An approximate quantum Hamiltonian identification algorithm using a Taylor expansion of the matrix exponential function

An approximate quantum Hamiltonian identification algorithm using a Taylor expansion of the matrix exponential function *

Yuanlong Wang[1,2], Daoyi Dong[1] and Ian R. Petersen[3]

***Abstract*— An approximate quantum Hamiltonian identification algorithm is presented with the assumption that the system initial state and observation matrix can be set appropriately. We sample the system with a fixed period and using the sampled data we estimate the Hamiltonian based on a Taylor expansion of the matrix exponential function. We prove the estimation error is linear in the variance of the additive Gaussian noise. We also propose a heuristic formula to find the order of magnitude of the optimal sampling period. Two numerical examples are presented to validate the theoretical results on robustness analysis.**

I. Introduction

Quantum tomography has been receiving increasing attention as it provides a way to characterize an unknown quantum object [1–6]. When the object is a quantum process, the task is called quantum process tomography [1]. Standard quantum process tomography methods are designed for general quantum process. It is possible to design more efficient algorithms for specific quantum processes. The system Hamiltonian can be taken as an important special class of quantum processes that are of primary interest for quantum systems [2]. The task of identifying parameters in the system Hamiltonian is called Quantum Hamiltonian Identification (QHI) or Hamiltonian Tomography.

Some QHI methods have already been designed for special classes of Hamiltonians. For example, Sone and Cappellaro [9] employed the Gröbner basis to investigate the Hamiltonian identifiability of a many-body spin system assisted by measuring a single quantum probe. Based on quantum process tomography, Wang *et al.* [7] designed a general iterative identification method for time-independent Hamiltonians, which is then improved in [8] as a two-step optimization QHI method. Bonnabel *et al.* [10] proposed a symmetry-preserving observer-based quantum Hamiltonian identification and proved an exponential convergence result for 2-level systems with the atom-laser frequency detuning and coupling constant being the unknown parameters. Bris *et al.* [11] investigated the problem of identifying the field free Hamiltonian and/or the dipole moment of a quantum system. They proved the well-posedness of the problem and introduced a numerical approach to estimate the parameters. Mohseni *et al.* [12] presented an approach to directly estimate single- and two-qubit Hamiltonian parameters using a single measurement device. Cole *et al.* [13] developed a Hamiltonian estimation method for some two-state systems and provided uncertainty bounds on the parameters. Cole *et al.* [14] also proposed a scheme to characterize the general Heisenberg Hamiltonian with non-uniform couplings. Holzäpfel *et al.* [15] designed a scalable method to reconstruct one-dimensional local Hamiltonians, which requires at most linearly many states to be prepared and linearly many observables to be measured. Rudinger and Joynt [16] applied compressed sensing methods to estimate Hamiltonians which are sparse in a well-defined sense. Franco *et al.* [17] presented a method to determine the coupling parameters in a chain of interacting spins that requires only time-resolved measurements over a single particle and no state initialization. Wang *et al.* [18] employed dynamical decoupling to determine all the coupling terms in a many-body Hamiltonian with finite energy density, which requires rounds of measurements varying linearly with the coupling term number in the Hamiltonian.

Zhang and Sarovar [19] proposed a QHI method from temporal records of system observables (time traces). They established the QHI problem as a system identification one, which is more familiar to the control systems community. Then they used the eigenstate realization algorithm (ERA) to construct a system realization from measurement results. By solving the polynomial equations obtained from the transfer function, they identified the unknown parameters in the Hamiltonian. Recently, Wang *et al.* [20] proposed an approximate QHI method based on time traces and a matrix logarithm expansion. Using this method, the truncation error in the final estimation decreases exponentially with the length of experimental data.

In this paper, we follow the idea in [19] and [20] to perform QHI from measurement time traces. Based on a Taylor expansion of the matrix exponential function, we design a new QHI algorithm. We consider the robustness of the proposed algorithm in the presence of Gaussian additive noise, which was not considered in [20]. We prove theoretically that the estimation error in this algorithm is linear in the variance of the noise. We perform numerical simulations to validate the analysis results.

The organization of this paper is as follows. Section II formulates the quantum Hamiltonian identification problem. Section III presents our QHI algorithm, analyzes its ro-

*This work was supported by the Australian Research Council's Discovery Projects funding scheme under Project DP130101658 and Laureate Fellowship FL110100020, and the AFOSR under grant FA2386-16-1-4065.

[1]School of Engineering and Information Technology, University of New South Wales, Canberra, ACT 2600, Australia yuanlong.wang.qc@gmail.com, daoyidong@gmail.com

[2]Centre for Quantum Computation and Communication Technology, Australian Research Council, Canberra, ACT 2600, Australia

[3]Research School of Engineering, Australian National University, Canberra, ACT 0200, Australia i.r.petersen@gmail.com

bustness, and discusses the optimization of the sampling period. Numerical results on the estimation error versus noise variance and sampling period are given in Section IV. Section V concludes this paper and proposes possible directions for future research.

II. Problem Formulation

We first rephrase the framework in [19] to formulate the QHI problem. Let H denote the Hamiltonian to be identified and let $\mathfrak{su}(d)$ denote the Lie algebra consisting of all $d \times d$ skew-Hermitian matrices. Then $i\mathrm{H} \in \mathfrak{su}(d)$ where $i = \sqrt{-1}$. Let $\{i\mathrm{H_j}\}$ $(j = 1, 2, ..., d^2-1)$ be a set of orthonormal bases of $\mathfrak{su}(d)$, with $d \times d$ Hermitian matrices $\mathrm{H_j}$ known and the inner product defined as $\langle i\mathrm{H_j}, i\mathrm{H_k}\rangle = \mathrm{Tr}(\mathrm{H_j}^\dagger \mathrm{H_k})$. Then we parameterize the system Hamiltonian H as

$$\mathrm{H} = \sum_{m=1}^{M} h_m \mathrm{H_m}, \tag{1}$$

where $h_m \in \mathcal{R}$ are unknown parameters to be estimated. M is a known number determined by the specific structure of the considered quantum system.

Let C_{jkl} denote the structure constants of $\mathfrak{su}(d)$, which satisfy

$$[i\mathrm{H_j}, i\mathrm{H_k}] = \sum_{l=1}^{d^2-1} C_{jkl}(i\mathrm{H_l}), \qquad j, k = 1, ..., d^2-1, \tag{2}$$

where $[A, B] = AB - BA$. Without loss of generality we assume that the C_{jkl} are real. Let ρ be the system state, whose evolution is determined by the Liouville-von Neumann equation

$$\dot{\rho} = -i[\mathrm{H}, \rho]. \tag{3}$$

If $\mathrm{H_j}$ is an observable, the experimental data can be obtained from Born's rule

$$x_j = \mathrm{Tr}(\mathrm{H_j}\rho). \tag{4}$$

Combining (1)-(4), we obtain

$$\dot{x}_k = \sum_{l=1}^{d^2-1} (\sum_{m=1}^{M} C_{mkl} h_m) x_l. \tag{5}$$

Define a matrix A with its element on k^{th} row and l^{th} column as

$$\mathrm{A}_{kl} = \sum_{m=1}^{M} C_{mkl} h_m, \tag{6}$$

and we rewrite (5) in matrix form as

$$\dot{\mathbf{x}} = \mathrm{A}\mathbf{x}, \tag{7}$$

where $\mathbf{x} = (x_1, x_2, ..., x_{d^2-1})^T$. We can further write the observation equation as

$$y = \mathbf{c}^T \mathbf{x}. \tag{8}$$

For example, if we only observe $\mathrm{H_2}$, then $\mathbf{c}^T = (0, 1, 0, ..., 0)$. If we design an algorithm to identify A_{kl}, then we can estimate h_m and finally reconstruct H.

Remark 1: To further reduce the dimension of A, one can focus on the Lie subalgebra generated by H ($m = 1, 2, ..., M$). For specific procedures, one can refer to [19] and [21].

It is possible to have $M \ll d^2 - 1$ due to practical requirements (e.g., focusing on several parameters) or physical structures (e.g., spin chain). In such situations, (6) implies that we may only need to estimate some of the parameters in A to reconstruct H. We define the matrix $\bar{\mathrm{C}}$ as

$$\begin{pmatrix} C_{111} & C_{211} & \cdots & C_{M11} \\ C_{121} & C_{221} & \cdots & C_{M21} \\ \cdots & \cdots & \cdots & \cdots \\ C_{1(d^2-1)1} & C_{2(d^2-1)1} & \cdots & C_{M(d^2-1)1} \\ C_{1(d^2-1)2} & C_{2(d^2-1)2} & \cdots & C_{M(d^2-1)2} \\ \cdots & \cdots & \cdots & \cdots \\ C_{1(d^2-1)(d^2-1)} & C_{2(d^2-1)(d^2-1)} & \cdots & C_{M(d^2-1)(d^2-1)} \end{pmatrix}.$$

We take M rows from $\bar{\mathrm{C}}$ to form a nonsingular matrix $\tilde{\mathrm{C}}$. For those A_{kl} whose corresponding $C_{mkl} \in \tilde{\mathrm{C}}$, we write them into an $M \times 1$ vector $\tilde{\mathbf{a}}$. Let

$$\mathbf{h} = (h_1, h_2, ..., h_M)^T.$$

Then we have

$$\tilde{\mathbf{a}} = \tilde{\mathrm{C}}\mathbf{h}. \tag{9}$$

To estimate $\tilde{\mathbf{a}}$, which may have a much lower dimension than $\mathbf{x}$, we aim to design an efficient algorithm to estimate one element of $\tilde{\mathbf{a}}$ at each time. Let I denote the identity matrix. We formulate the QHI problem as follows:

Problem 1: Consider a real linear system

$$\begin{cases} \dot{\mathbf{x}}(t) = \mathrm{A}\mathbf{x}(t), \quad \mathbf{x}(0) = \mathbf{x}_0, \\ y(t) = \mathbf{c}^T \mathbf{x}(t). \end{cases} \tag{10}$$

Let $\mathbf{e_j}$ denote the j^{th} column of I. We assume that $\mathbf{c}$ and $\mathbf{x}_0$ can be chosen as any $\mathbf{e_j}$ $(1 \le j \le d^2-1)$ with a proper experimental setup. The QHI problem is to design an efficient method to identify A_{ab} $(1 \le a, b \le d^2-1)$.

III. Hamiltonian Identification Algorithm

A. Identification Algorithm

In classical control theory, the methods to solve Problem 1 usually take A as a whole and estimate all of its elements [22], and the algorithm efficiency is severely restricted by the dimension of A. In quantum systems, the dimension increases exponentially with the number of least information unit (qubit), which makes many dimension-dependent algorithms impractical for many-qubit systems. Furthermore, when people are only interested in some (instead of all) of the unknown parameters, it will be unnecessary to reconstruct all the elements in A. Here we propose an effective algorithm on the basis of proper prior knowledge and experimental setting.

Let $\hat{x}$ denote the estimation of the variable x in this paper. We assume that the experimental data is obtained through sampling the system with a period Δt. Suppose $\mathbf{x}_0 = \mathbf{e_k}$. For the observable $\mathrm{H_i}$, the j^{th} data value is

$$\begin{aligned} \hat{y}(j\Delta t) &= \mathbf{c}^T e^{\mathrm{A}j\Delta t}\mathbf{x}_0 \\ &= \textstyle\sum_{r=0}^{\infty} \frac{j^r \Delta t^r}{r!} \mathbf{c}^T \mathrm{A}^r \mathbf{x}_0 \\ &= \delta_{ik} + \textstyle\sum_{r=1}^{\infty} \frac{j^r \Delta t^r}{r!} (\mathrm{A}^r)_{ik}, \end{aligned} \tag{11}$$

where δ is the Kronecker delta function.

Let $\theta = (\theta_1, \theta_2, ..., \theta_n)^T$ where $\theta_r = (\mathrm{A}^r)_{ik}$. The determination of the number n will be illustrated later. Suppose the data length is N, which is usually determined by experiments. We let

$$\hat{\mathbf{y}}^N = [\hat{y}(\Delta t) - \delta_{ik}, \hat{y}(2\Delta t) - \delta_{ik}, ..., \hat{y}(N\Delta t) - \delta_{ik}]^T.$$

We truncate the infinite series in (11) and rewrite it into a matrix form

$$\hat{\mathbf{y}}^N \approx \mathrm{K}\theta, \tag{12}$$

where

$$\mathrm{K} = \begin{pmatrix} \frac{1^1\Delta t^1}{1!} & \frac{1^2\Delta t^2}{2!} & \cdots & \frac{1^n\Delta t^n}{n!} \\ \frac{2^1\Delta t^1}{1!} & \frac{2^2\Delta t^2}{2!} & \cdots & \frac{2^n\Delta t^n}{n!} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{N^1\Delta t^1}{1!} & \frac{N^2\Delta t^2}{2!} & \cdots & \frac{N^n\Delta t^n}{n!} \end{pmatrix}_{N\times n}. \tag{13}$$

Then we use a least squares method to obtain an estimate

$$\hat{\theta} = (\mathrm{K}^T\mathrm{K})^{-1}\mathrm{K}^T\hat{\mathbf{y}}, \tag{14}$$

and we have $\hat{\mathrm{A}}_{jk} = \hat{\theta}_1$.

The procedure of our algorithm is outlined as follows:

Algorithm 1: Step 1. Determine $\tilde{\mathbf{a}}$, $\tilde{\mathrm{C}}$ and the sampling period Δt. n should be chosen such that $n \leq N$.

Step 2. For $C_{mab} \in \tilde{\mathrm{C}}$, set the initial state as $\mathbf{x}_0 = \mathbf{e_b}$ and observe $\mathrm{H_a}$. Record the sampled data value $\hat{\mathbf{y}}^N$.

Step 3. Estimate $\hat{\theta}$ using (14). Then $\hat{\mathrm{A}}_{ab} = \hat{\theta}_1$.

Step 4. Change a and b and repeat Step 2 and Step 3 to estimate all elements in $\tilde{\mathbf{a}}$.

Step 5. $\hat{\mathrm{H}}$ is obtained using (1) and (9).

B. Robustness Analysis

We present the following theorem to characterize the robustness of our algorithm.

Theorem 1: Assume the experimental data is subject to additive Gaussian noise with zero mean and correlation matrix $\sigma^2 I$. Using our algorithm, the mean squared error (MSE) $E[\mathrm{Tr}(\hat{\mathrm{H}} - \mathrm{H})^2]$ is linear in σ^2, where $E(\cdot)$ denotes expectation.

Proof: Let η denote the noise vector such that $\hat{\mathbf{y}}^N = \mathbf{y}^N + \eta$. Also let

$$\mathrm{R} = \sum_{r=n+1}^{\infty} \frac{\Delta t^r}{r!}(\mathrm{A}^r)_{ik}(1^r, 2^r, ..., N^r)^T.$$

Its convergence can be seen from the fact that the factorial function increases much faster than the power function. The estimated vector is

$$\begin{aligned} \hat{\theta} &= (\mathrm{K}^T\mathrm{K})^{-1}\mathrm{K}^T(\mathbf{y}^N + \eta) \\ &= (\mathrm{K}^T\mathrm{K})^{-1}\mathrm{K}^T(\mathrm{K}\theta + \mathrm{R} + \eta) \\ &= \theta + (\mathrm{K}^T\mathrm{K})^{-1}\mathrm{K}^T\mathrm{R} + (\mathrm{K}^T\mathrm{K})^{-1}\mathrm{K}^T\eta. \end{aligned} \tag{15}$$

We then have

$$\begin{aligned} &E[(\hat{\theta}_1 - \theta_1)^2] \\ &= E[(\mathbf{e_1}^T\hat{\theta} - \mathbf{e_1}^T\theta)^2] \\ &= \mathrm{R}^T\mathrm{K}(\mathrm{K}^T\mathrm{K})^{-1}\mathbf{e_1}\mathbf{e_1}^T(\mathrm{K}^T\mathrm{K})^{-1}\mathrm{K}^T\mathrm{R} \\ &\quad + \mathrm{Tr}[\mathrm{K}(\mathrm{K}^T\mathrm{K})^{-1}\mathbf{e_1}\mathbf{e_1}^T(\mathrm{K}^T\mathrm{K})^{-1}\mathrm{K}^T\eta\eta^T] \\ &= [\mathrm{R}^T\mathrm{K}(\mathrm{K}^T\mathrm{K})^{-1}\mathbf{e_1}]^2 + \sigma^2\mathbf{e_1}^T(\mathrm{K}^T\mathrm{K})^{-1}\mathbf{e_1}. \end{aligned} \tag{16}$$

Therefore $E[(\hat{\mathrm{A}}_{ik} - \mathrm{A}_{ik})^2]$ is linear in σ^2. Similarly,

$$E[(\hat{\mathrm{A}}_{ik} - \mathrm{A}_{ik})(\hat{\mathrm{A}}_{ab} - \mathrm{A}_{ab})] \quad ((i,k) \neq (a,b))$$

is also linear in σ^2. Furthermore,

$$\begin{aligned} &E[\mathrm{Tr}(\hat{\mathrm{H}} - \mathrm{H})^2] \\ &= E\{\mathrm{Tr}[(\hat{\mathbf{h}} - \mathbf{h})(\hat{\mathbf{h}} - \mathbf{h})^T]\} \\ &= E\{\mathrm{Tr}[\tilde{\mathrm{C}}^{-T}\tilde{\mathrm{C}}^{-1}(\hat{\tilde{\mathbf{a}}} - \tilde{\mathbf{a}})(\hat{\tilde{\mathbf{a}}} - \tilde{\mathbf{a}})^T]\}, \end{aligned} \tag{17}$$

which is also linear in σ^2. ■

C. Optimization of the Sampling Period

The sampling period is a key index affecting the final estimation error. We present two factors guiding the choice of Δt.

First, as illustrated in the supplementary material of [19], the Nyquist Sampling Theorem leads to an upper bound for Δt. Assume that we have the prior knowledge $||\mathrm{A}|| \leq F$, where $||\cdot||$ is the Frobenius norm. Then we require

$$\Delta t < \frac{\pi}{F}. \tag{18}$$

Second, (16) leads to a critical value that Δt is not recommended to surpass. Let

$$D_1 = \mathrm{R}^T\mathrm{K}(\mathrm{K}^T\mathrm{K})^{-1}\mathbf{e_1}.$$

We can say that D_1 is associated with the norm of R. Using Stirling's Formula, the absolute value of each item in the summation defining R can be approximated as

$$\begin{aligned} &|\tfrac{j^r\Delta t^r}{r!}(\mathrm{A}^r)_{ik}| \\ &\approx \tfrac{1}{\sqrt{2\pi r}}\tfrac{(j\Delta te)^r}{r^r}|(\mathrm{A}^r)_{ik}| \\ &= \tfrac{1}{\sqrt{2\pi r}}(\tfrac{j\Delta te}{r})^r|\mathbf{e_i}^T\mathrm{A}^r\mathbf{e_k}| \\ &\leq \tfrac{1}{\sqrt{2\pi r}}(\tfrac{j\Delta te}{r})^r||\mathbf{e_i}^T|| \cdot ||\mathrm{A}||^r \cdot ||\mathbf{e_k}|| \\ &\leq \tfrac{1}{\sqrt{2\pi r}}(\tfrac{NF\Delta te}{r})^r. \end{aligned} \tag{19}$$

To add up these terms in (19) from $r = n+1$ to infinity, one can anticipate that if $\frac{NF\Delta te}{r}$ is less than 1, then the summation would quickly converge, making this residual error R small enough to reduce the identification error in our algorithm. Therefore it is recommended to have

$$\frac{NF\Delta te}{n+1} \leq 1,$$

which indicates

$$\Delta t \leq \frac{n+1}{NFe}. \tag{20}$$

Remark 2: It is worth mentioning that only the first critical point is strict. The second point is heuristic and relies on proper prior knowledge. It can provide suggestions on choosing the order of magnitude of Δt.

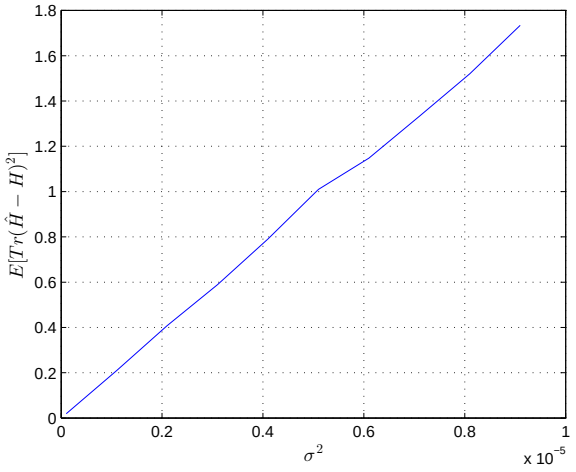

Fig. 1. Identification error $E[\mathrm{Tr}(\hat{\mathrm{H}}-\mathrm{H})^2]$ versus noise variance σ^2 for a single-qubit system.

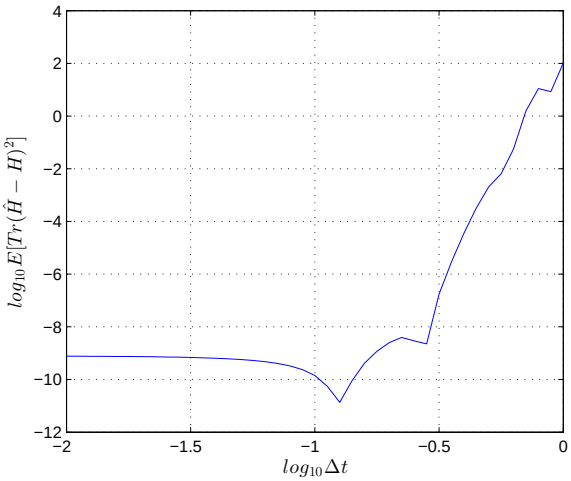

Fig. 2. Truncation error $\log_{10} E[\mathrm{Tr}(\hat{\mathrm{H}}-\mathrm{H})^2]$ versus sampling period $\log_{10}\Delta t$ for a single-qubit system.

IV. Numerical Results

A. Case Study for a Single-qubit System

We consider a single-qubit system with Hamiltonian

$$\mathrm{H}=\sum_{i=x,y,z} f_i\sigma_{\mathrm{i}}, \tag{21}$$

where f_i $(i=x,y,z)$ are real unknown parameters and the following Pauli matrices are used:

$$\sigma_x=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_y=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad \sigma_z=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}.$$

We have

$$\mathbf{h}=\frac{1}{\sqrt{2}}(f_x,f_y,f_z)^T$$

and the true value is $(0.1,0.3,-0.8)^T$ (units 1/sec). The corresponding basis matrices are

$$\mathrm{H}_1=\sigma_{\mathrm{x}},\ \mathrm{H}_2=\sigma_{\mathrm{y}} \text{ and } \mathrm{H}_3=\sigma_{\mathrm{z}}.$$

Then the structure constants C_{jkl} are proportional to Levi-Civita symbols. We have

$$\mathrm{A}=\sqrt{2}\begin{pmatrix}0 & -f_3 & f_2\\ f_3 & 0 & -f_1\\ -f_2 & f_1 & 0\end{pmatrix},$$

$$\tilde{\mathbf{a}}=(\mathrm{A}_{32},\mathrm{A}_{13},\mathrm{A}_{21})^T$$

and

$$\tilde{\mathrm{C}}=\begin{pmatrix}-1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1\end{pmatrix}.$$

We first use the proposed algorithm to identify the Hamiltonian under different noise variances. The sampling period used is 0.05 (unit s is omitted henceforth). The data length N is 25 and n is 20 in the simulation. The simulation results are shown in Fig. 1, which verifies the conclusion of Theorem 1. Each point is repeated 500 times.

If we make $\sigma=0$, the estimation error will mainly come from the truncation error in our algorithm. We keep the sampling period and data length the same as those in Fig. 1. A plot of the truncation error versus sampling period is shown in Fig. 2. As the sampling period increases, the truncation error has an increasing trend, which is in agreement with the analysis in Subsection III-C.

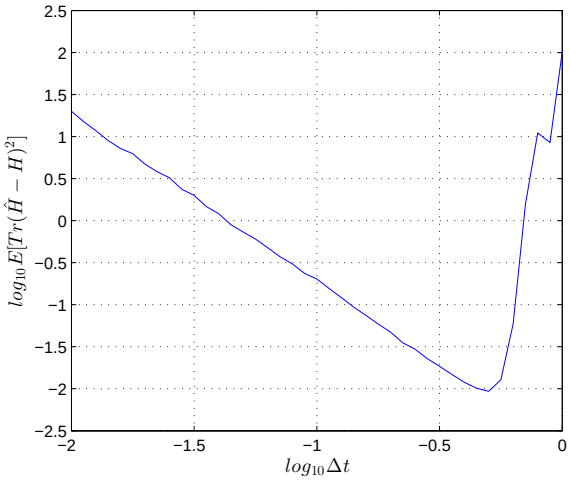

Fig. 3. Identification error $\log_{10} E[\mathrm{Tr}(\hat{\mathrm{H}}-\mathrm{H})^2]$ versus sampling period $\log_{10}\Delta t$ for a single-qubit system.

We then simulate the effect of different sampling periods on the estimation error with additive Gaussian noise. We fix the variance of the noise as $\sigma^2=4\times10^{-6}$ and apply the identification algorithm with different sampling periods. The simulation result is shown in Fig. 3 where each point is repeated 500 times. Assume that we have prior knowledge $||\mathrm{A}||\le 2$. Then (18) gives $\Delta t<2.5824$. Furthermore, (20) gives $\Delta t\le 0.1472$, which is of the same order of magnitude as the optimal value in Fig. 3.

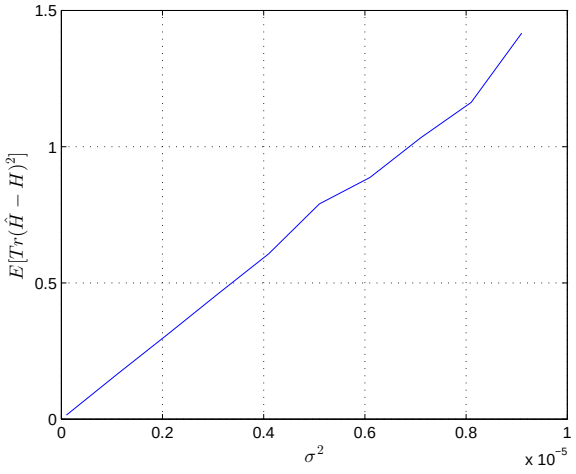

Fig. 4. Identification error $E[\mathrm{Tr}(\hat{\mathrm{H}}-\mathrm{H})^2]$ versus noise variance σ^2 for a 1D Chain System.

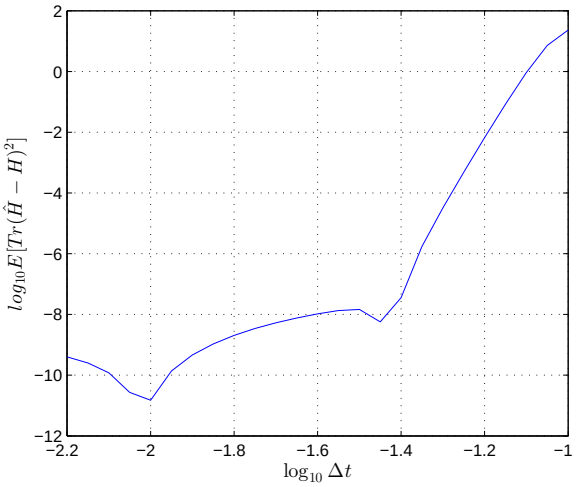

Fig. 5. Truncation error $\log_{10} E[\mathrm{Tr}(\hat{\mathrm{H}}-\mathrm{H})^2]$ versus sampling period $\log_{10}\Delta t$ for a 1D Chain System.

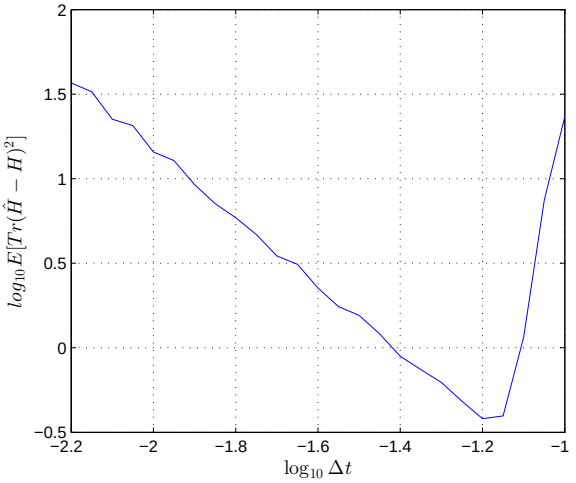

Fig. 6. Identification error $\log_{10} E[\mathrm{Tr}(\hat{\mathrm{H}}-\mathrm{H})^2]$ versus sampling period $\log_{10}\Delta t$ for a 1D Chain System.

B. Case Study for a 1D Chain System

For multi-qubit systems, we present numerical results for a 1D chain system with N_q qubits:

$$\mathrm{H}=\sum_{k=1}^{N_q}\frac{\omega_k}{2}\sigma_{\mathrm{z}}^{\mathrm{k}}+\sum_{k=1}^{N_q-1}\delta_k(\sigma_{+}^{\mathrm{k}}\sigma_{-}^{\mathrm{k+1}}+\sigma_{-}^{\mathrm{k}}\sigma_{+}^{\mathrm{k+1}}), \qquad (22)$$

where ω_k and δ_k are the unknown real parameters and $\sigma_{\pm}=\sigma_x\pm i\sigma_y$. This is also the model used in [19]. We focus on $N_q=3$. To normalize the basis matrices, we have

$$\mathbf{h}=(\frac{\omega_1}{2},\frac{\omega_2}{2},\frac{\omega_3}{2},2\delta_1,2\delta_2)^T$$

and the true value is $(3.8,-4,0.4,5.3,-1.1)^T$ (units 1/sec). The corresponding basis matrices are

$$\mathrm{H}_1=\sigma_{\mathrm{z}}^1,\ \mathrm{H}_2=\sigma_{\mathrm{z}}^2,\ \mathrm{H}_3=\sigma_{\mathrm{z}}^3,\ \mathrm{H}_4=\sigma_{\mathrm{x}}^1\sigma_{\mathrm{x}}^2,$$
$$\mathrm{H}_5=\sigma_{\mathrm{x}}^2\sigma_{\mathrm{x}}^3,\ \mathrm{H}_6=\sigma_{\mathrm{y}}^1\sigma_{\mathrm{x}}^2,\ \mathrm{H}_7=\sigma_{\mathrm{y}}^2\sigma_{\mathrm{x}}^3,\ \mathrm{H}_8=\sigma_{\mathrm{x}}^1,$$
$$\mathrm{H}_9=\sigma_{\mathrm{y}}^1,\ \mathrm{H}_{10}=\sigma_{\mathrm{x}}^1\sigma_{\mathrm{y}}^2,\ \mathrm{H}_{11}=\sigma_{\mathrm{x}}^3,\ \mathrm{H}_{12}=\sigma_{\mathrm{y}}^3.$$

We then have

$$\tilde{\mathbf{a}}=(\mathrm{A}_{27},\mathrm{A}_{16},\mathrm{A}_{89},\mathrm{A}_{4,10},\mathrm{A}_{11,12})^T$$

and

$$\tilde{\mathrm{C}}=\begin{pmatrix}0&0&0&0&2\\0&0&0&2&0\\-2&0&0&0&0\\0&-2&0&0&0\\0&0&-2&0&0\end{pmatrix}.$$

We use the proposed algorithm to identify the Hamiltonian under different noise variances. The sampling period we used is 0.05. The data length N is 25. n is taken as 20 in the simulation. The simulation result is shown in Fig. 4, which is consistent with the conclusion of Theorem 1. Each point is repeated 500 times.

We then set $\sigma=0$ to test the truncation error of our algorithm. We keep the sampling period and data length the same as those in Fig. 4. The result of the truncation error versus sampling period is shown in Fig. 5. As the sampling period increases, the truncation error has an increasing trend.

We finally simulate the estimation error with additive Gaussian noise in the measured data under different sampling periods. We fix the variance of the noise as $\sigma^2=4\times10^{-6}$ and apply the identification algorithm under different sampling periods. The numerical result is shown in Fig. 6 and each point is repeated 500 times. Assume that we have prior knowledge $||\mathrm{A}||\le 12$. Then (18) gives $\Delta t<0.5589$. Furthermore, (20) gives $\Delta t\le 0.0258$, which is of the same order of magnitude as the optimal value in Fig. 6.

V. Conclusion

We have presented a quantum Hamiltonian identification algorithm under the assumption that the system initial state and observation matrix can be set appropriately. We proved theoretically that the estimation error is linear in the variance of the additive Gaussian noise and performed simulations to validate this conclusion. We also proposed a heuristic formu-

la to suggest the order of magnitude of the optimal sampling period. Future work includes a better characterization of the relationship between the estimation error and the sampling period, and possible improvement on the robustness of the algorithm.

REFERENCES

[1] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* Cambridge, Cambridge University Press, 2000.

[2] D. Burgarth and K. Yuasa, "Quantum system identification," *Phys. Rev. Lett.*, vol. 108, no. 8, 080502, 2012.

[3] B. Qi, Z. Hou, L. Li, D. Dong, G.-Y. Xiang, G.-C. Guo, "Quantum state tomography via linear regression estimation," *Sci. Rep.*, vol. 3, no. 3496, 2013.

[4] Z. Hou, H.-S. Zhong, Y. Tian, D. Dong, B. Qi, L. Li, Y. Wang, F. Nori, G.-Y. Xiang, C.-F. Li and G.-C. Guo, "Full reconstruction of a 14-qubit state within four hours," *New J. Phys.*, vol. 18, 2016, Art. ID 083036.

[5] B. Qi, Z. Hou, Y. Wang, D. Dong, H.-S. Zhong, L. Li, G.-Y. Xiang, H. M. Wiseman, C.-F. Li and G.-C. Guo, "Adaptive quantum state tomography via linear regression estimation: Theory and two-qubit experiment," *npj Quantum Inform.*, 3:19, 2017.

[6] M. Guţă and N. Yamamoto, "System identification for passive linear quantum systems," *IEEE Trans. Autom. Control*, vol. 61, no. 4, pp. 921-936, 2016.

[7] Y. Wang, B. Qi, D. Dong and I. R. Petersen, "An iterative algorithm for Hamiltonian identification of quantum systems," in *Proc. 55th IEEE Conf. Decision Control*, pp. 2523-2528, Las Vegas, NV, USA, Dec. 12-14, 2016.

[8] 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*, in press, doi: 10.1109/TAC.2017.2747507, arXiv: 1610.08841, 2016.

[9] A. Sone and P. Cappellaro, "Hamiltonian identifiability assisted by single-probe measurement," *Phys. Rev. A*, vol. 95, no. 2, 022335, 2017.

[10] S. Bonnabel, M. Mirrahimi and P. Rouchon, "Observer-based Hamiltonian identification for quantum systems," *Automatica*, vol. 45, no. 5, pp. 1144-1155, 2009.

[11] C. Le Bris, M. Mirrahimi, H. Rabitz and G. Turinici, "Hamiltonian identificaiton for quantum systems: well-posedness and numerical approaches," *ESAIM: COCV*, vol. 13, no. 2, pp. 378-395, 2007.

[12] M. Mohseni, A. T. Rezakhani and A. Aspuru-Guzik, "Direct estimation of single- and two-qubit Hamiltonians and relaxation rates," *Phys. Rev. A*, vol. 77, no. 4, 042320, 2008.

[13] J. H. Cole, S. G. Schirmer, A. D. Greentree, C. J. Wellard, D. K. L. Oi and L. C. L. Hollenberg, "Identifying an experimental two-state Hamiltonian to arbitrary accuracy," *Phys. Rev. A*, vol. 71, no. 6, 062312, 2005.

[14] J. H. Cole, S. J. Devitt and L. C. L. Hollenberg, "Precision characterization of two-qubit Hamiltonians via entanglement mapping," *J. Phys. A: Math. Gen.*, vol. 39, no. 47, 14649, 2006.

[15] M. Holzäpfel, T. Baumgratz, M. Cramer and M. B. Plenio, "Scalable reconstruction of unitary processes and Hamiltonians," *Phys. Rev. A*, vol. 91, no. 4, 042129, 2015.

[16] K. Rudinger and R. Joynt, "Compressed sensing for Hamiltonian reconstruction," *Phys. Rev. A*, vol. 92, no. 5, 052322, 2015.

[17] 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, 187203, 2009.

[18] S. T. Wang, D. L. Deng and L. M. Duan, "Hamiltonian tomography for quantum many-body systems with arbitrary couplings," *New J. Phys.*, vol. 17, no. 9, 093017, 2015.

[19] J. Zhang and M. Sarovar, "Quantum Hamiltonian identification from measurement time traces," *Phys. Rev. Lett.*, vol. 113, no. 8, 080401, 2014.

[20] Y. Wang, D. Dong, I. R. Petersen and J. Zhang, "An approximate algorithm for quantum Hamiltonian identification, its complexity and error analysis," *Proc. 20th IFAC World Congr.*, Toulouse, France, 9-14 July, 2017.

[21] A. Sone and P. Cappellaro, "Dimension estimability via single-probe measurement," *arXiv preprint*, quant-ph, arXiv: 1702.03280, 2017.

[22] L. Ljung, *System Identification: Theory for the User*, New Jersey, Prentice Hall, 1999.