

## Quantum Hamiltonian Identification from Measurement Time Traces

Jun Zhang<sup>1</sup> and Mohan Sarovar<sup>2,\*</sup>

<sup>1</sup>Joint Institute of UM-SJTU and Key Laboratory of System Control and Information Processing (MOE), Shanghai Jiao Tong University, Shanghai 200240, China

<sup>2</sup>Department of Scalable and Secure Systems Research (08961), Sandia National Laboratories, Livermore, California 94550, USA  
(Received 24 January 2014; published 18 August 2014)

Precise identification of parameters governing quantum processes is a critical task for quantum information and communication technologies. In this Letter, we consider a setting where system evolution is determined by a parametrized Hamiltonian, and the task is to estimate these parameters from temporal records of a restricted set of system observables (time traces). Based on the notion of system realization from linear systems theory, we develop a constructive algorithm that provides estimates of the unknown parameters directly from these time traces. We illustrate the algorithm and its robustness to measurement noise by applying it to a one-dimensional spin chain model with variable couplings.

DOI: 10.1103/PhysRevLett.113.080401

PACS numbers: 03.65.Wj, 02.30.Yy, 03.67.-a

The promise of quantum technologies for tasks such as computation, communication, and metrology is motivating the construction of devices that are precisely engineered at the nanoscale, and whose quantum dynamics are exceptionally well characterized and controlled [1]. The fragility and sensitivity of typical quantum devices make achieving such objectives extremely challenging, and significant research efforts over the past two decades have focused on addressing these challenges.

Process tomography is the most generally applied technique for characterizing an unknown quantum dynamical process [1,2]. However, all variants of process tomography are very resource demanding, e.g., in the required number of measurements settings and number of input state preparations. In addition, it is often unsuitable in resource-constrained situations where one may only have measurement access to certain observables or subsystems; e.g., see Fig. 1. Furthermore, process tomography does not utilize often available partial information about the system. One such common scenario is when the structure of a dynamical model can be obtained from underlying physics, and what is to be determined are some unknown parameters in the model. This is the quantum version of parameter estimation in classical system sciences, and some previous work has considered variants to quantum tomography for this problem [3].

In this work, we consider a new approach to quantum parameter estimation. Whereas process tomography typically measures a complete basis of system observables at one time instant, we ask what can be achieved if a temporal record of a small set of system observables is collected? We refer to such a successive record of observable expectations as a measurement time trace, and develop a method that enables information about dynamical parameters to be extracted from such time traces. Our method takes into account *a priori* information and fits naturally into resource

constrained situations, and as such, we expect that it will be very experimentally relevant and feasible. Additionally, because our scheme utilizes a time trace, it can identify the generator of dynamics (e.g., a Hamiltonian) as opposed to the dynamical map (e.g., a unitary at a fixed time), which is typically what process tomography achieves. This is advantageous since, in physically realistic scenarios, the generator of dynamics is more compactly specified than the map. This will be discussed in more detail below.

Several authors have considered parameter estimation from various types of time-dependent measurement records [4–14]. Particularly relevant to this work, Cole *et al.* used Fourier analysis to identify a single qubit Hamiltonian from one measurement observable [5], and Devitt *et al.* presented a scheme to identify any two-qubit Hamiltonian from the temporal evolution of the concurrence measure of entanglement [6]. Subsequent work by Burgarth *et al.* [8,9] and Di Franco *et al.* [10] generalized this approach to estimate the coupling strengths in a many-qubit network from measurements on a small part of the network. Recently, Burgarth *et al.* presented a framework for quantum system identification based on input-output

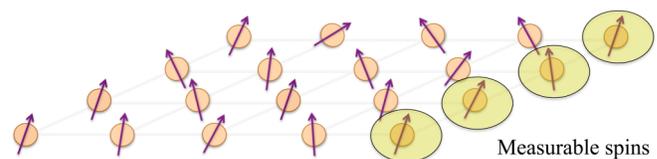


FIG. 1 (color online). A spin (or qubit) lattice as an example illustrating the type of system considered in this work. The spins interact with each other through nearest-neighbor or long-range couplings and certain local observables are measurable for a subset of the spins (circled above). The task is to identify the parameters defining the Hamiltonian of the interconnected system from a time trace of expectation values of these observables.

information and formalized the notion of equivalence between system realizations [15].

Our approach differs from existing work on quantum system identification in two critical aspects. First, we develop a constructive algorithm for identification of arbitrary Hamiltonian quantum dynamics that takes advantage of available prior knowledge of the system (e.g., network structure or partial knowledge of parameters). The technique can also be employed when such prior information is absent. Second, in contrast to most existing system identification schemes, we do not require state tomography of a restricted set of subsystems, but rather develop a technique that produces parameter estimates based only on the collected measurement time traces.

*Setup.*—We consider the task of identifying the Hamiltonian of an unknown quantum dynamical process. Assume that the dimension of the system is finite and known, and that the dynamical process can be prepared at some well-characterized initial states. Further, we assume that the dynamical evolution of the process is unitary (no decoherence). This condition can be relaxed and the approach will be extended to the nonunitary case in a future publication.

A parametrized form of the Hamiltonian governing the quantum dynamical process can be written as

$$H = \sum_{m=1}^M a_m(\theta) X_m, \quad (1)$$

where  $\theta$  is a vector consisting of unknown parameters,  $a_m \in \mathbb{R}$  are some known functions of  $\theta$ , and  $X_m$  are known Hermitian operators [16]. Assume that the dimension of the quantum process is  $N$ , and thus,  $iH \in \mathfrak{su}(N)$ , i.e., the Lie algebra consisting of all the  $N \times N$  skew-Hermitian matrices. An orthonormal basis of  $N^2 - 1$  matrices  $\{iX_m\}$  can be chosen for  $\mathfrak{su}(N)$ , where the Hilbert-Schmidt inner product is defined as  $\langle iX_m, iX_n \rangle \equiv \text{tr}(X_m^\dagger X_n)$ , and hence,  $a_m = \text{tr}(HX_m)$ . For example,  $(i/2)\sigma_\alpha^\dagger \otimes \sigma_\beta^\dagger$  form a basis for the two-qubit algebra  $\mathfrak{su}(4)$ , where  $\sigma_\alpha, \sigma_\beta$  can be Pauli matrices  $\sigma_x, \sigma_y, \sigma_z$ , or the identity matrix  $I_2$ , and superscripts label the qubits [17]. The numbers  $C_{jkl}$  such that

$$[iX_j, iX_k] = \sum_{l=1}^{N^2-1} C_{jkl} (iX_l), \quad j, k = 1, \dots, N^2 - 1,$$

are the structure constants of the Lie algebra  $\mathfrak{su}(N)$  with respect to this basis. Each element  $X_m$  is Hermitian and, thus, can be considered an observable for the system. Furthermore, we can consider the  $a_m$  as our unknown parameters, because solving for  $\theta$  from  $a_m$  is simply an algebraic problem.

Note that in Eq. (1), typically  $M \ll N^2 - 1$  because of physical constraints on system energy, locality, and weight of interactions. For instance, the Hamiltonian for the spin

lattice system in Fig. 1 contains only weight-one and weight-two basis elements  $X_m$  [18], and furthermore, the weight-two interactions might be restricted to only being between nearest-neighbor spins on the lattice. By utilizing measurement time traces our identification algorithm can estimate the process at the Hamiltonian level where there are only  $M$  unknown parameters. In contrast, process tomography generally does not consider time traces and, therefore, must estimate the process at the unitary level where there are, in general,  $N^2 - 1$  unknown parameters.

*Observable dynamics.*—The dynamics of the expectation value of an observable  $X_k$ , written as  $x_k = \langle \psi | X_k | \psi \rangle$ , can be derived as

$$\dot{x}_k = \sum_{l=1}^{N^2-1} \left( \sum_{m=1}^M C_{mkl} a_m \right) x_l. \quad (2)$$

Collecting the  $x_k$  in a vector  $\mathbf{x} \in \mathbb{R}^{N^2-1}$ , we obtain a linear equation describing the complete dynamics

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x}, \quad x_k(0) = \langle \psi(0) | X_k | \psi(0) \rangle, \quad (3)$$

where the matrix  $\mathbf{A} \in \mathbb{R}^{(N^2-1) \times (N^2-1)}$  has elements  $A_{kl} = \sum_{m=1}^M C_{mkl} a_m$ . Using the antisymmetries of the structure constants, it can be shown that  $\mathbf{A}^T = -\mathbf{A}$ . The vector  $\mathbf{x}$ , often called the coherence vector [19], is a complete representation of the quantum state. Equation (3) explicitly describes the quantum dynamics as a linear time invariant system, and hence, it enables application of results from classical linear systems theory.

Typically, some observable expectation values may be easily measured; e.g., local observables of a collection of spins are tracked as a function of time; see Fig. 1. Often the measured observables belong to the chosen  $\mathfrak{su}(N)$  basis, but if not, each observable  $O_i$  can be expanded in this basis as  $O_i = \sum_j o_j^{(i)} X_j$ . Collect the unique basis elements present in the expansion of all measured observables in the set  $\mathcal{M} = \{X_{\nu_1}, X_{\nu_2}, \dots, X_{\nu_p}\}$ , where  $\nu$  is a vector of length  $p$ . For example, if  $O_1 = o_3^{(1)} X_3 + o_5^{(1)} X_5$  and  $O_2 = o_2^{(2)} X_2 + o_3^{(2)} X_3$ , with  $o_k^{(j)} \in \mathbb{R}$ , then  $p = 3$  and  $\mathcal{M} = \{X_2, X_3, X_5\}$ . Generally,  $p \ll N^2 - 1$ .

In the following, we will use time traces of the measured observable expectation values to identify the unknown Hamiltonian parameters. To this end, we first need to derive the dynamical equation governing the time evolution of these observables. Parallel to the study of controllability in classical nonlinear systems theory [20], we give a constructive procedure to obtain the closed dynamics for these observables. For the Hamiltonian in Eq. (1), let  $\Delta = \{X_m\}_{m=1}^M$ . Define an iterative procedure as

$$G_0 = \mathcal{M}, \quad \text{and} \quad G_i = [G_{i-1}, \Delta] \cup G_{i-1}, \quad (4)$$

where  $[G_{i-1}, \Delta] \equiv \{X_j : \text{tr}(X_j^\dagger [g, h]) \neq 0, \text{ where } g \in G_{i-1}, h \in \Delta\}$  [21]. In geometric control theory, the sequence

of  $G_i$  are referred to as the filtration associated to  $\Delta$  [20]. Since  $\mathfrak{su}(N)$  is finite, this iteration will saturate at a maximal set  $\tilde{G}$  after finite steps, and we refer to this set as the accessible set. Intuitively, the set  $\tilde{G}$  contains the elements of the system that couple to the measured observables. Then, writing all the  $x_k$  with  $X_k \in \tilde{G}$  in a vector  $\mathbf{x}_a$  of dimension  $K \leq N^2 - 1$ , the dynamics for this vector is given by

$$\dot{\mathbf{x}}_a = \tilde{\mathbf{A}}\mathbf{x}_a, \quad (5)$$

where  $\tilde{\mathbf{A}}$  is a  $K \times K$  submatrix of  $\mathbf{A}$ , i.e., only the elements necessary to describe the evolution of the subset of observable averages collected in  $\mathbf{x}_a$ .

*Identification algorithm.*—A necessary condition for the identifiability of  $a_m$  is that it be present in the matrix  $\tilde{\mathbf{A}}$ , because, otherwise, it would not participate in the dynamical equation (5), and there would be no way to infer its value from examining the observables in  $\mathcal{M}$ . In order to estimate these identifiable parameters, we utilize the notion of a system realization constructed from the measurement time traces. In linear systems theory, there are many methods for constructing a realization of a linear dynamical system based on measurement results [22], and in the following, we adapt one of these, the eigenstate realization algorithm (ERA) [23], for the purposes of Hamiltonian parameter estimation.

The estimation setting we consider is the following. Suppose we have access to the expectation values of the observables in  $\mathcal{M}$  at regular time instants  $j\Delta t$  for some sampling period  $\Delta t$  [24]. Denote these values as  $\{\mathbf{y}(j\Delta t)\}$ , and they may have to be collected from averaging measurements on several runs of the experiment under the same initial state. Note that  $\mathbf{y}(j\Delta t)$  is the output of the following discretized form of Eq. (5):

$$\mathbf{x}_a(j+1) = \tilde{\mathbf{A}}_d\mathbf{x}_a(j), \quad \mathbf{y}(j) = \mathbf{C}\mathbf{x}_a(j), \quad (6)$$

where for brevity of notation we use  $\mathbf{x}_a(j) \equiv \mathbf{x}_a(j\Delta t)$  and  $\mathbf{y}(j) \equiv \mathbf{y}(j\Delta t)$ , and  $\tilde{\mathbf{A}}_d = e^{\tilde{\mathbf{A}}\Delta t}$ . The  $p \times K$  matrix  $\mathbf{C}$  picks up the entries in  $\mathbf{x}_a(j)$  that correspond to expectation values of elements of  $\mathcal{M}$ . Also, assume that the system is prepared at a fixed, known initial state  $\mathbf{x}(0)$ , and the corresponding initial state for Eq. (6) is  $\mathbf{x}_a(0)$ . Then, these relations can be solved easily to obtain an explicit form for the outputs:  $\mathbf{y}(j) = \mathbf{C}\tilde{\mathbf{A}}_d^j\mathbf{x}_a(0)$ . Having access to the time trace  $\mathbf{y}(j)$ , one may try to solve this set of equations directly. However, since  $\tilde{\mathbf{A}}_d$  is a transcendental function of  $a_m$ , determining the parameters this way is usually infeasible. Instead, we will utilize ERA and formulate a new relationship so that parameter estimation only requires solving polynomial equations.

The first stage of the estimation algorithm is to construct a minimal realization of the system based on input-output information. This is achieved by ERA in three steps, as

follows. Step (1) Collect the measured data into an  $rp \times s$  matrix (generalized Hankel matrix) as

$$\mathbf{H}_{rs}(k) = \begin{bmatrix} \mathbf{y}(k) & \mathbf{y}(k+t_1) & \cdots & \mathbf{y}(k+t_{s-1}) \\ \mathbf{y}(j_1+k) & \mathbf{y}(j_1+k+t_1) & \cdots & \mathbf{y}(j_1+k+t_{s-1}) \\ \vdots & \vdots & & \vdots \\ \mathbf{y}(j_{r-1}+k) & \mathbf{y}(j_{r-1}+k+t_1) & \cdots & \mathbf{y}(j_{r-1}+k+t_{s-1}) \end{bmatrix},$$

with arbitrary integers  $j_i$  ( $i = 1, \dots, r-1$ ) and  $t_l$  ( $l = 1, \dots, s-1$ ). Step (2) Find the singular value decomposition of  $\mathbf{H}_{rs}(0)$  as

$$\mathbf{H}_{rs}(0) = P \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix} Q^T = [P_1 \quad P_2] \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} Q_1^T \\ Q_2^T \end{bmatrix},$$

where  $P \in \mathbb{R}^{rp \times rp}$ ,  $Q \in \mathbb{R}^{s \times s}$  are both orthonormal, and  $\Sigma$  is a diagonal matrix with the nonzero singular values of  $\mathbf{H}_{rs}(0)$  determined up to numerical accuracy  $\epsilon$ , i.e.,  $\Sigma_{ii} > \epsilon$  for all  $i \leq n_\Sigma$  where  $n_\Sigma$  is the dimension of  $\Sigma$ . The matrices  $P_1, P_2, Q_1, Q_2$  are partitions with compatible dimensions. Step (3) Form a realization of the system (6) as  $\hat{\mathbf{A}}_d = \Sigma^{-(1/2)} P_1^T \mathbf{H}_{rs}(1) Q_1 \Sigma^{-(1/2)}$ ,  $\hat{\mathbf{C}} = \mathbf{E}_p^T P_1 \Sigma^{(1/2)}$ , where  $\mathbf{E}_p^T = [\mathbf{I}_p, 0_p, \dots, 0_p]$ . The pair  $(\hat{\mathbf{A}}_d, \hat{\mathbf{C}})$  reproduces the input-output relations specified by Eq. (6), that is,

$$\mathbf{y}(j) = \mathbf{C}\tilde{\mathbf{A}}_d^j\mathbf{x}_a(0) = \hat{\mathbf{C}}\hat{\mathbf{A}}_d^j\hat{\mathbf{x}}(0), \quad \text{for all } j \geq 0, \quad (7)$$

provided that  $\hat{\mathbf{x}}(0) \equiv \Sigma^{(1/2)} Q_1^T e_1$ , where  $e_1$  is the first column of  $\mathbf{I}_s$ .

This completes the specification of the ERA algorithm. Then let  $\hat{\mathbf{A}} = \log \hat{\mathbf{A}}_d / \Delta t$  [24]. This results in a realization of the continuous-time linear system in the form of the triple  $(\hat{\mathbf{A}}, \hat{\mathbf{C}}, \hat{\mathbf{x}}(0))$ . Now, to estimate the Hamiltonian parameters we use an invariant of different realizations, the transfer function [22], to form equations for the unknown parameters. Specifically, the transfer function from an initial state  $\mathbf{x}(0)$  to the measurement observables specified by  $\mathbf{C}$  can be written as  $G(s) = \mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{x}(0)$ , where  $s \in \mathbb{C}$  is the Laplace variable. Equating the transfer functions for the original system with unknown parameters and the ERA realization, we get

$$\mathbf{C}(s\mathbf{I} - \tilde{\mathbf{A}})^{-1}\mathbf{x}_a(0) = \hat{\mathbf{C}}(s\mathbf{I} - \hat{\mathbf{A}})^{-1}\hat{\mathbf{x}}(0). \quad (8)$$

The right-hand side of Eq. (8) is completely determined by the measured data, and the left-hand side can be simplified as the ratio  $Q(s)/P(s)$  [22], where

$$P(s) = \det(s\mathbf{I} - \tilde{\mathbf{A}}),$$

$$Q(s) = \det \left( s \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} - \begin{bmatrix} \tilde{\mathbf{A}} & \mathbf{x}_a(0) \\ \mathbf{C} & \mathbf{0} \end{bmatrix} \right). \quad (9)$$



$(\bar{\theta}_i - \theta_i)/\theta_i \times 100\%$  [27], remains small, whereas the standard deviation of the estimates scales approximately linearly with  $\sigma$ . Further characterization of the robustness of the procedure to measurement noise is presented in the Supplemental Material [24]. We note that the robustness of our method is a function of the realization algorithm (ERA) and realization invariant used to construct the polynomial equations. In fact, we experimented with another invariant, the Markov parameters of a system, and discovered that it is not as robust to noise as the transfer function approach presented here.

*Conclusion.*—We have developed a robust algorithm to identify the unknown parameters of a quantum Hamiltonian from the time traces of a set of system observables, which naturally takes into account prior information and restrictions on measurement access. A direction for future work is the generalization of this algorithm to parameter estimation for open quantum systems governed by Lindblad evolution [28], in which case the evolution of the coherence vector is described by an affine time-invariant system of equations [19].

M. S. thanks Akshat Kumar for information on techniques for solving multivariate polynomial systems. This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the United States Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000. J. Z. acknowledges financial support from NSFC under Grant No. 61174086, and State Key Laboratory of Precision Spectroscopy, ECNU, China. The authors are grateful for the hospitality of KITP at UCSB, where this work was initiated. This research was supported in part by the National Science Foundation under Grant No. NSF PHY11-25915.

---

\*mnsarov@sandia.gov

- [1] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, England, 2001).
- [2] M. Mohseni, A. T. Rezakhani, and D. A. Lidar, *Phys. Rev. A* **77**, 032322 (2008).
- [3] M. P. da Silva, O. Landon-Cardinal, and D. Poulin, *Phys. Rev. Lett.* **107**, 210404 (2011).
- [4] N. Boulant, T. F. Havel, M. A. Pravia, and D. G. Cory, *Phys. Rev. A* **67**, 042322 (2003).
- [5] J. H. Cole, S. G. Schirmer, A. D. Greentree, C. J. Wellard, D. K. L. Oi, and L. C. L. Hollenberg, *Phys. Rev. A* **71**, 062312 (2005).
- [6] S. J. Devitt, J. H. Cole, and L. C. L. Hollenberg, *Phys. Rev. A* **73**, 052317 (2006).
- [7] K. C. Young, M. Sarovar, R. Kosut, and K. B. Whaley, *Phys. Rev. A* **79**, 062301 (2009).
- [8] D. Burgarth, K. Maruyama, and F. Nori, *Phys. Rev. A* **79**, 020305 (2009).
- [9] D. Burgarth and K. Maruyama, *New J. Phys.* **11**, 103019 (2009).
- [10] C. Di Franco, M. Paternostro, and M. S. Kim, *Phys. Rev. Lett.* **102**, 187203 (2009).
- [11] C. E. Granade, C. Ferrie, N. Wiebe, and D. G. Cory, *New J. Phys.* **14**, 103013 (2012).
- [12] Y. Kato and N. Yamamoto, *New J. Phys.* **16**, 023024 (2014).
- [13] J. M. Dominy, L. C. Venuti, A. Shabani, and D. A. Lidar, [arXiv:1312.0973v1](https://arxiv.org/abs/1312.0973v1).
- [14] V. Jagadish and A. Shaji, [arXiv:1401.1058v1](https://arxiv.org/abs/1401.1058v1).
- [15] D. Burgarth and K. Yuasa, *Phys. Rev. Lett.* **108**, 080502 (2012).
- [16] We set  $\hbar = 1$ , and therefore, the  $a_m$  have units  $1/s$ .
- [17] In the following, we will omit the tensor product when writing multiqubit Pauli operators for brevity.
- [18] The weight of a multiqubit Pauli operator is the number of nonidentity terms in the tensor product.
- [19] K. Lendi, *J. Phys. A* **20**, 15 (1987).
- [20] S. Sastry, *Nonlinear Systems* (Springer, New York, 1999).
- [21] We do not need to keep track of multiplicative constants, only the operators generated by these commutators.
- [22] F. M. Callier and C. A. Desoer, *Linear System Theory* (Springer, New York, 1991).
- [23] J. N. Juang and R. S. Pappa, *J. Guid. Control Dyn.* **8**, 620 (1985).
- [24] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevLett.113.080401>, which includes Refs. [29–30], for discussion of appropriate choice of  $\Delta t$  and an application of the system identification algorithm.
- [25] S. Bose, *Contemp. Phys.* **48**, 13 (2007).
- [26] Y. Guan and J. Verschelde, *PHClab: A MATLAB/Octave Interface to PHCpack*, IMA: Software for Alge. Geom. Vol. 148 (Springer-Verlag, Berlin, 2008).
- [27]  $\bar{X}$  is the empirical mean of the random variable  $X$ .
- [28] H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, New York, 2002).
- [29] G. F. Franklin, J. D. Powell, and M. L. Workman, *Digital Control of Dynamic Systems* (Addison-Wesley, Reading, MA, 1997).
- [30] N. J. Higham, *Functions of Matrices: Theory and Computation* (SIAM, Philadelphia, 2008).