Quantum Hamiltonian Identifiability via a Similarity Transformation Approach and Beyond

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***Abstract*—The identifiability of a system is concerned with whether the unknown parameters in the system can be uniquely determined with all the possible data generated by a certain experimental setting. A test of quantum Hamiltonian identifiability is an important tool to save time and cost when exploring the identification capability of quantum probes and experimentally implementing quantum identification schemes. In this article, we generalize the identifiability test based on the similarity transformation approach (STA) in classical control theory and extend it to the domain of quantum Hamiltonian identification. We employ the STA to prove the identifiability of spin-1/2 chain systems with arbitrary dimension assisted by single-qubit probes. We further extend the traditional STA method by proposing a structure preserving transformation (SPT) method for nonminimal systems. We use the SPT method to introduce an indicator for the existence of economic quantum Hamiltonian identification algorithms, whose computational complexity directly depends on the number of unknown parameters (which could be much smaller than the system dimension). Finally, we give an example of such an economic Hamiltonian identification algorithm and perform simulations to demonstrate its effectiveness.**

***Index Terms*—Hamiltonian identifiability, quantum Hamiltonian identification, quantum system, similarity transformation approach (STA).**

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I. Introduction

THERE is growing interest in quantum system research, aiming to develop advanced technology, including quantum computation, quantum communication [1], and quantum sensing [2]. Before exploiting a quantum system as a quantum device, it is usually necessary to estimate the state and identify key variables of the system [3]–[7]. The Hamiltonian is a fundamental quantity that governs the evolution of a quantum system. Hamiltonian identification is, thus, critical for tasks such as calibrating quantum devices [8] and characterizing quantum channels [9], [10].

Before performing identification experiments, a natural question arises: Are the available data from a given experimental setting enough to identify (or determine) all the desired parameters in the Hamiltonian? In this article, we refer to such a problem as Hamiltonian identifiability. The solution to this problem is fundamental and necessary for designing efficient experiments and investigating the capability of quantum sensors [2] and also gives us insights on information extraction of certain probe systems.

There are several existing approaches to investigating the problem of quantum system identification [11]–[14]. For example, Burgarth and Yuasa [15] proved that controllable quantum systems are indistinguishable if and only if they are related through a unitary transformation, which can be developed as an identifiability method for controllable systems. The identifiability problem for a Hamiltonian corresponding to a dipole moment was investigated in [16]. The identification problem of spin chains has been extensively investigated in [17]–[22]. For example, Di Franco *et al.* [17], [18] proposed a spin chain Hamiltonian identification scheme requiring no state initialization but only time-resolved measurements on one terminal qubit. By employing measurement on a terminal qubit of the chain, Burgarth *et al.* [19] designed a coupling strength identification algorithm for one class of spin chain models. The Zeeman effect was employed in [20] to reconstruct Hamiltonian, which requires no time-resolved dynamics of the system. Burgarth and Maruyama [21] proposed a sufficient condition for a many-body Hamiltonian to be identifiable through a limited access to a small subsystem using prior topology knowledge about the system (extended to combinatorially symmetric Hidden Markov Models in [22]). Moreover, Guţă and Yamamoto [23] presented identifiable conditions for parameters in passive linear quantum systems and further disposed of the requirement of "passive" in [24]. Control signals to enhance the observability of the quantum dipole moment matrix were introduced in [25]. Zhang and Sarovar [26] proposed a Hamiltonian identification method based on measurement time traces. Sone and Cappellaro [27] employed Gröbner basis to test the Hamiltonian identifiability of spin-1/2 systems, and their method is also applicable to general finite-dimensional systems.

We assume that the dimension [28] and structure (e.g., the coupling types) [29] of the Hamiltonian are already determined, and the task is to identify unknown parameters in the Hamiltonian. It is natural to resort to identifiability test methods in classical (nonquantum) control field to tackle the quantum Hamiltonian identifiability problem. Common classical methods include the Laplace transform approach [30], the Taylor series expansion approach [31], and the similarity transformation approach (STA) [32]–[34] (for a review, see [35]–[38]). The main idea of the Laplace transform approach is to determine the number of solutions of the multivariate equations composed by coefficients of the transfer function. In contrast, the STA method transforms the identifiability problem into finding the existence of unequal solutions of similarity equations generated by a minimal system's equivalent realizations, thus providing a chance to avoid directly solving multivariate polynomial equations, a considerable advantage in the case of high-dimensional or incomplete prior information. In this article, we extend the STA method to quantum Hamiltonian identifiability. We generalize and improve STA-based identifiability criteria, which are applicable to both classical control and quantum identification domains. We employ the STA method to analyze all physical cases in [27] and present proofs for the associated identifiability conclusions. Although the identification problem of similar systems has been investigated, existing results mainly focus on either designing identification algorithms [17]–[20], or presenting sufficient conditions for a system to be identifiable [21], [22].

We further propose a structure preserving transformation (SPT) method for the STA-based identifiability analysis in nonminimal systems. In classical control, when faced with nonminimal systems, one usually prefers to change the system settings such that it becomes minimal. In other words, the original settings are abandoned. This indirect solution is not applicable when the experimental settings are difficult to change or when we only expect to explore the information extraction capability of some particular physical probe systems. Such situations are often confronted in the quantum domain, since only some well-chosen measurement operations may be easy to realize and measurement operations usually destroy the quantum states themselves. Here, the SPT method provides a chance to preserve most of the system key properties after transformations, while still performing identifiability analysis on its minimal subsystem. Hence, we employ the SPT method to prove that it is always possible to estimate one unknown parameter in the system matrix using a specifically designed experimental setting. This conclusion serves as an indicator for the existence of "economic" quantum Hamiltonian identification algorithms, whose computational complexity directly depends on the number of unknown parameters.

As an example, we provide a specific economic identification algorithm. The computational complexity $O(\mathcal{M}^2 + q\mathcal{M}\mathcal{N})$ only depends on the number of unknown parameters $\mathcal{M}$ and data length $\mathcal{N}$ (q is a variable not larger than $\mathcal{N}$). Therefore, for physical systems with a small number of unknown parameters in the Hamiltonian, this identification algorithm can be efficient.

The main contributions of this article are summarized as follows.

1) The identifiability test method based on the STA is generalized and extended to the quantum Hamiltonian identifiability problem. Improved identifiability test criteria are provided, and the analysis method based on SPT is developed for nonminimal systems when the system settings are difficult to change.
2) Based on the STA method, the Hamiltonian identifiability problem of the three physical cases in [27] is analyzed in detail, and concrete identifiability conclusions are proved. These results as illustrative examples show the effectiveness of the STA method for analyzing Hamiltonian identifiability of closed quantum systems with arbitrary dimension.
3) To analyze general nonminimal systems, an SPT application is developed to present an indicator for the existence of economic Hamiltonian identification algorithms, which have computational complexity directly depending on the number of unknown parameters. One example of such identification algorithms is then presented.

The structure of this article is as follows. In Section II, we present some preliminaries, formulate the identifiability problem, and briefly introduce the classical Laplace transform approach. Section II-B presents the identifiability test method employing the STA. Based on the STA method, we present the identifiability proof for two spin models, the exchange model without and with transverse field in Sections IV and V, respectively. In Section VI, we employ the SPT method to present an indicator for the existence of economic quantum Hamiltonian identification algorithms and also give a concrete example of developing such an algorithm. Finally, Section VII concludes this article.

Notation: Let $*$ denote an indeterminate variable or matrix. For a matrix A, $A_{\sigma i}$ and $A_{j\sigma}$ denote its ith column and jth row, respectively. Real and complex domains are denoted by $\mathbb{R}$ and $\mathbb{C}$, respectively. Let $\otimes$ denote the tensor product. Define the vectorization function as $\text{vec}(A_{m\times n}) = [A_{\sigma 1}^T, A_{\sigma 2}^T, \ldots, A_{\sigma n}^T]^T$. Let $\lambda_i(A)$ denote the ith eigenvalue of A and $\Lambda(A)$ is the set of all the eigenvalues of A (repeated eigenvalues appear multiple times in $\Lambda(A)$). Let $||\cdot||$ denote the Frobenius norm. Define δ as the Dirac delta function or the Kronecker delta function, in the continuous or discrete sense, respectively. Denote the estimation value of the true value x as $\hat{x}$. Define $\lfloor x \rfloor$ the largest integer that is not larger than x.

II. Preliminaries and Problem Formulation

A. Quantum State and Measurement

The state of a quantum system is represented by a complex Hermitian matrix ρ in a Hilbert space, and its dynamics are described by the Liouville–von Neumann equation

$$\dot{\rho} = -\mathrm{i}[H, \rho] \tag{1}$$

where $\mathrm{i} = \sqrt{-1}$, H is the system Hamiltonian, $[A, B] = AB - BA$ is the commutator, and we set $\hbar = 1$ using atomic units in this article. Matrix ρ is positive semidefinite, satisfying $\mathrm{Tr}(\rho) = 1$.

To extract information from a quantum state, it is normally necessary to perform a positive-operator valued measure (POVM), which is a set $\{M_i\}$, where all the elements are Hermitian positive-semidefinite matrices and $\sum_i M_i = I$. When a set $\{M_i\}$ of the POVM is performed, the probability of outcome i occurring is determined by the Born rule, $p_i = \mathrm{Tr}(\rho M_i)$. The data in actual experiments are the approximation values of p_i.

B. Problem Formulation of Hamiltonian Identifiability and Identification

We first rephrase the framework in [26] to recast the problem of Hamiltonian identification as a linear system identification problem. Let H be the d-dimensional Hamiltonian to be identified, which can be parametrized as

$$H = \sum_{m=1}^{\mathcal{M}} a_m(\theta) H_m \tag{2}$$

where $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_{\mathcal{M}})^T$ is a vector consisting of all the unknown parameters, $\mathcal{M}$ is the number of unknown parameters, a_m are known functions of $\boldsymbol{\theta}$, and H_m are known Hermitian matrices (also called basis matrices). Let $\mathfrak{su}(d)$ denote the Lie algebra consisting of all $d \times d$ skew-Hermitian traceless matrices. Then, $\{\mathrm{i}H_m\}$ can be chosen as an orthonormal basis of $\mathfrak{su}(d)$, where the inner product is defined as $\langle \mathrm{i}H_m, \mathrm{i}H_n \rangle = \mathrm{Tr}(H_m^\dagger H_n)$. The traceless assumption is reasonable because H has an intrinsic degree of freedom (see [39] for details).

Let S_{jkl} be the real structure constants of $\mathfrak{su}(d)$, which satisfy

$$[\mathrm{i}H_j, \mathrm{i}H_k] = \sum_{l=1}^{d^2-1} S_{jkl}(\mathrm{i}H_l) \tag{3}$$

where $j, k = 1, \ldots, d^2 - 1$. If H_k is the observable, then the experimental data are obtained from Born's rule

$$x_k = \mathrm{Tr}(H_k \rho). \tag{4}$$

The identifiability is determined by the system structure. Hence, it is usually assumed that there are no imperfections in the available experimental data, which is the reason we identify theoretical values with practical data in (4).

From (1)–(4), we have

$$\dot{x_k} = \sum_{l=1}^{d^2-1} \left(\sum_{m=1}^{\mathcal{M}} S_{mkl} a_m(\theta) \right) x_l. \tag{5}$$

If we directly rewrite (5) into a matrix form, the dimension of the system matrix would be $d^2 - 1$, which is large for multiqubit systems. To reduce the dimension, first consider the operators O_i that we can directly measure in practice. We expand O_i as $O_i = \sum_j o_j H_j$ and collect all the H_j that appear in the expansion of O_i as $\mathbb{M} = \{H_{v_1}, \ldots, H_{v_p}\}$. Also, we collect all the H_j that appear in the expansion of H as $\mathbb{L} = \{H_m\}_{m=1}^{\mathcal{M}}$. Define an iterative procedure as

$$G_0 = \mathbb{M}, \quad G_i = \{G_{i-1}, \mathbb{L}\} \cup G_{i-1}$$

where $\{G_{i-1}, \mathbb{L}\} \triangleq \{H_j | \mathrm{Tr}(H_j^\dagger [g, h]) \neq 0, \quad \text{for some} \quad g \in G_{i-1}, h \in \mathbb{L}\}$. This iteration will terminate at a maximal set $\bar{G}$ (called the *accessible set*) because $\mathfrak{su}(d)$ is finite dimensional. We collect all the x_i with $H_i \in \bar{G}$ in a vector $\mathbf{x}$ of dimension n, and its dynamics satisfy the linear system equation

$$\dot{\mathbf{x}} = A\mathbf{x}. \tag{6}$$

The elements in A are the coefficients in (5), which are linear combinations of $a_m(\boldsymbol{\theta})$. For some types of physical systems, the dimension n can be much smaller than $d^2 - 1$. Real matrix A is antisymmetric due to the antisymmetry of the structure constants. The output data can be denoted as

$$\mathbf{y} = C\mathbf{x} \tag{7}$$

where C is a known matrix that selects the entries in $\mathbf{x}$ corresponding to the expectation values of the elements in $\mathbb{M}$. Therefore, the quantum Hamiltonian identification problem can be established as follows.

Problem 1: Given the system matrix $A = A(\theta)$, initial state $\mathbf{x}(0) = \mathbf{x}_0$, and observation matrix C, design an algorithm to obtain an estimate $\hat{\theta}$ of $\boldsymbol{\theta}$ from measurement data $\hat{\mathbf{y}}$.

Before designing specific identification algorithms, a natural question arises: For a system A, can we uniquely determine the unknown parameters, based on a given experimental setup (i.e., $\mathbf{x}_0$ and C)? If not, then it may be required to redesign the experimental setup before starting the experiment. This is especially significant for quantum system identification, since implementing quantum experiments is usually expensive. This induces the problem of identifiability. Denote by $\boldsymbol{\theta}$ the true value of the unknown parameter vector to be identified. Assume that the system under consideration has some parametric model structure with output data $\mathcal{S}(\theta)$, for a given experimental setup. The equation

$$\mathcal{S}(\boldsymbol{\theta}) = \mathcal{S}(\theta') \tag{8}$$

means that the model with parameter set θ' outputs *exactly* the same data as the model with parameter set $\boldsymbol{\theta}$. Identifiability then depends on the number of solutions to (8) for θ'. We use the following definition from [38].

Definition 1 (see [38]): The model $\mathcal{S}$ is *structurally globally identifiable* (abbreviated as *identifiable* in the rest of this article), if for almost any value of $\boldsymbol{\theta}$, (8) has only one solution $\theta' = \boldsymbol{\theta}$.

Definition 1 is in essence the same as the definition of identifiability in [27]. It is necessary to ensure that identifiability holds for almost any value of the parameters because the number of solutions to (8) might change for some particular values of $\boldsymbol{\theta}$, which are called *atypical* cases (to be illustrated later). Also, identifiability is determined by the system structure. Hence, we do not consider noise or uncertainty in the experimental data. A trivial necessary condition for a parameter to be identifiable is that it should appear in the system model $\mathcal{S}$, and in the following, we only focus on this class of parameters.

C. Laplace Transform Approach and Atypical Cases

One of the most intuitive ways to solve identifiability problems is through the Laplace transform, which is also helpful in understanding concepts like *atypical* cases. Hence, we first briefly introduce the Laplace transform approach [38]. Consider the following standard multiple-input multiple-output linear system with zero initial condition:

$$\begin{cases} \dot{\mathbf{x}} = A(\theta)\mathbf{x} + B(\theta)\mathbf{u}, \ \ \mathbf{x}(0) = \mathbf{0} \\ \mathbf{y} = C(\theta)\mathbf{x} + D(\theta)\mathbf{u}. \end{cases} \tag{9}$$

Throughout this article, we use 4-tuples $\Sigma = (A, B, C, D)$ to denote linear systems with the form of (9). The Laplace transform solution to (9) is

$$\mathbf{Y}(s,\theta) = \mathbf{T}(s,\theta)\mathbf{U}(s)$$

where the transfer function matrix is $\mathbf{T}(s,\theta) = C(\theta)[sI - A(\theta)]^{-1}B(\theta) + D(\theta)$.

Remark 1: Now, we know that the system (6) and (7) with initial state $\mathbf{x}(0) = \mathbf{x}_0$ is equivalent to the system $\dot{\mathbf{x}} = A\mathbf{x} + Bu$ and $\mathbf{y} = C\mathbf{x}$ with a zero-initial state $\mathbf{x}(0) = \mathbf{0}$, where $B = \mathbf{x}_0$ and $u = \delta(t)$. The reason is that these two systems share the same Laplace domain solution $\mathbf{Y}(s) = C[sI - A]^{-1}\mathbf{x}_0$. In this way, we can transform a system without control to a controlled zero-initial-state system. Kalman decomposition to be introduced later will be more natural in a system with a control term. Hence, we introduce the Laplace transform approach and the STA based on the standard form (9).

In the frequency domain, (8) is now

$$\mathbf{T}(s,\boldsymbol{\theta})\mathbf{U}(s) = \mathbf{T}(s,\theta')\mathbf{U}(s).$$

By cancelling $\mathbf{U}(s)$, (8) is equivalent to

$$\mathbf{T}(s,\boldsymbol{\theta}) = \mathbf{T}(s,\theta') \ \ \forall s. \tag{10}$$

Hence, the transfer function is exactly a tool to characterize identifiability. By writing (10) in a canonical form (e.g., transforming the numerators and denominators into monic polynomials) and equating coefficients on both sides of (10), one obtains a series of algebraic equations in $\boldsymbol{\theta}$ and θ'. If for almost any value of $\boldsymbol{\theta}$, the solutions always satisfy $\theta' = \boldsymbol{\theta}$, then the system is identifiable. In order to investigate identifiability, Sone and Cappellaro [27] employed the Gröbner basis to determine the conditions of identifiability. By directly solving (10), where the RHS is replaced by a specific transfer function reconstructed from experimental data, one can develop algorithms like that in [26] to identify the Hamiltonian.

The following property of the transfer function will be frequently used in the following.

Property 1: When a system undergoes a similarity transformation $\mathbf{x}' = P\mathbf{x}$, where P is a nonsingular matrix, the transfer function remains the same, and thus, the identifiability does not change.

We specifically illustrate *atypical* cases and *hypersurfaces*. Assume that the number of unknown parameters is $\mathcal{M}$, and we have no prior knowledge of the true values, which indicates that the candidate space for the parameters is $\mathbb{R}^{\mathcal{M}}$. A hypersurface is a manifold or an algebraic variety with dimension $\mathcal{M} - 1$, and it is usually obtained by adding an extra polynomial equation about the unknown parameters. Hypersurface sets have Lebesgue measure zero, and they can, thus, be neglected in practice. Atypical cases are subsets of hypersurfaces. Hence, analysis on atypical cases can also be omitted. When the complement of a hypersurface is open and dense in $\mathbb{R}^{\mathcal{M}}$ and has full measure, it is often called a *generic* set [40]. For strictness, the phrase "almost always" is usually employed to indicate that atypical cases have already been neglected. We give an example of atypical cases from the point of view of transfer functions such as [38, Example 3.1]. Consider a system with unknown parameters θ_1 and θ_2 and the transfer function

$$\mathbf{T}(s,\boldsymbol{\theta}) = \frac{\theta_1}{s + \theta_1 + \theta_2}. \tag{11}$$

The algebraic equations from (10) are, thus, $\theta_1 = \theta_1'$ and $\theta_1 + \theta_2 = \theta_1' + \theta_2'$. Therefore, the system (11) is generally identifiable, except the case of $\theta_1 = 0$, which leads to a zero transfer function and erases all the information about θ_2. Since $\theta_1 = 0$ is an atypical case, we can omit it and conclude that this system is (almost always) identifiable. In the rest of this article, we omit "almost always" if there is no ambiguity.

III. Hamiltonian Identifiability via the STA

A. General Procedures for Minimal Systems

Strictly speaking, the word "minimal" is used to describe system realizations that are both controllable and observable. In this article, we call a system "minimal" if it is both controllable and observable.

Let $\boldsymbol{\theta}$ be the true value generating the system (9). Suppose that there is an alternative value θ' generating the same output data. Then, θ' gives an alternative realization

$$\begin{cases} \dot{\mathbf{x}}' = A(\theta')\mathbf{x}' + B(\theta')\mathbf{u}, \ \mathbf{x}'(0) = \mathbf{0} \\ \mathbf{y} = C(\theta')\mathbf{x}' + D(\theta')\mathbf{u}. \end{cases} \tag{12}$$

Suppose that the system realization (9) is minimal. Then, (12) is also minimal, since they have the same dimension. From Kalman's algebraic equivalence theorem [41], minimal realizations of a transfer function are equivalent, i.e., they are related by a similarity transformation

$$\begin{cases} A(\theta) = S^{-1}A(\theta')S \\ B(\boldsymbol{\theta}) = S^{-1}B(\theta') \\ C(\boldsymbol{\theta}) = C(\theta')S \\ D(\boldsymbol{\theta}) = D(\theta') \end{cases} \tag{13}$$

where S is an invertible matrix. We call equations in (13) the *STA equations*. We take S, θ, and θ' as unknown variables and search for their solution. The solvability of (13) can be guaranteed because it always has a trivial solution $S = I$ and $\boldsymbol{\theta} = \theta'$. If all the solutions satisfy $\boldsymbol{\theta} = \theta'$, then the system (9) is identifiable. Otherwise, it is unidentifiable. In cases when the signs of $\boldsymbol{\theta}$ are not considered, one can check whether all the solutions to the STA equations satisfy $|\theta| = |\theta'|$ to determine the identifiability.

B. Nonminimal Systems

If the system is not minimal, Kalman's algebraic equivalence theorem (and hence the STA equations) can only be applied to the controllable and observable part of the system. If one ignores whether the system is minimal or not and directly employs the solution to the STA equations to test the identifiability, an incorrect conclusion might be obtained. For example, consider the following 2-D system.

Example 1:

$$\begin{cases} \dot{\mathbf{x}} = \begin{pmatrix} \theta_1 & 0 \\ 0 & \theta_2 \end{pmatrix} \mathbf{x} + \begin{pmatrix} 1 \\ 0 \end{pmatrix} u, \ \mathbf{x}(0) = \mathbf{0} \\ y = (1 \ \ 0)\mathbf{x}. \end{cases} \tag{14}$$

This system (14) is uncontrollable and unobservable. If one directly solves the STA equations, the conclusion is that it is identifiable. However, since the output y never contains any information about x_2, which evolves independently as $\dot{x}_2 = \theta_2 x_2$, θ_2 is, in fact, unidentifiable.

The fact that (10) is equivalent to (8) in Section II-C means that a linear system's identifiability is uniquely and completely determined by its transfer function. Therefore, unlike in the situation using the STA, nonminimal systems do not introduce extra requirements in the Laplace transform approach.

Regardless of controllability or observability, the transfer function of a system remains the same under similarity transformation. Therefore, for uncontrollable or unobservable systems, the solution using the STA is [33]: i) perform Kalman decomposition and obtain the controllable and observable (minimal) subsystem; ii) write down the STA equations for the minimal subsystem; and iii) the original system is identifiable if and only if the solutions to the STA equations in (ii) all satisfy $\boldsymbol{\theta} = \theta'$.

For Example 1, (14) is already in the Kalman canonical form, and the minimal subsystem is $\dot{x}_1 = \theta_1 x_1 + u, y = x_1$. Hence, θ_1 is identifiable and θ_2 is unidentifiable. This example also implies the following identifiability Criterion 1, which corresponds to the fact in [27] that the parameters that do not appear in the transfer function are unidentifiable.

Criterion 1: Suppose a system is nonminimal. Perform Kalman decomposition to obtain its minimal subsystem and nonminimal subsystem. The unknown parameters that do not appear in the minimal subsystem are unidentifiable.

For a nonminimal system, even if all the unknown parameters appear in the minimal subsystem and the STA equations for the original system (rather than the minimal subsystem) exclude the solutions $\boldsymbol{\theta} \neq \theta'$, it is not sufficient for guaranteeing the identifiability of the original system. A straightforward example can be obtained by substituting θ_1 and θ_2 in Example 1 with $\theta_1 + \theta_2$ and $\theta_1 - \theta_2$, respectively.

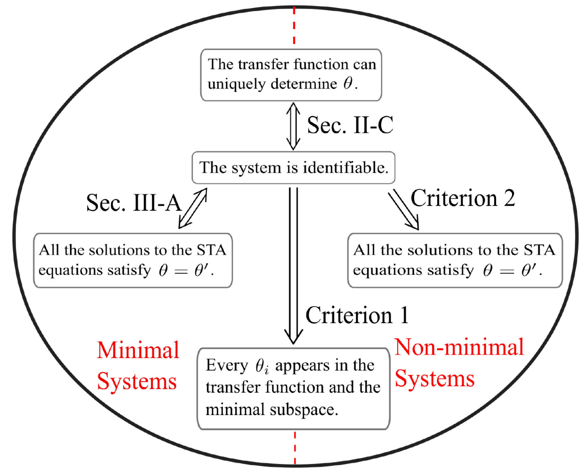

Fig. 1. Relationships between identifiability criteria.

Although it is necessary to analyze the minimality before solving the STA equations in most situations, we find a shortcut for some special cases.

Criterion 2: If the STA equations for a system have a (nonatypical) solution $\boldsymbol{\theta_0} \neq \boldsymbol{\theta_0'}$, the system is unidentifiable regardless of whether it is minimal or not.

For the proof of Criterion 2, we consider two specific realizations $(A(\boldsymbol{\theta_0}), B(\boldsymbol{\theta_0}), C(\boldsymbol{\theta_0}), D(\boldsymbol{\theta_0}))$ and $(A(\boldsymbol{\theta_0'}), B(\boldsymbol{\theta_0'}), C(\boldsymbol{\theta_0'}), D(\boldsymbol{\theta_0'}))$ for the system. According to the form of STA equations (13), these two different (possibly nonminimal) realizations are related by a similarity transformation. Using Property 1, they result in the same transfer function. Therefore, different system parameters are generating the same system model. This means that the system must be unidentifiable, which proves Criterion 2.

As pointed out in [42], the controllability and observability properties are neither sufficient nor necessary for identifiability. Example 1 has shown that nonminimal systems may be unidentifiable. If one replaces θ_2 in the system matrix of (14) with θ_1, then the system becomes identifiable, which indicates that nonminimal systems can also be identifiable.

In Fig. 1, we summarize all the results of Sections III-A and III-B. Note that for nonminimal systems, Criterion 2 is necessary but not sufficient, different from the case for minimal systems.

C. SPT Method

The SPT method is an idea we develop for identifiability analysis in nonminimal systems. Suppose there is a nonminimal system $\Sigma = (A, B, C, D)$ with state vector $\mathbf{x}$. If Criterion 2 fails, traditionally, we have to perform Kalman decomposition. We let $\bar{\mathbf{x}} = P\mathbf{x}$ such that the equivalent system $\bar{\Sigma} = (\bar{A}, \bar{B}, \bar{C}, \bar{D})$ has the Kalman canonical form. Then, we employ the STA equations for its minimal subsystem $\bar{\Sigma}_1 = (\bar{A}_1, \bar{B}_1, \bar{C}_1, \bar{D}_1)$, with the corresponding state vector $\bar{\mathbf{x}}_1$ having a dimension smaller than $\mathbf{x}$.

Quantum systems usually generate clear structure properties in A. These structure properties may be completely disguised in the system $\bar{\Sigma}$, making the STA equations difficult to solve. This problem is seldom investigated in classical control theory, because, classically, one prefers to change the system structure (A, B, C, D) so that the system becomes minimal when faced with such problems. On the contrary, quantum research sometimes investigates the physical capability of a certain fixed system setting, and the initial quantum system states or the observables may be difficult to change. Therefore, changing (A, B, C, D) may not be practical. How can we keep (some of) the structure properties of the original system Σ and meanwhile perform STA analysis?

The idea of SPT is to further perform a similarity transformation on $\bar{\Sigma}$ to recover (some of) the structure properties of Σ, meanwhile preserving the canonically decomposed form. To do this, we let $\tilde{\mathbf{x}} = (\tilde{P}^{-1} \oplus I)\bar{\mathbf{x}}$ and obtain a system $\tilde{\Sigma} = (\tilde{A}, \tilde{B}, \tilde{C}, \tilde{D})$, where $\tilde{P}^{-1}$ acts only on the minimal subsystem $\bar{\Sigma}_1$. Since the second transformation $\tilde{P}^{-1} \oplus I$ is block-diagonal, $\tilde{\Sigma}$ is still in the Kalman canonical form, and the matrices $(\tilde{A}_1, \tilde{B}_1, \tilde{C}_1, \tilde{D}_1)$ are submatrices of those in $\tilde{\Sigma}$, respectively. If $\tilde{P}$ is close to P (in the form/appearance, not in norm), or $\tilde{P}^{-1}$ is close to P^{-1}, then we are likely to regain an $\tilde{A}_1$ similar to A, thus recovering key structure properties. Then, we solve the STA equations for the minimal subsystem $\tilde{\Sigma}_1$ to determine the identifiability.

In the SPT method, $\tilde{P}$ can never be exactly equal to P, because their dimensions are different. The choice of $\tilde{P}$ is not unique and should depend on specific problems. One common choice is to let $\tilde{P}$ be a submatrix of P. An example using the SPT method is provided in Section VI-A.

D. Quantum Hamiltonian Identifiability via the STA

We clarify several points when using the STA for analyzing Hamiltonian identifiability. For simplicity, we only consider single input systems (i.e., the matrix B has only one column), while the result can be straightforwardly extended to multi-input systems. From Remark 1, a quantum system of (6) and (7) with the initial state $\mathbf{x}(0) = \mathbf{x}_0$ is equivalent to the following zero-initial-state system:

$$\begin{cases} \dot{\mathbf{x}} = A\mathbf{x} + Bu, \quad \mathbf{x}(0) = \mathbf{0} \\ \mathbf{y} = C\mathbf{x} \end{cases}$$

where $B = \mathbf{x}_0$ and $u = \delta(t)$.

For a quantum Hamiltonian, $\mathbf{x}_0$ and C are usually determined and A is antisymmetric. We rewrite (13) as

$$SA(\theta) = A(\theta')S \tag{15}$$

$$S\mathbf{x}_0 = \mathbf{x}_0 \tag{16}$$

$$C = CS \tag{17}$$

together with the requirement that S is nonsingular and other possible constraints on θ and θ'. Equations (15)–(17) are the starting point for STA analysis for the rest of this article.

Next, we use the STA to test the identifiability for single-probe-assisted spin-1/2 chain systems in [27], which have the form of a 1-D chain, composed of multiqubits with their interaction governed by the system Hamiltonian. It is usually assumed that only the first qubit (the probe qubit) can be initialized and measured, while the rest qubits are all inaccessible (and thus, they are assumed to be in the maximally mixed state initially). The probe qubit can be used as a quantum sensor, and the identifiability problem is also relevant to the capability evaluation of the quantum sensor. As in [27], we identify only the magnitude of the unknown parameters in the Hamiltonian, i.e., a system is identifiable if and only if all the solutions to the STA equations for the minimal subsystem satisfy $|\theta_i| = |\theta_i'|$. There are four physical models in [27], where the transfer function on the Ising model without transverse field can be directly calculated and we omit the STA analysis for this model. The Ising model with the transverse field can also be skipped, because the system matrix has the same structure as that in the exchange model without transverse field. Hence, we only analyze two exchange models, with and without transverse field. Let $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_n)^T$ be the unknown parameters. We choose $\{H_m\} = \{\sigma_{\alpha_1} \otimes \sigma_{\alpha_2} \otimes \ldots \otimes \sigma_{\alpha_n}\}_{\alpha_i \in \{0,1,2,3\}}$ as the same as those in [26], where $\sigma_0 = I_{2\times 2}$, and Pauli matrices $\sigma_1 = X$, $\sigma_2 = Y$, and $\sigma_3 = Z$. Then, the accessible sets are the same as those in [27] for each of the following cases. For the exchange model without transverse field, $n+1$ is the total qubit number, and the Hamiltonian can be written as

$$H = \sum_{i=1}^{n} \frac{(-1)^{i+1}\theta_i}{2}(X_i X_{i+1} + Y_i Y_{i+1}) \tag{18}$$

where the subscript i denotes the ith qubit, and X and Y are the single-qubit Pauli matrices

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

The observable is X_1 with the initial state being an eigenstate of X_1 (i.e., the system state is $|X_+\rangle\langle X_+| \otimes I/2^n$, where $|X_+\rangle = (1,1)^T/\sqrt{2}$). For the exchange model with transverse field, n must be odd and $\frac{n+1}{2}$ is the total qubit number. The Hamiltonian can be written as

$$H = \sum_{i=1}^{\frac{n+1}{2}} \frac{\theta_{2i-1}}{2} Z_i + \sum_{i=1}^{\frac{n-1}{2}} \frac{\theta_{2i}}{2}(X_i X_{i+1} + Y_i Y_{i+1}) \tag{19}$$

where $Z = \mathrm{diag}(1, -1)$. With the initial state being the eigenstate of X_1, the observable can be X_1 or Y_1. Therefore, there are altogether three situations to be analyzed, which are summarized as Theorems 1–3. These three situations were first investigated in [27] and only verified numerically for several specific cases. Here, we provide a mathematical proof for arbitrary dimension. Also, Theorems 1–3 contain various situations to showcase the power of the STA: Theorems 1 and 3 characterize identifiable minimal systems, while Theorem 2 corresponds to an unidentifiable minimal system. An example of dealing with identifiable nonminimal systems will be presented in Theorem 4.

IV. Exchange Model Without Transverse Field

The Hamiltonian for this spin system is described in [27], which also derives the system model (18). Therefore, we start from the linear system form (9). In the system matrix A, only the elements directly above or below the main diagonal are nonzero:

$$A = \begin{pmatrix} 0 & \theta_1 & 0 & 0 & \cdots \\ -\theta_1 & 0 & \theta_2 & 0 & \cdots \\ 0 & -\theta_2 & 0 & \ddots & \\ 0 & 0 & \ddots & & \theta_n \\ \vdots & \vdots & & -\theta_n & 0 \end{pmatrix}_{(n+1)\times(n+1)}. \tag{20}$$

The initial state of the probe is an eigenstate of X_1. Hence, $B = \mathbf{x}_0 = (1, 0, \ldots, 0)^T$. We measure X_1, and $C = (1, 0, \ldots, 0)$. We have the following theorem.

Theorem 1: The exchange model without transverse field is identifiable when measuring X_1 on the single-qubit probe, with the initial state of the probe in an eigenstate of X_1.

Proof: We first prove this system is minimal for almost any value of the unknown parameters and, then, test the identifiability.

1) Proof for Minimality:

Lemma 1: With (20) and $B = (1, 0, \ldots, 0)^T$, the controllability matrix $\text{CM} = (B, AB, \ldots, A^n B)$ has full rank for almost any value of θ.

The proof of Lemma 1 is provided in Appendix A. Then, given the observability matrix $\text{OM} = (C, CA, \ldots, CA^n)^T = \text{diag}(1, -1, 1, -1, \ldots, (-1)^n) \cdot \text{CM}^T$, the system is also almost always observable. Therefore, it is almost always minimal.

2) Identifiability Test: We now employ the STA equations to test the identifiability. Using (16) and (17), we know that S is of the form

$$S = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & * & \cdots & * \\ \vdots & \vdots & & \vdots \\ 0 & * & \cdots & * \end{pmatrix}_{(n+1)\times(n+1)} \tag{21}$$

and (15) is now

$$\begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & * & \cdots & * \\ \vdots & \vdots & & \vdots \\ 0 & * & \cdots & * \end{pmatrix} \begin{pmatrix} 0 & \theta_1 & 0 & \cdots & 0 \\ -\theta_1 & 0 & \ddots & & \\ 0 & \ddots & & & \\ \vdots & & & & \end{pmatrix}$$

$$= \begin{pmatrix} 0 & \theta_1' & 0 & \cdots & 0 \\ -\theta_1' & 0 & \ddots & & \\ 0 & \ddots & & & \\ \vdots & & & & \end{pmatrix} \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & * & \cdots & * \\ \vdots & \vdots & & \vdots \\ 0 & * & \cdots & * \end{pmatrix}. \tag{22}$$

Denote the partitioned S and A as

$$S = \begin{pmatrix} 1_{1\times 1} & (\mathbf{0}_{n\times 1})^T \\ \mathbf{0}_{n\times 1} & \tilde{S}_{n\times n} \end{pmatrix}, \quad A = \begin{pmatrix} 0_{1\times 1} & (\mathbf{E}_{n\times 1})^T \\ -\mathbf{E}_{n\times 1} & \tilde{A}_{n\times n} \end{pmatrix}.$$

Then, (22) is equivalent to

$$\mathbf{E}^T = \mathbf{E}'^T \tilde{S} \tag{23}$$

$$-\tilde{S}\mathbf{E} = -\mathbf{E}' \tag{24}$$

$$\tilde{S}\tilde{A} = \tilde{A}'\tilde{S}. \tag{25}$$

From the first elements in (23) and (24), we have $\theta_1 = \theta_1' \tilde{S}_{11}$ and $-\tilde{S}_{11}\theta_1 = -\theta_1'$. Since the atypical case of $\theta_1 = 0$ is not considered, we have $\theta_1' \neq 0$ and $|\tilde{S}_{11}| = 1$, which indicates $|\theta_1| = |\theta_1'|$. Then, from the remaining elements in (23) and (24), we have $\tilde{S}_{12} = \tilde{S}_{13} = \cdots = \tilde{S}_{1n} = 0$ and $\tilde{S}_{21} = \tilde{S}_{31} = \cdots = \tilde{S}_{n1} = 0$.

If $\tilde{S}_{11} = 1$, (25) is now of the same form as (22) but with dimension decreased by 1; otherwise, if $\tilde{S}_{11} = -1$, (25) is equivalent to $(-\tilde{S})\tilde{A} = \tilde{A}'(-\tilde{S})$, which is also of the same form as (22) with the dimension decreased by 1. Therefore, these procedures can be performed inductively, and finally, we know all the solutions to (22) satisfy $S = \text{diag}(1, \pm 1, \ldots, \pm 1)$ and $|\theta_i| = |\theta_i'|$ for all $1 \leq i \leq n$. ■

Remark 2: The relevant result in Theorem 1 was also presented in [18], where a specific Hamiltonian identification algorithm for the same system setting was proposed. Here, we use it as an example to illustrate the effectiveness of the STA.

V. Exchange Model With Transverse Field

The Hamiltonian for this system is as in (19), and we start from the linear system form (9). In A, each θ_{2k+1} appears twice and each θ_{2k} appears four times, which is different from (20)

$$A = \begin{pmatrix} 0 & \theta_1 & 0 & -\theta_2 & \cdots \\ -\theta_1 & 0 & \theta_2 & 0 & \cdots \\ 0 & -\theta_2 & 0 & \ddots & \\ \theta_2 & 0 & \ddots & & \theta_n \\ \vdots & \vdots & & -\theta_n & 0 \end{pmatrix}_{(n+1)\times(n+1)} \tag{26}$$

where n must be odd. The initial state of the probe is an eigenstate of X_1. Hence, $B = \mathbf{x}_0 = (1, 0, \ldots, 0)^T$. With Property 1, we can first rearrange A as follows: we take its odd rows in ascending sequence and then take its even rows in ascending sequence, and we apply the same procedures to its columns. We may rewrite A into

$$A = \begin{pmatrix} 0 & \bar{A} \\ -\bar{A} & 0 \end{pmatrix} \tag{27}$$

where

$$\bar{A} = \begin{pmatrix} \theta_1 & -\theta_2 & 0 & \cdots & 0 \\ -\theta_2 & \theta_3 & -\theta_4 & & \vdots \\ 0 & -\theta_4 & \theta_5 & \ddots & 0 \\ \vdots & & \ddots & \ddots & -\theta_{n-1} \\ 0 & \cdots & 0 & -\theta_{n-1} & \theta_n \end{pmatrix} \tag{28}$$

is symmetric. After this transformation, we have $B = (1, 0, \ldots, 0)^T$ unchanged.

A. Measuring X_1

First, we consider measuring X_1. Then, $C = (1, 0, \ldots, 0)$. We have the following conclusion.

Theorem 2: The exchange model with transverse field is unidentifiable when measuring X_1 on the single-qubit probe, with the initial state of the probe in an eigenstate of X_1.

Proof: We employ Criterion 2 to prove the conclusion and, thus, do not need to analyze its minimality. When A in (26) is transformed to (27), C is unchanged, and we assume S is transformed to $\bar{S}$. Now, (16) and (17) imply that $\bar{S}$ is of the same form as (21). We do not need to find all the solutions to (15). Instead, we only need to find a special solution to (15), which gives $|\theta_i| \neq |\theta_i'|$ for some i. We assume

$$\bar{S} = 1_{1\times 1} \oplus N_{\frac{n-1}{2}\times\frac{n-1}{2}} \oplus M_{\frac{n+1}{2}\times\frac{n+1}{2}}$$

which satisfies the form (21). Now, (15) is

$$\begin{pmatrix} 1 & & \\ & N & \\ & & M \end{pmatrix} \begin{pmatrix} & \bar{A} \\ -\bar{A} & \end{pmatrix} = \begin{pmatrix} & \bar{A}' \\ -\bar{A}' & \end{pmatrix} \begin{pmatrix} 1 & & \\ & N & \\ & & M \end{pmatrix}. \qquad (29)$$

We further assume that N and M are orthogonal, which guarantees that $\bar{S}$ is nonsingular, and now, (29) is in essence only one equation

$$\begin{pmatrix} 1 & \\ & N \end{pmatrix} \bar{A} M^T = \bar{A}'. \qquad (30)$$

We perform spectral decomposition on $\bar{A}$ to have $\bar{A} = PEP^T$, where P is orthogonal and E is diagonal. We have the following lemma (the proof is given in Appendix B) to exclude the atypical cases.

Lemma 2: Given arbitrary $\lambda_0 \in \mathbb{C}$, it is atypical that $\lambda_0 \in \Lambda(\bar{A})$.

Lemma 2 is nontrivial. For example, if we change the structure of $\bar{A}$ as $\left(\begin{smallmatrix} \theta_1 & \theta_2 \\ \theta_1 & \theta_2 \end{smallmatrix}\right)$, then it is always true that $0 \in \Lambda(\bar{A})$.

Denote $\mathbb{I}_k = \mathrm{diag}(1, \ldots, 1, -1, 1, \ldots, 1)$, where only the kth element is -1. We have the following assertion.

Lemma 3: There is at least one $k \in \{1, 2, \ldots, n\}$ such that $|\theta_1| \neq |(PE\mathbb{I}_k P^T)_{11}|$.

The proof of Lemma 3 is given in Appendix C. Using Lemma 3, suppose $|\theta_1| \neq |(PE\mathbb{I}_m P^T)_{11}|$. We let

$$M^T = P\mathbb{I}_m P^T \begin{pmatrix} 1 & \\ & N^T \end{pmatrix}.$$

As long as N is orthogonal, M is orthogonal. We denote the LHS of (30) as $\bar{L}$ and have

$$\begin{aligned} \bar{L} &= \begin{pmatrix} 1 & \\ & N \end{pmatrix} \bar{A} M^T \\ &= \begin{pmatrix} 1 & \\ & N \end{pmatrix} PEP^T P\mathbb{I}_m P^T \begin{pmatrix} 1 & \\ & N^T \end{pmatrix} \\ &= \begin{pmatrix} 1 & \\ & N \end{pmatrix} PE\mathbb{I}_m P^T \begin{pmatrix} 1 & \\ & N^T \end{pmatrix}. \end{aligned} \qquad (31)$$

We, thus, know

$$\begin{aligned} |\bar{L}_{11}| &= \left| I_{1\sigma} \begin{pmatrix} 1 & \\ & N \end{pmatrix} PE\mathbb{I}_m P^T \begin{pmatrix} 1 & \\ & N^T \end{pmatrix} I_{\sigma 1} \right| \\ &= |I_{1\sigma} PE\mathbb{I}_m P^T I_{\sigma 1}| = |(PE\mathbb{I}_m P^T)_{11}| \neq |\theta_1|. \end{aligned}$$

From (31), we know that $\bar{L}$ is always symmetric. Then, we only need to find an appropriate orthogonal N to make $\bar{L}$ have the same positions of zeros as $\bar{A}$. Denote $Z = PE\mathbb{I}_m P^T$, which is symmetric. We design a series of orthogonal matrices $N^{(1)}_{\frac{n-1}{2}\times\frac{n-1}{2}}, N^{(2)}_{\frac{n-3}{2}\times\frac{n-3}{2}}, \ldots, N^{(\frac{n-3}{2})}_{2\times 2}$ such that

$$N = \begin{pmatrix} I_{\frac{n-5}{2}\times\frac{n-5}{2}} & \\ & N^{(\frac{n-3}{2})} \end{pmatrix} \cdots \begin{pmatrix} I_{1\times 1} & \\ & N^{(2)} \end{pmatrix} N^{(1)}.$$

We further denote a series of $\frac{n+1}{2}$-dimensional matrices $Z^{(1)}, Z^{(2)}, \ldots, Z^{(\frac{n-3}{2})}$ such that

$$Z^{(1)} = \begin{pmatrix} 1 & \\ & N^{(1)} \end{pmatrix} Z \begin{pmatrix} 1 & \\ & [N^{(1)}]^T \end{pmatrix} \qquad (32)$$

and $Z^{(i+1)} = (I_{i+1} \oplus N^{(i+1)}) Z^{(i)} (I_{i+1} \oplus [N^{(i+1)}]^T)$ for $1 \leq i \leq \frac{n-5}{2}$. Then, $Z^{(\frac{n-3}{2})} = \bar{L}$. We start from the innermost layer (32).

We partition Z as

$$Z = \begin{pmatrix} Z_{11} & J_{1\times\frac{n-1}{2}} \\ (J_{1\times\frac{n-1}{2}})^T & \mathcal{J}_{\frac{n-1}{2}\times\frac{n-1}{2}} \end{pmatrix}$$

and have

$$Z^{(1)} = \begin{pmatrix} Z_{11} & J[N^{(1)}]^T \\ N^{(1)} J^T & N^{(1)} \mathcal{J} [N^{(1)}]^T \end{pmatrix}. \qquad (33)$$

In (33), Z_{11} is unchanged, and we need to make $J[N^{(1)}]^T$ have the form

$$J[N^{(1)}]^T = (*, 0, \ldots, 0). \qquad (34)$$

We perform spectral decomposition to set

$$J^T J = U^{(1)} \mathrm{diag}(*, 0, \ldots, 0) [U^{(1)}]^T.$$

Then, $N^{(1)} = [U^{(1)}]^T$ is orthogonal and (34) holds.

For the next layer, we partition $Z^{(1)}$ as

$$Z^{(1)} = \begin{pmatrix} Z_{11} & * & 0_{1\times\frac{n-3}{2}} \\ * & * & K_{1\times\frac{n-3}{2}} \\ 0_{\frac{n-3}{2}\times 1} & (K_{1\times\frac{n-3}{2}})^T & \mathcal{K}_{\frac{n-3}{2}\times\frac{n-3}{2}} \end{pmatrix}.$$

We then have

$$\begin{aligned} Z^{(2)} &= \begin{pmatrix} 1 & & \\ & 1 & \\ & & N^{(2)} \end{pmatrix} Z^{(1)} \begin{pmatrix} 1 & & \\ & 1 & \\ & & [N^{(2)}]^T \end{pmatrix} \\ &= \begin{pmatrix} Z_{11} & * & 0_{1\times\frac{n-3}{2}} \\ * & * & K[N^{(2)}]^T \\ 0_{\frac{n-3}{2}\times 1} & N^{(2)} K^T & N^{(2)} \mathcal{K} [N^{(2)}]^T \end{pmatrix}. \end{aligned}$$

Z_{11} is unchanged, and we need to make $K[N^{(2)}]^T$ take the form

$$K[N^{(2)}]^T = (*, 0, \ldots, 0).$$

We perform spectral decomposition to make

$$K^T K = U^{(2)} \mathrm{diag}(*, 0, \ldots, 0) [U^{(2)}]^T$$

and then $N^{(2)} = [U^{(2)}]^T$ is what we need. Continuing the above procedure, we can finally determine an orthogonal N such that $\bar{L} = Z^{(\frac{n-3}{2})}$ has the same structure as $\bar{A}$. Since Z_{11} is unchanged and $|Z_{11}| \neq |\theta_1|$, we know that $|\bar{L}_{11}| \neq |\theta_1|$, which implies that we have found a special unequal solution to the STA equations. Thus, the system is unidentifiable. ■

B. Measuring Y_1

Now, we consider measuring Y_1, which sets $C = (0, 1, 0, \ldots, 0)$. We have the following theorem to correct the conclusion in [27].

Theorem 3: The exchange model with transverse field is identifiable when measuring Y_1 on the single-qubit probe, with the initial state of the probe in an eigenstate of X_1.

Proof:

1) Proof for Minimality: After A in (26) is transformed to (27), C is transformed to

$$C = (0_{1\times\frac{n+1}{2}}, \bar{C}), \;\; \bar{C} = (1, 0_{1\times\frac{n-1}{2}}). \tag{35}$$

Denote

$$B = (\bar{B}^T, 0_{1\times\frac{n+1}{2}})^T, \;\; \bar{B} = (1, 0_{1\times\frac{n-1}{2}})^T. \tag{36}$$

We have the following lemma (the proof is given in Appendix B) to show that the system is minimal.

Lemma 4: With (27), (28), (35), and (36), both the controllability matrix $\mathrm{CM} = [B, AB, \ldots, A^n B]$ and the observability matrix $\mathrm{OM} = [C^T, A^T C^T, \ldots, A^{nT} C^T]^T$ have full rank for almost any value of $\boldsymbol{\theta}$.

2) Identifiability Test: By Property 1, we use the STA to prove that the system (27) and (28) is identifiable with (35) and (36). We partition S as

$$S = \begin{pmatrix} X_{\frac{n+1}{2}\times\frac{n+1}{2}} & *_{\frac{n+1}{2}\times\frac{n+1}{2}} \\ \frac{n+1}{2}\times\frac{n+1}{2} & Y_{\frac{n+1}{2}\times\frac{n+1}{2}} \end{pmatrix}.$$

Then, (15) is

$$\begin{pmatrix} X & * \\ & Y \end{pmatrix} \begin{pmatrix} 0 & \bar{A} \\ -\bar{A} & 0 \end{pmatrix} = \begin{pmatrix} 0 & \bar{A}' \\ -\bar{A}' & 0 \end{pmatrix} \begin{pmatrix} X & * \\ & Y \end{pmatrix} \tag{37}$$

which is

$$X\bar{A} = \bar{A}'Y \tag{38}$$

$$Y\bar{A} = \bar{A}'X \tag{39}$$

where the other two equations on the indeterminate submatrices are omitted. Using (16) and (17), we have

$$X_{\sigma 1} = (1, 0, \ldots, 0)^T, \;\; Y_{1\sigma} = (1, 0, \ldots, 0). \tag{40}$$

From (38) and (39), we have

$$X^T X\bar{A} = X^T \bar{A}'Y = \bar{A}Y^T Y \tag{41}$$

$$Y^T Y\bar{A} = Y^T \bar{A}'X = \bar{A}X^T X. \tag{42}$$

From (41) and (42), the following relationship holds:

$$\left(X^T X - Y^T Y\right)\bar{A} = -\bar{A}\left(X^T X - Y^T Y\right) \tag{43}$$

which is a special form of Sylvester equation. We rephrase the general solving procedures for the Sylvester equation [43] to solve (43). Considering that $\bar{A}$ is a symmetric matrix, as shown in (28), we vectorize (43) to have

$$\left(\bar{A} \otimes I_{\frac{n+1}{2}} + I_{\frac{n+1}{2}} \otimes \bar{A}\right) \mathrm{vec}\left(X^T X - Y^T Y\right) = 0.$$

Using the same idea in Appendixes B and D, it is straightforward to prove that $\bar{A} \otimes I + I \otimes \bar{A}$ is almost always nonsingular by considering $\bar{A} = I$. An equivalent expression is that we almost always have

$$\lambda_i(\bar{A}) + \lambda_j(\bar{A}) \neq 0 \tag{44}$$

for any $1 \leq i, j \leq \frac{n+1}{2}$. Therefore, we can almost always have

$$X^T X = Y^T Y. \tag{45}$$

Similarly, we have

$$\left(XX^T - YY^T\right)\bar{A}' = -\bar{A}'(XX^T - YY^T)$$

and thus

$$\left(\bar{A}' \otimes I_{\frac{n+1}{2}} + I_{\frac{n+1}{2}} \otimes \bar{A}'\right) \mathrm{vec}\left(XX^T - YY^T\right) = 0. \tag{46}$$

Lemma 5: With (27), (28), and (37), $\bar{A}' \otimes I_{\frac{n+1}{2}} + I_{\frac{n+1}{2}} \otimes \bar{A}'$ is almost always nonsingular.

The proof of Lemma 5 is provided in Appendix E. With Lemma 5, we can almost always solve (46) to have

$$XX^T = YY^T. \tag{47}$$

Considering (40), we partition X and Y as

$$X = \begin{pmatrix} 1_{1\times 1} & E_{1\times\frac{n-1}{2}} \\ 0_{\frac{n-1}{2}\times 1} & \tilde{X}_{\frac{n-1}{2}\times\frac{n-1}{2}} \end{pmatrix}, \;\; Y = \begin{pmatrix} 1_{1\times 1} & 0_{1\times\frac{n-1}{2}} \\ F_{\frac{n-1}{2}\times 1} & \tilde{Y}_{\frac{n-1}{2}\times\frac{n-1}{2}} \end{pmatrix}.$$

From (45), $(X^T X)_{11} = 1 = (Y^T Y)_{11} = 1 + F^T F$, which means $F = 0$. Similarly, from (47), we have $E = 0$. We partition $\bar{A}$ as

$$\bar{A} = \begin{pmatrix} \theta_1 & G_{1\times\frac{n-1}{2}} \\ \left(G_{1\times\frac{n-1}{2}}\right)^T & \tilde{A}_{\frac{n-1}{2}\times\frac{n-1}{2}} \end{pmatrix}.$$

Then, (38) is

$$\begin{pmatrix} 1 & 0 \\ 0 & \tilde{X} \end{pmatrix} \begin{pmatrix} \theta_1 & G \\ G^T & \tilde{A} \end{pmatrix} = \begin{pmatrix} \theta_1' & G' \\ G'^T & \tilde{A}' \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & \tilde{Y} \end{pmatrix}$$

which implies $\theta_1 = \theta_1'$

$$G = G'\tilde{Y} \tag{48}$$

$$\tilde{X}G^T = G'^T \tag{49}$$

$$\tilde{X}\tilde{A} = \tilde{A}'\tilde{Y}. \tag{50}$$

Equation (48) is $(-\theta_2, 0, \ldots, 0) = (-\theta_2', 0, \ldots, 0)\tilde{Y}$, which implies that $\tilde{Y}_{1\sigma} = (\theta_2/\theta_2', 0, \ldots, 0)$. Similarly, (49) gives $\tilde{X}_{\sigma 1} = (\theta_2'/\theta_2, 0, \ldots, 0)^T$. With similar procedures, (39) gives $\tilde{X}_{1\sigma} = (\theta_2/\theta_2', 0, \ldots, 0)$, $\tilde{Y}_{\sigma 1} = (\theta_2'/\theta_2, 0, \ldots, 0)^T$, and

$$\tilde{Y}\tilde{A} = \tilde{A}'\tilde{X}. \tag{51}$$

Equating $\tilde{X}_{11}$ (or $\tilde{Y}_{11}$), we find $|\theta_2| = |\theta_2'|$. If $\theta_2 = \theta_2'$, we have

$$\tilde{Y}_{1\sigma} = (1, 0, \ldots, 0) = (\tilde{X}_{\sigma 1})^T. \tag{52}$$

Now, (50)–(52) have the same structures as (38)–(40), respectively, while with the dimension decreased by 1. If $\theta_2 = -\theta_2'$, we have $-\tilde{Y}_{1\sigma} = (1, 0, \ldots, 0) = (-\tilde{X}_{\sigma 1})^T$, and we can rewrite (50) and (51) as $(-\tilde{X})\tilde{A} = \tilde{A}'(-\tilde{Y})$ and $(-\tilde{Y})\tilde{A} = \tilde{A}'(-\tilde{X})$. Therefore, either $\{\tilde{X}, \tilde{Y}, \tilde{A}, \tilde{A}'\}$ or $\{-\tilde{X}, -\tilde{Y}, \tilde{A}, \tilde{A}'\}$ have the same structure and property as $\{X, Y, \bar{A}, \bar{A}'\}$, but with the dimension decreased by 1. This procedure can, thus, be performed recursively, until we finally reach $X = Y = \text{diag}(1, \pm 1, \ldots, \pm 1)$ and $|\theta_i| = |\theta_i'|$ for every $1 \le i \le n$. ∎

Remark 3: Theorems 2 and 3 indicate that when the system matrix A has periodically repeated structure properties, STA analysis can avoid the curse of dimensionality and provide identifiability results for arbitrary dimension. It is worth mentioning that the STA analysis is not limited to spin chain systems, but is also applicable to general closed quantum systems, as exemplified in Section VI.

VI. Economic Quantum Hamiltonian Identification Algorithms

If a system is identifiable, we may develop an appropriate identification algorithm to identify the parameters. In this section, we provide another application of the STA and SPT to quantum Hamiltonian identification. Generally, the dimension of a quantum system is exponential in the number of qubits. Hence, identification algorithms that have polynomial complexity in the system dimension will in essence have exponential computational complexity in the number of qubits, which has been referred to as the exponential problem, one of the central problems in quantum research [1]. To avoid this problem, one method is to design identification algorithms with computational complexity directly depending on quantities that increase much slower than the system dimension. Typically, such quantities include the number of qubits in multiqubit systems, or the number of unknown parameters for special physical systems (in which case the corresponding algorithms are referred to as "economic" ones in this article). The STA can be a useful tool to indicate the existence of such economic algorithms.

A. Indicator for the Existence of Economic Identification Algorithms

We aim to design an identification algorithm that has computational complexity that only depends on the number of unknown parameters. Suppose that we have a d-dimensional Hamiltonian H with $\mathcal{M}$ unknown parameters θ_i. In most cases, the a_is in (2) are linear functions of θ_i. Hence, we can expand H directly using $\boldsymbol{\theta}$, $H = \sum_{i=1}^{\mathcal{M}} \theta_i H_i$. Using the procedures in Section II-B, we can model the evolution of the state as an n-dimensional linear system model

$$\dot{\mathbf{x}} = A\mathbf{x}, \quad \mathbf{x}(0) = \mathbf{x_0} \tag{53}$$

where the elements of A are linear combinations of θ_i. Without loss of generality, the identification of all θ_i is equivalent to identifying certain $\mathcal{M}$ elements of A. We hope that the algorithm can identify one unknown element in A under one set of B and C, with computational complexity $f(\mathcal{M})$ that is a function of $\mathcal{M}$ but not of d. Then, the total computational complexity to identify the Hamiltonian is $\mathcal{M}f(\mathcal{M})$, which does not directly depend on d.

We start by investigating the identification capability of the fundamental setting of $B = I_{\sigma i}$ and $C = I_{j\sigma}$. By changing indices, we assume that $B = I_{\sigma 2}$ and $C = I_{1\sigma}$. In the most general case, there are no special properties for the structure of A. Assume that this system (A, B, C) is already minimal. Then, from (16) and (17), we know that the transformation matrix S is

$$S = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ * & 1 & * & \cdots & * \\ * & 0 & * & \cdots & * \\ \vdots & \vdots & \vdots & & \vdots \\ * & 0 & * & \cdots & * \end{pmatrix}$$

and (15) is now

$$\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ * & 1 & * & \cdots & * \\ * & 0 & * & \cdots & * \\ \vdots & \vdots & \vdots & & \vdots \\ * & 0 & * & \cdots & * \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \cdots \\ \vdots & \vdots & \end{pmatrix} = \begin{pmatrix} A_{11}' & A_{12}' & \cdots \\ A_{21}' & A_{22}' & \cdots \\ \vdots & \vdots & \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ * & 1 & * & \cdots & * \\ * & 0 & * & \cdots & * \\ \vdots & \vdots & \vdots & & \vdots \\ * & 0 & * & \cdots & * \end{pmatrix}. \tag{54}$$

By equating the elements on the first row and second column of both sides of (54), we have $A_{12} = A_{12}'$, which indicates this fundamental setting of B and C has the capability of identifying one parameter for minimal systems. Interestingly, we succeed in extending this conclusion to nonminimal systems using the STA.

Theorem 4: Given a linear system (A, B, C), A_{ij} is identifiable (including its sign) if $B = I_{\sigma j}$ and $C = I_{i\sigma}$.

Proof: Without loss of generality, we can always assume that we are identifying A_{12} or A_{11} after appropriately changing the element order of $\mathbf{x}$.

For the case of identifying A_{12}, $C = (1, 0, \ldots, 0)$ and $B = (0, 1, 0, \ldots, 0)^T$. Without loss of generality, we assume that the system is neither controllable nor observable. We tentatively calculate the first two rows of the observability matrix, which are

$$\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ * & A_{12} & * & \cdots & * \end{pmatrix}. \tag{55}$$

Since $A_{12} = 0$ is atypical, it is almost always true that (55) has rank 2. Assume that the observable subsystem of (53) has dimension m. We, thus, have $2 \le m < n$.

Let

$$T = \begin{pmatrix} 1 & & & & & \\ & 1 & & & & \\ -A_{32}/A_{12} & & 1 & & & \\ -A_{42}/A_{12} & & & 1 & & \\ \vdots & & & & \ddots & \\ -A_{n2}/A_{12} & & & & & 1 \end{pmatrix}_{n\times n}$$

and perform a similarity transformation $\bar{\mathbf{x}} = T\mathbf{x}$. Using Property 1, the equivalent system is

$$\bar{A} = TAT^{-1} = \begin{pmatrix} * & A_{12} & * & \cdots & * \\ * & * & * & \cdots & * \\ * & 0 & * & \cdots & * \\ \vdots & \vdots & \vdots & & \vdots \\ * & 0 & * & \cdots & * \end{pmatrix}$$

$\bar{B} = TB = (0, 1, 0, \ldots, 0)^T$ and $\bar{C} = CT^{-1} = (1, 0, \ldots, 0)$. The former two rows in the observability matrix $\overline{\text{OM}}$ of the new system $(\bar{A}, \bar{B}, \bar{C})$ have the same form as (55). Since $\overline{\text{OM}}$ has rank m, there exists a reordering $(j_3, j_4, \ldots, j_n)$ of $(3, 4, \ldots, n)$ such that the matrix $(\overline{\text{OM}}_{\sigma 1}, \overline{\text{OM}}_{\sigma 2}, \overline{\text{OM}}_{\sigma j_3}, \overline{\text{OM}}_{\sigma j_4}, \ldots, \overline{\text{OM}}_{\sigma j_m})$ is column full ranked. Let the matrix $U = (I_{\sigma 1}, I_{\sigma 2}, I_{\sigma j_3}, I_{\sigma j_4}, \ldots, I_{\sigma j_n})^{-1}$ and perform a further similarity transformation $\tilde{\mathbf{x}} = U\bar{\mathbf{x}}$. Then, the equivalent system is

$$\tilde{A} = U\bar{A}U^{-1} = \begin{pmatrix} * & A_{12} & * & \cdots & * \\ * & * & * & \cdots & * \\ * & 0 & * & \cdots & * \\ \vdots & \vdots & \vdots & & \vdots \\ * & 0 & * & \cdots & * \end{pmatrix}_{n\times n} \quad (56)$$

$\tilde{B} = U\bar{B} = (0, 1, 0, \ldots, 0)^T$ and $\tilde{C} = \bar{C}U^{-1} = (1, 0, \ldots, 0)$. Now, the observability matrix of the system $\tilde{\Sigma} = (\tilde{A}, \tilde{B}, \tilde{C})$ is

$$\widetilde{\text{OM}} = \begin{pmatrix} \tilde{C} \\ \tilde{C}\tilde{A} \\ \vdots \\ \tilde{C}\tilde{A}^{n-1} \end{pmatrix} = \begin{pmatrix} \bar{C}U^{-1} \\ \bar{C}\bar{A}U^{-1} \\ \vdots \\ \bar{C}\bar{A}^{n-1}U^{-1} \end{pmatrix} = \overline{\text{OM}} \cdot U^{-1}.$$

Therefore, the first m columns of $\widetilde{\text{OM}}$ are of full rank. We can now employ the SPT method. To perform observability decomposition for the system $\tilde{\Sigma}$, first, we select the first two rows and other $m-2$ rows from $\widetilde{\text{OM}}$ to form a full-row-rank matrix $\tilde{E}_{m\times n}$ such that the former m columns of $\tilde{E}$ are also full rank. We partition $\tilde{E}$ as $\tilde{E} = [\tilde{F}_{m\times m}\ \mathbf{f}_{m\times(n-m)}]$, and then, $\tilde{F}$ is invertible. The transformation matrix $\left(\begin{smallmatrix} \tilde{F} & \mathbf{f} \\ \mathbf{0} & I \end{smallmatrix}\right)$ can decompose the system $\tilde{\Sigma}$ into observable and unobservable parts. We choose the second transformation matrix as $\tilde{F}^{-1} \oplus I$. The total transformation is

$$Q = \begin{pmatrix} \tilde{F}^{-1} & \mathbf{0} \\ \mathbf{0}^T & I \end{pmatrix} \begin{pmatrix} \tilde{F} & \mathbf{f} \\ \mathbf{0}^T & I \end{pmatrix} = \begin{pmatrix} I & \tilde{F}^{-1}\mathbf{f} \\ \mathbf{0}^T & I \end{pmatrix}$$

and its inversion is

$$Q^{-1} = \begin{pmatrix} I & -\tilde{F}^{-1}\mathbf{f} \\ \mathbf{0}^T & I \end{pmatrix}.$$

Let $\acute{\mathbf{x}} = Q\tilde{\mathbf{x}}$ generate the system $\acute{\Sigma} = (\acute{A}, \acute{B}, \acute{C})$:

$$\begin{cases} \dot{\acute{\mathbf{x}}} = \acute{A}\acute{\mathbf{x}} + \acute{B}\delta(t), \ \acute{\mathbf{x}}(0) = \mathbf{0} \\ y = \acute{C}\bar{\mathbf{x}}. \end{cases}$$

We partition $\tilde{A}$ as

$$\tilde{A} = \begin{pmatrix} \widetilde{UL}_{m\times m} & \widetilde{UR}_{m\times(n-m)} \\ \widetilde{DL}_{(n-m)\times m} & \widetilde{DR}_{(n-m)\times(n-m)} \end{pmatrix}.$$

Then, we have

$$\acute{A} = Q\tilde{A}Q^{-1} = \begin{pmatrix} I & \tilde{F}^{-1}\mathbf{f} \\ \mathbf{0}^T & I \end{pmatrix} \begin{pmatrix} \widetilde{UL} & \widetilde{UR} \\ \widetilde{DL} & \widetilde{DR} \end{pmatrix} \begin{pmatrix} I & -\tilde{F}^{-1}\mathbf{f} \\ \mathbf{0}^T & I \end{pmatrix}$$

$$= \begin{pmatrix} \widetilde{UL} + \tilde{F}^{-1}\mathbf{f}\widetilde{DL} & *_{m\times(n-m)} \\ _{(n-m)\times m} & *_{(n-m)\times(n-m)} \end{pmatrix}$$

$\acute{B} = Q\tilde{B} = (0, 1, 0, \ldots, 0)^T$ and $\acute{C} = \tilde{C}Q^{-1} = (1, \underbrace{0, \ldots, 0}_{m-1}, *, \ldots, *)$. We partition $\acute{\mathbf{x}} = (\grave{\mathbf{x}}^T, *)^T$, where $\grave{\mathbf{x}}$ is m-dimensional. Since the second transformation $\tilde{F}^{-1} \oplus I$ is block-diagonal, we know $\acute{\Sigma}$ is in the observable canonical form. Therefore, $\grave{\mathbf{x}}$ corresponds to the observable subsystem of $\acute{\Sigma}$. We denote this m-dimensional observable subsystem as $\grave{\Sigma} = (\grave{A}, \grave{B}, \grave{C})$ where $\grave{A} = \widetilde{UL} + \tilde{F}^{-1}\mathbf{f}\widetilde{DL}$, $\grave{B} = (0, 1, 0, \ldots, 0)^T$ and $\grave{C} = (1, 0, \ldots, 0)$. From (56), we know $\widetilde{DL}_{\sigma 2} = (0, 0, \ldots, 0)^T$, and $\grave{A}_{\sigma 2} = \widetilde{UL}_{\sigma 2}$. Therefore, $\grave{A}_{12} = A_{12}$.

Similarly, we can employ the SPT method again to perform a controllability decomposition on $\grave{\Sigma}$ to finally obtain a t-dimensional $(2 \le t \le m)$ minimal system $(\check{A}, \check{B}, \check{C})$, where we still have $\check{A}_{12} = A_{12}$, $\check{B} = (0, 1, 0, \ldots, 0)^T$ and $\check{C} = (1, 0, \ldots, 0)$.

For $(\check{A}, \check{B}, \check{C})$, we can employ the STA method. Using (16) and (17), we know the transformation matrix S is

$$S = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ * & 1 & * & \cdots & * \\ * & 0 & * & \cdots & * \\ \vdots & \vdots & \vdots & & \vdots \\ * & 0 & * & \cdots & * \end{pmatrix}_{t\times t}$$

and (15) is now

$$\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ * & 1 & * & \cdots & * \\ * & 0 & * & \cdots & * \\ \vdots & \vdots & \vdots & & \vdots \\ * & 0 & * & \cdots & * \end{pmatrix} \begin{pmatrix} * & A_{12} & * & \cdots & * \\ * & * & * & \cdots & * \\ \vdots & \vdots & \vdots & & \vdots \\ * & * & * & \cdots & * \end{pmatrix}$$

$$= \begin{pmatrix} * & A'_{12} & * & \cdots & * \\ * & * & * & \cdots & * \\ \vdots & \vdots & \vdots & & \vdots \\ * & * & * & \cdots & * \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ * & 1 & * & \cdots & * \\ * & 0 & * & \cdots & * \\ \vdots & \vdots & \vdots & & \vdots \\ * & 0 & * & \cdots & * \end{pmatrix}. \quad (57)$$

Equating the elements on the first row and second column of both sides of (57), we have $A_{12} = A'_{12}$. Thus, A_{12} is identifiable.

For the case identifying A_{11}, $B^T = C = (1, 0, \dots, 0)$. Its observability matrix is now

$$\mathrm{OM} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ A_{11} & * & \cdots & * \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix}.$$

If $\mathrm{OM}_{2\sigma}$ has nonzero elements other than A_{11}, then the former two rows of OM are linearly independent, and we can use similar procedures to the case of identifying A_{12} to prove that A_{11} is identifiable. Otherwise, if $\mathrm{OM}_{2\sigma} = (A_{11}, 0, \dots, 0)$, then $A_{1\sigma} = (A_{11}, 0, \dots, 0)$, which means (A, B, C) now is already of the observable canonical form, where the observable subsystem is 1-D:

$$\begin{cases} \dot{x}_1 = A_{11}x_1 + 1 \cdot \delta(t), \ x_1(0) = 0 \\ y = 1 \cdot x_1. \end{cases}$$

Hence, A_{11} is certainly identifiable, which completes the proof. ■

Remark 4: Note that Theorem 4 provides a sufficient condition for identifiability. In Theorem 4, we assume that we have the capability to set $B = I_{\sigma j}$ and $C = I_{i\sigma}$. This assumption on the system setting depends on the specific requirement. For example, if one is not interested in any elements in $A_{3\sigma}$ (even if there are indeed some unknown parameters in the third row of A), then we do not require the ability to set $C = I_{3\sigma}$.

B. Economic Hamiltonian Identification Algorithm

Theorem 4 indicates the existence of economic quantum Hamiltonian identification algorithms. A natural following question is whether we can develop an economic algorithm. In fact, the proof of Theorem 4 has already implied how to prepare the initial state of the system and select the observable. Here, we present an identification algorithm based on the Taylor expansion of matrix exponential function [44].

We start from the system (53) that has a solution $y(t) = Ce^{At}\mathbf{x_0}$. We assume that in actual experiments, we can sample the system output with a fixed period of time Δt, and the data length is $\mathcal{N}$. Then, the data we obtain are denoted as $D = (y(\Delta t), y(2\Delta t), \dots, y(\mathcal{N}\Delta t))^T$ and its ith element is $D_i = y(i\Delta t)$. To estimate A_{jk}, we prepare the system initial value in a state corresponding to $B = \mathbf{x_0} = I_{\sigma k}$ and measure the observable corresponding to $C = I_{j\sigma}$.

We rewrite the data as

$$\begin{aligned} D_p = Ce^{pA\Delta t}B &= \sum_{r=0}^{\infty} \frac{p^r \Delta t^r}{r!} I_{j\sigma} A^r I_{\sigma k} \\ &= \delta_{jk} + \sum_{r=1}^{\infty} \frac{p^r \Delta t^r}{r!} (A^r)_{jk} \approx \delta_{jk} + \sum_{r=1}^{q} \frac{p^r \Delta t^r}{r!} (A^r)_{jk} \end{aligned}$$

where we should choose $q \le \mathcal{N}$.

Denote $w = \mathcal{N}||\mathrm{A}||\Delta te$ and $z = 1 + \max(\lfloor w \rfloor, q)$ for simplicity. We bound the truncated terms as

$$\begin{aligned} &\left| \sum_{r=q+1}^{\infty} \frac{p^r \Delta t^r}{r!} (\mathrm{A}^r)_{jk} \right| \\ &\le \sum_{r=q+1}^{\infty} \left| \frac{1}{\sqrt{2\pi r}} \frac{(p\Delta te)^r}{r^r} (\mathrm{A}^r)_{jk} \right| \\ &= \sum_{r=q+1}^{\infty} \frac{1}{\sqrt{2\pi r}} \left(\frac{p\Delta te}{r} \right)^r |I_{j\sigma} \mathrm{A}^r I_{\sigma k}| \\ &\le \sum_{r=q+1}^{\infty} \frac{1}{\sqrt{2\pi r}} \left(\frac{p\Delta te}{r} \right)^r ||I_{j\sigma}|| \cdot ||\mathrm{A}||^r \cdot ||I_{\sigma k}|| \\ &= \sum_{r=q+1}^{\infty} \frac{1}{\sqrt{2\pi r}} \left(\frac{p||\mathrm{A}||\Delta te}{r} \right)^r \\ &\le \frac{1}{\sqrt{2\pi(q+1)}} \sum_{r=q+1}^{\infty} \left(\frac{w}{r} \right)^r \\ &\le \frac{1}{\sqrt{2\pi(q+1)}} \sum_{r=q+1}^{z-1} \left(\frac{w}{r} \right)^r + \frac{1}{\sqrt{2\pi(q+1)}} \sum_{r=z}^{\infty} \left(\frac{w}{z} \right)^r \\ &= \frac{1}{\sqrt{2\pi(q+1)}} \sum_{r=q+1}^{z-1} \left(\frac{w}{r} \right)^r + \frac{\left(\frac{w}{z}\right)^z}{\sqrt{2\pi(q+1)}(1 - \frac{w}{z})} \end{aligned}$$

where the first line comes from Stirling's approximation. Hence, the summation of the truncated items is never divergent.

Denote $\Psi^{(q)} = (\psi_1, \psi_2, \dots, \psi_q)^T$ where $\psi_i = (A^i)_{jk}$. Then, we need to identify $A_{jk} = \psi_1$. Denote

$$L = \begin{pmatrix} \frac{1^1 \Delta t^1}{1!} & \frac{1^2 \Delta t^2}{2!} & \cdots & \frac{1^q \Delta t^q}{q!} \\ \frac{2^1 \Delta t^1}{1!} & \frac{2^2 \Delta t^2}{2!} & \cdots & \frac{2^q \Delta t^q}{q!} \\ \\ \frac{\mathcal{N}^1 \Delta t^1}{1!} & \frac{\mathcal{N}^2 \Delta t^2}{2!} & \cdots & \frac{\mathcal{N}^q \Delta t^q}{q!} \end{pmatrix}_{\mathcal{N} \times q}.$$

We have $D \approx L\Psi^{(q)}$. We use a least-squares method to obtain an estimate

$$\hat{\Psi}^{(q)} = (L^T L)^{-1} L^T D$$

and $\hat{A}_{jk} = \hat{\psi}_1$. To fully reconstruct any H, this algorithm has online computational complexity $O(\mathcal{M}^2 + q\mathcal{M}\mathcal{N})$, because $(L^T L)^{-1} L^T$ can be computed offline in advance. In the worst case, there is no prior knowledge on H, and the computational complexity becomes $O(d^4 + d^2 q\mathcal{N})$. As long as $\mathcal{N} = o(d^2)$, this computational complexity is lower than the $O(d^6)$ of the identification algorithm in [39]. For another example of such economic Hamiltonian identification algorithms, refer to [45].

C. Numerical Example

We perform numerical simulations to illustrate the performance of the identification algorithm. Consider a 5-qubit exchange model without transverse field [$n = 4$ in (18)], and the values of the Hamiltonian parameters are $\boldsymbol{\theta} = (0.1, 1.5, -0.8, 3.1)$. The accessible set is $\bar{G} = \{X_1, Z_1Y_2, Z_1Z_2X_3, Z_1Z_2Z_3Y_4, Z_1Z_2Z_3Z_4X_5\}$. We set the initial states of the system as the eigenstates of Z_1Y_2, $Z_1Z_2X_3$, $Z_1Z_2Z_3Y_4$, $Z_1Z_2Z_3Z_4X_5$ and observe X_1, Z_1Y_2, $Z_1Z_2X_3$, $Z_1Z_2Z_3Y_4$, respectively. From Theorem 4, we know all the parameters are identifiable. Then, we identify the Hamiltonian using the Taylor expansion identification algorithm. The sampling period is $\Delta t = 0.1$ s and the parameter

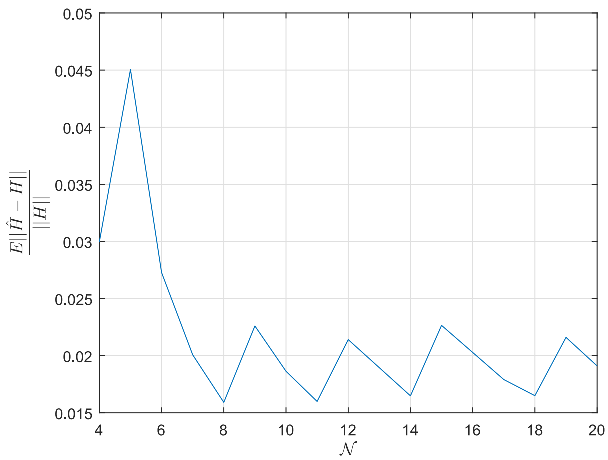

Fig. 2. Relative identification error $\frac{E\|\hat{H}-H\|}{\|H\|}$ versus data length $\mathcal{N}$.

$q = \lfloor 0.3\mathcal{N} \rfloor + 3$. We add zero-mean Gaussian noise with standard deviation 0.001 into the sampling data. The identification result is shown in Fig. 2, where each point is repeated 500 times. In Fig. 2, the horizontal axis is the data length $\mathcal{N}$ and the vertical axis is the relative identification error $\frac{E\|\hat{H}-H\|}{\|H\|}$, where $E(\cdot)$ is the expectation on all the possible measurement results. The numerical result shows that the identification algorithm can effectively identify the Hamiltonian.

VII. Conclusion

We have extended the STA method in classical control theory to the domain of quantum Hamiltonian identification and employed the STA method to study the concept of identifiability of time-independent Hamiltonians. For a concrete analysis, we focus on the spin-1/2 chain model with a single-qubit probe (also partly investigated in [17], [18], and [27]). The STA has been demonstrated to be a powerful tool to analyze the identifiability for quantum systems with arbitrary dimension, which is also helpful for further designing identification algorithms. The STA can also serve as a useful method for physicists to investigate the information extraction capability of quantum subsystems (like the single-qubit probe in [17]–[19] and [27]). An SPT method was developed to efficiently test the identifiability for nonminimal systems. We further employed the SPT method to provide an indicator for the existence of economic quantum Hamiltonian identification algorithms. The SPT method is proved to be a strong supplement to the STA. SPT can also be applicable to classical control systems, especially when the experimental settings are difficult to change. We proposed an example of economic quantum Hamiltonian identification algorithms and presented a numerical example to illustrate the performance of the identification algorithm.

Future work includes developing a general framework using the STA to characterize the amount of identifiable information for an unidentifiable system. It will also be helpful to propose more sufficient or necessary conditions for a system to be identifiable. Furthermore, it is useful to develop other efficient Hamiltonian identification algorithms with good performance.

Appendix A
Proof of Lemma 1

Proof: By induction, for $1 \le k \le n$, we have

$$A^k B = \left[(\underbrace{*, \ldots, *}_{k}, (-1)^k \prod_{i=1}^{k} \theta_i, \underbrace{0, \ldots, 0}_{n-k})^T \right]_{(n+1)\times 1}$$

where $*$ are polynomials in θ_i. Therefore, CM is an upper triangular matrix, and its determinant is

$$\det(\mathrm{CM}) = \prod_{k=1}^{n} (-1)^k \prod_{i=1}^{k} \theta_i$$

which is nonzero for almost any value of θ. Hence, CM is almost always full ranked. ∎

Appendix B
Proof of Lemma 2

Proof: We consider $\det(\bar{A} - \lambda_0 I)$, which must equal to one of the following three possibilities: a) a nontrivial polynomial in θ_is $(i = 1, 2, \ldots, n)$; b) a nonzero constant; and c) the constant zero. We let $\theta_2 = \theta_4 = \cdots = \theta_{n-1} = 0$ and $\theta_1 = \theta_3 = \cdots = \theta_n = \lambda_0 + 1$. Then, from (28), we know that $\det(\bar{A} - \lambda_0 I) = \det(I) = 1$. Therefore, (c) is excluded. No matter which of (a) and (b) is valid, $\det(\bar{A} - \lambda_0 I) \neq 0$ for almost any value of $\boldsymbol{\theta}$, which implies that it is atypical to assume $\lambda_0 \in \Lambda(\bar{A})$. ∎

Appendix C
Proof of Lemma 3

Proof: Since $\bar{A} = PEP^T = \sum_{i=1}^{n} E_{ii} P_{\sigma i} (P^T)_{i\sigma}$, we have $\theta_1 = I_{1\sigma} \bar{A} I_{\sigma 1} = \sum_{i=1}^{n} E_{ii} I_{1\sigma} P_{\sigma i} (P^T)_{i\sigma} I_{\sigma 1} = \sum_{i=1}^{n} E_{ii} P_{1i}^2$. Since $\sum_{i=1}^{n} P_{1i}^2 = 1$, $P_{1\sigma}$ cannot be all zero. Suppose that there are m nonzero elements in $P_{1\sigma}$, where $1 \le m \le n$. If $m = 1$, we suppose it is $P_{1t} \neq 0$. Then, $P_{1t} = \pm 1$ and $P_{1i} = 0$ for every $i \neq t$. Since $\sum_{j=1}^{n} P_{jt}^2 = 1$, $P_{jt} = 0$ for every $j \neq 1$. We calculate

$$-\theta_2 = I_{1\sigma} \bar{A} I_{\sigma 2} = \sum_{i=1}^{n} E_{ii} I_{1\sigma} P_{\sigma i} (P^T)_{i\sigma} I_{\sigma 2}$$

$$= \sum_{i=1}^{n} E_{ii} P_{1i} P_{2i} = E_{tt} P_{1t} P_{2t} = 0$$

which is atypical and can be ignored. Hence, it is almost always true that $m \ge 2$. We assume that $P_{1i_j} \neq 0$ for $i_j = i_1, i_2, \ldots, i_m$ and otherwise $P_{1i} = 0$.

We prove the conclusion of Lemma 3 by contradiction. Suppose that for every $1 \le k \le n$, $|\theta_1| = |(P E \mathbb{I}_k P^T)_{11}|$. Since $(P E \mathbb{I}_k P^T)_{11} = I_{1\sigma} \left[PEP^T - PE(I - \mathbb{I}_k) P^T \right] I_{\sigma 1}$

$$= I_{1\sigma} \left[\sum_{i=1}^{n} E_{ii} P_{\sigma i} (P^T)_{i\sigma} - 2 E_{kk} P_{\sigma k} (P^T)_{k\sigma} \right] I_{\sigma 1}$$

$$= \sum_{i=1}^{n} E_{ii} P_{1i}^2 - 2 E_{kk} P_{1k}^2$$

$$= \theta_1 - 2 E_{kk} P_{1k}^2$$

we always have

$$|\theta_1| = |\theta_1 - 2E_{kk}P_{1k}^2|. \tag{58}$$

We let $k = i_1$ in (58). From Lemma 2, we have $E_{i_1i_1} \neq 0$. Since $P_{1i_1} \neq 0$, we take the square of both sides of (58) and obtain $\theta_1 = E_{i_1i_1}P_{1i_1}^2$. For the same reason, we have $\theta_1 = E_{i_2i_2}P_{1i_2}^2 = \cdots = E_{i_mi_m}P_{1i_m}^2$. Then, we have $\theta_1 = mE_{i_1i_1}P_{1i_1}^2$, which means $E_{i_1i_1}P_{1i_1}^2 = 0$ and implies a contradiction. ■

Appendix D
Proof of Lemma 4

Proof: The controllability matrix is

$$\text{CM} = \begin{pmatrix} \bar{B} & 0 & -\bar{A}^2\bar{B} & 0 & \dots & 0 \\ 0 & -\bar{A}\bar{B} & 0 & \bar{A}^3\bar{B} & \dots & -\bar{A}(-\bar{A}^2)^{\frac{n-1}{2}}\bar{B} \end{pmatrix}.$$

From Lemma 2, we know $\bar{A}$ is almost always nonsingular. Hence, it suffices to prove that $Q = (\bar{B}, \bar{A}^2\bar{B}, \dots, \bar{A}^{n-1}\bar{B})$ is almost always nonsingular. Similar to the analysis in Appendix B, $\det(Q)$ has only three possibilities, where the possibility of $\det(Q) \equiv 0$ needs to be excluded. Hence, we only need to find a special $\bar{A}$ such that $\det(Q) \neq 0$.

We take

$$\bar{A} = \begin{pmatrix} 0 & 1 & & & \\ 1 & 0 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & 0 & 1 \\ & & & 1 & 1 \end{pmatrix}.$$

Then, we have

$$\bar{A}^2 = \begin{pmatrix} 1 & 0 & 1 & & & & \\ 0 & 2 & 0 & 1 & & & \\ 1 & 0 & 2 & 0 & \ddots & & \\ & 1 & & \ddots & & 0 & 1 \\ & & & \ddots & 0 & 2 & 1 \\ & & & & 1 & 1 & 2 \end{pmatrix}.$$

We can take Q as the controllability matrix of another system $(\bar{A}^2, \bar{B})$, which should be controllable. Since controllability is unchanged under similarity transformation, we transform $\bar{A}^2$ into

$$\tilde{A} = \begin{pmatrix} 1 & 1 & & & \\ 1 & 2 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & 2 & 1 \\ & & & 1 & 1 \end{pmatrix}. \tag{59}$$

This similarity transformation works in the following steps: i) we take all the odd rows of $\bar{A}^2$ in ascending order; ii) following (i), we take all the even rows of $\bar{A}^2$ in descending order; and iii) we repeat (i) and (ii) on the columns of $\bar{A}^2$. After steps (i) and (ii), each 2 (except the 2 in the last row) will have a 1 just above it and a 1 just below it, and this property does not change in step (iii). Also, the transformation is symmetric. Hence, $\tilde{A}$ is symmetric with all the 2s on the diagonal line. Therefore, $\tilde{A}$ has the form of (59). Under this transformation, $\tilde{B} = \bar{B}$ is unchanged.

For system $(\tilde{A}, \tilde{B})$, it can be proven by induction that the controllability matrix $\tilde{Q}$ is an upper triangular matrix with all the diagonal elements 1. Therefore, $\det(\tilde{Q}) \neq 0$, and thus, $\det(Q) \neq 0$, and the possibility (c) is excluded. Hence, CM is almost always full rank.

For the observability matrix, we have

$$\text{OM} = \begin{pmatrix} 0 & \bar{C} \\ -\bar{C}\bar{A} & 0 \\ 0 & -\bar{C}\bar{A}^2 \\ \dots & \dots \\ -\bar{C}\bar{A}(-\bar{A}^2)^{\frac{n-1}{2}} & 0 \end{pmatrix}.$$

Hence, it suffices to prove that $P = (\bar{C}^T, \bar{A}^{2\,T}\bar{C}^T, \dots, \bar{A}^{(n-1)T}\bar{C}^T)^T$ is almost always nonsingular. Since $\bar{A}$ is symmetric and $\bar{C}^T = \bar{B}$, we know $P = Q^T$. Therefore, OM is also almost always full rank. ■

Appendix E
Proof of Lemma 5

Proof: First, we investigate the relationship between $\Lambda(\bar{A})$ and $\Lambda(\bar{A})'$. Since A is similar to A', we know A^2 is similar to A'^2, which implies $\Lambda(A^2) = \Lambda(A'^2)$. Therefore, we have

$$\Lambda\begin{pmatrix} -\bar{A}^2 & 0 \\ 0 & -\bar{A}^2 \end{pmatrix} = \Lambda\begin{pmatrix} -\bar{A}'^2 & 0 \\ 0 & -\bar{A}'^2 \end{pmatrix}.$$

If we arrange the eigenvalues of $\bar{A}$ and $\bar{A}'$ both in ascending sequences, we have

$$\lambda_i(\bar{A}') = p_i\lambda_i(\bar{A}) \tag{60}$$

for $1 \leq i \leq \frac{n+1}{2}$ where $p_i = \pm 1$.

Second, we point out that it is atypical for $\bar{A}$ to have multiple eigenvalues. We consider $\det(\lambda I - \bar{A})$, which is a polynomial on λ, with the coefficients being polynomials on θ_is. Polynomial $\det(\lambda I - \bar{A})$ has multiple roots if and only if its discriminant, which is a polynomial function in the coefficients of $\det(\lambda I - \bar{A})$, equals to zero [46]. We can view this discriminant as a polynomial function in θ_is. If this discriminant is, in fact, the constant zero, then $\det(\lambda I - \bar{A})$ will always have multiple roots, which can be excluded by taking $\bar{A} = \text{diag}(1, 2, \dots, \frac{n+1}{2})$. Therefore, the discriminant does not degenerate to zero, and its solution set is of zero measure. Hence, the set of $\boldsymbol{\theta}$ that can make $\det(\lambda I - \bar{A})$ have multiple roots is of zero measure, which implies that it is atypical when $\bar{A}$ has multiple eigenvalues.

Third, we prove that we can almost always have $\lambda_i(\bar{A}') + \lambda_j(\bar{A}') \neq 0$ for any $1 \leq i, j \leq \frac{n+1}{2}$. Using (60), we have

$$\lambda_i(\bar{A}') + \lambda_j(\bar{A}') = p_i\lambda_i(\bar{A}) + p_j\lambda_j(\bar{A}). \tag{61}$$

If $i = j$, then the RHS of (61) is $2p_i\lambda_i(\bar{A})$, which is almost always nonzero according to Lemma 2. If $i \neq j$, the RHS of (61) is $p_i[\lambda_i(\bar{A}) \pm \lambda_j(\bar{A})]$, which is also almost always nonzero because of (44) and the fact that $\bar{A}$ almost always has no multiple eigenvalues. Therefore, we can almost always have $\lambda_i(\bar{A}') + \lambda_j(\bar{A}') \neq 0$ for any $1 \leq i, j \leq \frac{n+1}{2}$, which is equivalent to the statement that $\bar{A}' \otimes I_{\frac{n+1}{2}} + I_{\frac{n+1}{2}} \otimes \bar{A}'$ is almost always nonsingular. ■

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References

[1] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information*. Cambridge, U.K.: Cambridge Univ. Press, 2000.
[2] C. L. Degen, F. Reinhard, and P. Cappellaro, "Quantum sensing," *Rev. Mod. Phys.*, vol. 89, no. 3, 2017, Art. no. 035002.
[3] M. Paris and J. Řeháček, *Quantum State Estimation (Lecture Notes in Physics)*, vol. 649. Berlin, Germany: Springer, 2004.
[4] H. M. Wiseman and G. J. Milburn, *Quantum Measurement and Control*. Cambridge, U.K.: Cambridge Univ. Press, 2009.
[5] Z. Hou *et al.*, "Full reconstruction of a 14-qubit state within four hours," *New J. Phys.*, vol. 18, 2016, Art. no. 083036.
[6] B. Qi *et al.*, "Adaptive quantum state tomography via linear regression estimation: Theory and two-qubit experiment," *npj Quantum Inf.*, vol. 3, 2017, Art. no. 19.
[7] A. Sone, Q. Zhuang, and P. Cappellaro, "Quantifying precision loss in local quantum thermometry via diagonal discord," *Phys. Rev. A*, vol. 98, no. 1, 2018, Art. no. 012115.
[8] J. Wang *et al.*, "Experimental quantum Hamiltonian learning," *Nature Phys.*, vol. 13, no. 6, pp. 551–555, 2017.
[9] S. J. Devitt, J. H. Cole, and L. C. Hollenberg, "Scheme for direct measurement of a general two-qubit Hamiltonian," *Phys. Rev. A*, vol. 73, no. 5, 2006, Art. no. 052317.
[10] J. Zhang and M. Sarovar, "Identification of open quantum systems from observable time traces," *Phys. Rev. A*, vol. 91, no. 5, 2015, Art. no. 052121.
[11] Y. Fu, H. Rabitz, and G. Turinici, "Hamiltonian identification in presence of large control field perturbations," *J. Phys. A: Math. Theor.*, vol. 49, no. 49, 2016, Art. no. 495301.
[12] M. Levitt, M. Guţă, and H. I. Nurdin, "Power spectrum identification for quantum linear systems," *Automatica*, vol. 90, pp. 255–262, 2018.
[13] S. Bonnabel, M. Mirrahimi, and P. Rouchon, "Observer-based Hamiltonian identification for quantum systems," *Automatica*, vol. 45, no. 5, pp. 1144–1155, 2009.
[14] C.-C. Shu, K.-J. Yuan, D. Dong, I. R. Petersen, and A. D. Bandrauk, "Identifying strong-field effects in indirect photofragmentation reactions," *J. Phys. Chem. Lett.*, vol. 8, no. 1, pp. 1–6, 2016.
[15] D. Burgarth and K. Yuasa, "Quantum system identification," *Phys. Rev. Lett.*, vol. 108, no. 8, 2012, Art. no. 080502.
[16] C. Le Bris, M. Mirrahimi, H. Rabitz, and G. Turinici, "Hamiltonian identification for quantum systems: Well-posedness and numerical approaches," *ESAIM: Control Optim. Calculus Variations*, vol. 13, no. 2, pp. 378–395, 2007.
[17] C. Di Franco, M. Paternostro, and M. S. Kim, "Bypassing state initialization in Hamiltonian tomography on spin-chains," *Int. J. Quantum Inf.*, vol. 9, pp. 181–187, 2011.
[18] C. Di Franco, M. Paternostro, and M. S. Kim, "Hamiltonian tomography in an access-limited setting without state initialization," *Phys. Rev. Lett.*, vol. 102, no. 18, 2009, Art. no. 187203.
[19] D. Burgarth, K. Maruyama, and F. Nori, "Coupling strength estimation for spin chains despite restricted access," *Phys. Rev. A*, vol. 79, no. 2, 2009, Art. no. 020305.
[20] D. Burgarth and A. Ajoy, "Evolution-free Hamiltonian parameter estimation through Zeeman markers," *Phys. Rev. Lett.*, vol. 119, no. 3, 2017, Art. no. 030402.
[21] D. Burgarth and K. Maruyama, "Indirect Hamiltonian identification through a small gateway," *New J. Phys.*, vol. 11, no. 10, 2009, Art. no. 103019.
[22] D. K. Burgarth, "Identifying combinatorially symmetric hidden Markov models," *Electron. J. Linear Algebra*, vol. 34, pp. 393–398, 2018.
[23] M. Guţă and N. Yamamoto, "System identification for passive linear quantum systems," *IEEE Trans. Autom. Control*, vol. 61, no. 4, pp. 921–936, Apr. 2016.
[24] M. Levitt and M. Guţă, "Identification of single-input-single-output quantum linear systems," *Phys. Rev. A*, vol. 95, no. 3, 2017, Art. no. 033825.
[25] Z. Leghtas, G. Turinici, H. Rabitz, and P. Rouchon, "Hamiltonian identification through enhanced observability utilizing quantum control," *IEEE Trans. Autom. Control*, vol. 57, no. 10, pp. 2679–2683, Oct. 2012.
[26] J. Zhang and M. Sarovar, "Quantum Hamiltonian identification from measurement time traces," *Phys. Rev. Lett.*, vol. 113, no. 8, 2014, Art. no. 080401.
[27] A. Sone and P. Cappellaro, "Hamiltonian identifiability assisted by a single-probe measurement," *Phys. Rev. A*, vol. 95, no. 2, 2017, Art. no. 022335.
[28] A. Sone and P. Cappellaro, "Exact dimension estimation of interacting qubit systems assisted by a single quantum probe," *Phys. Rev. A*, vol. 96, no. 6, 2017, Art. no. 062334.
[29] Y. Kato and N. Yamamoto, "Structure identification and state initialization of spin networks with limited access," *New J. Phys.*, vol. 16, no. 2, 2014, Art. no. 023024.
[30] R. Bellman and K. J. Åström, "On structural identifiability," *Math. Biosci.*, vol. 7, nos. 3/4, pp. 329–339, 1970.
[31] H. Pohjanpalo, "System identifiability based on the power series expansion of the solution," *Math. Biosci.*, vol. 41, nos. 1/2, pp. 21–33, 1978.
[32] C. C. Travis and G. Haddock, "On structural identification," *Math. Biosci.*, vol. 56, nos. 3/4, pp. 157–173, 1981.
[33] E. Walter and Y. Lecourtier, "Unidentifiable compartmental models: What to do?" *Math. Biosci.*, vol. 56, nos. 1/2, pp. 1–25, 1981.
[34] S. Vajda, K. R. Godfrey, and H. Rabitz, "Similarity transformation approach to identifiability analysis of nonlinear compartmental models," *Math. Biosci.*, vol. 93, no. 2, pp. 217–248, 1989.
[35] L. Ljung, *System Identification—Theory for the User*. Upper Saddle River, NJ, USA: Prentice-Hall, 1999.
[36] K. R. Godfrey and J. J. DiStefano III, "Identifiability of model parameters," *IFAC Proc. Vol.*, vol. 18, no. 5, pp. 89–114, 1985.
[37] J. P. Norton, "An investigation of the sources of nonuniqueness in deterministic identifiability," *Math. Biosci.*, vol. 60, no. 1, pp. 89–108, 1982.
[38] L. Wang and H. Garnier, *System Identification, Environmental Modelling, and Control System Design*. London, U.K.: Springer-Verlag, 2012.
[39] Y. Wang, D. Dong, B. Qi, J. Zhang, I. R. Petersen, and H. Yonezawa, "A quantum Hamiltonian identification algorithm: Computational complexity and error analysis," *IEEE Trans. Autom. Control*, vol. 63, no. 5, pp. 1388–1403, May 2018.
[40] E. D. Sontag, "For differential equations with r parameters, $2r + 1$ experiments are enough for identification," *J. Nonlinear Sci.*, vol. 12, no. 6, pp. 553–583, 2002.
[41] R. E. Kalman, "Mathematical description of linear dynamical systems," *J. Soc. Ind. Appl. Math. Ser. A: Control*, vol. 1, no. 2, pp. 152–192, 1963.
[42] J. DiStefano, "On the relationships between structural identifiability and the controllability, observability properties," *IEEE Trans. Autom. Control*, vol. 22, no. 4, pp. 652–652, Aug. 1977.
[43] K. Zhou, J. C. Doyle, and K. Glover, *Robust Optimal Control*. Upper Saddle River, NJ, USA: Prentice-Hall, 1996.
[44] Y. Wang, D. Dong, and I. R. Petersen, "An approximate quantum Hamiltonian identification algorithm using a Taylor expansion of the matrix exponential function," in *Proc. 56th IEEE Conf. Decis. Control*, Melbourne, VIC, USA, Dec. 12-15, 2017, pp. 5523–5528.
[45] Y. Wang, D. Dong, I. R. Petersen, and J. Zhang, "An approximate algorithm for quantum Hamiltonian identification with complexity analysis," in *Proc. 20th IFAC World Congr.*, Toulouse, France, Jul. 9–14, 2017, pp. 11744–11748.
[46] I. M. Gelfand, M. Kapranov, and A. Zelevinsky, *Discriminants, Resultants, and Multidimensional Determinants*. Boston, MA, USA: Birkhäuser, 2008.

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