trajectory $\boldsymbol{Z}^\star(\cdot)$ and optimal control $\mu_\theta^\star(\cdot)$ satisfies

$$\dot{\boldsymbol{\Lambda}}^\star(t) = -\nabla_{\boldsymbol{Z}^\star(t)} h_\mathrm{c}(\boldsymbol{Z}^\star(t), \boldsymbol{\Lambda}^\star(t), \mu_\theta^\star(t), t) \quad \forall\, t \in [t_0, t_\mathrm{f}] \tag{35}$$

subject to the terminal condition $\boldsymbol{\Lambda}^\star(t_\mathrm{f}) = \nabla_{\boldsymbol{Z}^\star(t_\mathrm{f})} J_\theta^{-1}(t_\mathrm{f})$. The right-hand side of (35) becomes

$$-\nabla_{\boldsymbol{Z}^\star(t)} \langle \boldsymbol{\Lambda}^\star(t), F(\boldsymbol{Z}^\star(t), \mu_\theta^\star(t), t)\rangle \tag{36}$$

since $K_1(\mu_\theta^\star(t), t)$ that appears in the Hamiltonian functional (22) is not a function of $\boldsymbol{Z}^\star(t)$. At any given time $t \in [t_0, t_\mathrm{f}]$, the operator F is a linear operator mapping $\mathcal{L}(\mathcal{H})$ into itself. Applying the definition of the adjoint with respect to the Hilbert-Schmidt inner product

$$\begin{aligned}&\langle \boldsymbol{\Lambda}^\star(t), F(\boldsymbol{Z}^\star(t), \mu_\theta^\star(t), t)\rangle \\ &\qquad = \langle F^\ddagger(\boldsymbol{\Lambda}^\star(t), \mu_\theta^\star(t), t), \boldsymbol{Z}^\star(t)\rangle\end{aligned} \tag{37}$$

and subsequently

$$\dot{\boldsymbol{\Lambda}}^\star(t) = -F^\ddagger(\boldsymbol{\Lambda}^\star(t), \mu_\theta^\star(t), t)\,. \tag{38}$$

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