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Article

# Experimental quantum Hamiltonian identification from measurement time traces

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ABSTRACT

Identifying Hamiltonian of a quantum system is of vital importance for quantum information processing. In this article, we realized and benchmarked a quantum Hamiltonian identification algorithm recently proposed (Zhang and Sarovar, 2014). we realized the algorithm on a liquid nuclear magnetic resonance quantum information processor using two types of working media with different forms of Hamiltonian. Our experiment realized the quantum identification algorithm based on free induction decay signals. We also showed how to process data obtained in a practical experiment. We studied the influence of decoherence by numerical simulations. Our experiments and simulations demonstrate that the algorithm is effective and robust.



## 1. Introduction

One critical task in quantum information processing is to characterize a quantum system so that it can be used for tasks, such as quantum teleportation [1,2], quantum cryptography [3,4], quantum computation [5,6], quantum simulation [7–11] and quantum metrology [12,13]. One way of fully characterizing a quantum system is doing quantum state tomography (QST) and quantum processing tomography (QPT) [14–19]. The QPT approach requires an exponential number of experiments, which makes it difficult to be realized for even a small sized quantum system [20–23].

Meanwhile, various methods based on measurement time traces for Hamiltonian identification have been proposed for general quantum systems. Fourier transformation (FT) of only one measurement observable is used for a single qubit Hamiltonian identification [24]. Temporal evolution of concurrence measure of entanglement is employed to identify arbitrary two-qubit Hamiltonian [25]. Hamiltonian identification using dynamical decouplings was proposed [26]. Schemes of estimating the coupling parameters for a complex quantum network based on measurements of a small part of the network were proposed [27,28]. A basic and general quantum system identification framework has been established on how much knowledge that is attainable about a quantum system for a given experimental setup [29]. Very recently, Zhang and Sarovar [30] proposed an efficient approach (the ZS approach) for identifying arbitrary Hamiltonian quantum dynamics, taking advantage of available prior knowledge of the system.

One typical dynamical system is the nuclear magnetic resonance (NMR) system, which is well described by quantum mechanics. Moreover, its control technology has been well developed during the 50 years since the birth of NMR. These factors make the NMR system an appealing quantum system for sophisticated manipulation. Therefore, NMR systems are widely used for quantum information processing [31,32]. To obtain the information of an NMR system, modern NMR spectrometers acquire the free induction decay (FID) signals, which are the measurement time traces of certain observables. Schemes based on FT (e.g. FT-NMR) of the FID signals, which is one of the most robust ways of processing FID, have been developed [33,34]. Because the ZS approach is based on measurement time traces for an arbitrary quantum system, the NMR spectrometer provides a practical and controllable system for demonstrating and benchmarking the ZS approach.

In this article, we implemented the ZS approach on an NMR quantum information processor and compared the result with that of FT approach. The experiments were performed with two types of working media with different Hamiltonian forms. Because of different Hamiltonian forms, we have to choose different measurement observables which require distinct experimental setups.

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Unlike works of NMR quantum computing in last two decades, we started from the thermal equilibrium state rather than the pseudo-pure state, and directly processed the FID signals. Our experiments demonstrated that the ZS is an very efficient approach for Hamiltonian identification. We also analysed the influences of imperfect experiment conditions and decoherence on the results using numerical simulations.

## 2. Algorithm

Here we briefly describe the ZS approach.[1] Suppose now we have an $n$-qubit quantum system with Hamiltonian $\widehat{H}$. With the initial state $\rho(0)$, the system evolves, governed by the Hamiltonian $\widehat{H}$. During the evolution, the expectation value of an observable $O$ at time $t$ is measured and recorded as $\mathbf{y}(t)$. $\mathbf{y}(t)$ is also called the measurement time trace of observable $O$. The Hamiltonian can be written in a parametrized form,

$$\widehat{H} = \sum_m a_m X_m, \tag{1}$$

where $a_m$ is the unknown parameters to be acquired, $X_m \in S = \{X_k | X_k = \sigma_\alpha \otimes \sigma_\beta \otimes \cdots \otimes \sigma_\gamma$, and $X_k \neq \mathbf{I}\}$, and $\sigma_\alpha, \sigma_\beta$ and $\sigma_\gamma$ are the Pauli matrices $\sigma_x, \sigma_y$ and $\sigma_z$ and $2 \times 2$ identity operator $I_2$. The number of the elements in $S$ is $4^n - 1$. However, if taken into consideration of a practical physical system, the number of the non-zero $a_m$'s can be significantly decreased.

All the elements in set $S$ are Hermitian operators. However, because of the physical constraints, only some of them can be easily measured, e.g., only the transverse magnetization in NMR, denoted by operator $\sigma_x$ ($\sigma_y$), can be observed. The temporal record of the expectations of such an observable $O$ can be collected, which is called a measurement time trace, and denoted by $\mathbf{y}(t)$, then $\mathbf{y}(t) = \mathrm{Tr}\{O\rho(t)\}$, with $\rho(t)$ being the density matrix at time $t$. Let $\mathbf{y}(t)$ be treated as an output of a linear system, and if we can find a set of $[\mathbf{C}_0, \mathbf{A}_0, \mathbf{x}_0(0)]$, which satisfies $\mathbf{y}(t) = \mathbf{C}_0 e^{\mathbf{A}_0 t}\mathbf{x}_0(0)$, we call this set a *realization*. For a certain output, various realizations can be obtained. Among these realizations, an invariant function, called *transfer function* $Y(s)$ exists, which is actually the Laplace transformation of the output, i.e.

$$Y(s) = \mathcal{L}(\mathbf{y}(t)) = \mathbf{C}_0(s\mathbf{I} - \mathbf{A}_0)^{-1}\mathbf{x}_0(0), \tag{2}$$

where $s$ is Laplace variable, $\mathcal{L}$ denotes Laplace transformation, and $\mathbf{I}$ is the density matrix with the same dimension of $\mathbf{A}_0$. The basic idea of the ZS approach is to find two realizations, one with all the unknown parameters $a_m$ (called realization 1, denoted by $[\mathbf{C}, \widetilde{\mathbf{A}}, \mathbf{x}_a(0)]$) and the other (called realization 2, denoted by $[\widehat{\mathbf{C}}, \widehat{\mathbf{A}}, \hat{\mathbf{x}}(0)]$) with completely known numbers. With these two realizations, the coefficients of the Laplace variable $s$ can be compared, hence the unknown parameters can be obtained,[2] i.e.,

$$\mathbf{C}(s\mathbf{I} - \widetilde{\mathbf{A}})^{-1}\mathbf{x}_a(0) = \widehat{\mathbf{C}}(s\mathbf{I} - \widehat{\mathbf{A}})^{-1}\hat{\mathbf{x}}(0). \tag{3}$$

A schematic of the ZS approach is shown in Fig. 1.

Realization 1 is obtained from the parametrized Hamiltonian $\widehat{H}$, the observable $O$ and the initial state $\rho(0)$. The observable and the initial state are appropriately chosen artificially according to the structure of a physical system. In such case, the vector $\mathbf{x}_a(0)$ describes the initial system state $\rho(0)$, the matrix $\tilde{\mathbf{A}}$ describes the dynamical evolution driven by $\widehat{H}$, and the matrix $\mathbf{C}$ predicts the measurement outcome $\mathbf{y}(t)$ for the system state $\mathbf{x}_t$.

Realization 2 is obtained solely by performing numerical methods, without relying on specific knowledge of the underlying system. One way to do so is the eigenstate realization algorithm (ERA) [35]. Technical details on how to obtain the two realizations is out of the scope of this article and shown in the Electronic Supplementary Material.

## 3. Experiments setup and results.

The ZS approach was tested in a two-qubit and a three-qubit NMR system, which were implemented with $^{13}$C-labelled trichloroethylene (TCE) and $^{13}$C-labelled L-alanine (ALA) as the working media, respectively. The molecular structures and the thermal spectra of ALA and TCE are shown in Fig. 2.

The Hamiltonian of a liquid NMR system is ($\hbar = 1$)

$$\widehat{H}_{\mathrm{NMR}} = \sum_{j=1}^{N} \pi \nu_j \sigma_z^j + \sum_{j>i=1}^{N} \frac{\pi J_{ij}}{2} \boldsymbol{\sigma}^i \cdot \boldsymbol{\sigma}^j, \tag{4}$$

where $2\pi\nu_i$ is the Larmor frequency for the $i$th spin, $J_{ij}$ is the indirect coupling constant between the $i$th and $j$th spin. In weak coupling, $|\nu_i - \nu_j| \gg |J_{ij}|$, which is valid for ALA, only the secular components of the scalar coupling survive. Hence the Hamiltonian of ALA is parametrized as

$$\widehat{H}_{\mathrm{ALA}} = a_1^{\mathrm{A}}\sigma_z^1 + a_2^{\mathrm{A}}\sigma_z^2 + a_3^{\mathrm{A}}\sigma_z^3 + a_4^{\mathrm{A}}\sigma_z^1\sigma_z^2 + a_5^{\mathrm{A}}\sigma_z^1\sigma_z^3 + a_6^{\mathrm{A}}\sigma_z^2\sigma_z^3. \tag{5}$$

TCE is strongly coupled, and its parametrized Hamiltonian has a more complicated form,

$$\widehat{H}_{\mathrm{TCE}} = a_1^{\mathrm{T}}\sigma_z^1 + a_2^{\mathrm{T}}\sigma_z^2 + a_3^{\mathrm{T}}(\sigma_x^1\sigma_x^2 + \sigma_y^1\sigma_y^2 + \sigma_z^1\sigma_z^2). \tag{6}$$

Once the Hamiltonian is parametrized, the observable can be decided. For TCE, $O^{\mathrm{T}} = \sigma_x^2$ is chosen, and one qubit time trace is sufficient to identify the whole Hamiltonian because of strong coupling. Whereas for ALA, $O^{\mathrm{A}} = \sigma_x^1 + \sigma_x^2 + \sigma_x^3$ has to be chosen as the observable because of the nature of the weak coupling Hamiltonian.

Then we prepare the initial states. Different forms of Hamiltonian require different experimental strategies. Different from NMR quantum computing with pseudo-pure initial state [31], Hamiltonian characterization should start directly from states that are easily prepared without knowing the Hamiltonian details, e.g., state $\rho(0) = \sum_j \sigma_x^j$. For ALA, we repeated the experiments for three times with three different initial states $\sigma_x^1, \sigma_x^2$, and $\sigma_x^3$, each corresponds to a different $\mathbf{x}_a(0)$ for ALA. Choosing three initial states instead of one simplifies the data processing procedure. For TCE, a single input state $\sigma_x^2$ is enough.

After preparation, $\rho(0)$ starts to evolve under the system Hamiltonian, hence the macroscopic magnetization in NMR rotates. The rotation of the magnetization induces an electromagnetic wave which is received by a coil, and the signal received is called the free induction decay(FID) signal. The FID signal acquired by modern NMR spectrometers contains real and imaginary parts. The real part is

$$V_R(t) = \alpha \mathrm{Tr}\{F_x \rho(t)\}, \tag{7}$$

where $\alpha$ is a coefficient related to the spectrometer, $\rho(t)$ is the density matrix of the system at time $t$, and $F_x = \sum_j \sigma_x^j$, where the summation includes the spins in the chosen observable. For TCE, only the second spin is observed and for ALA, all three qubits are observed. Thus the observable for TCE is $F_x^{\mathrm{T}} = \sigma_x^2$ and for ALA is $F_x^{\mathrm{A}} = \sigma_x^1 + \sigma_x^2 + \sigma_x^3$, which are exactly the observables we chose for

[1] Detailed information is given in the Electronic Supplementary Material, which also includes the details of the experiment and numerical simulations.

[2] Theoretically, the equation $\mathbf{y}(t) = \mathbf{C}e^{\mathbf{A}t}\mathbf{x}_a(0)$ can be solved to obtain all the unknown parameters in $\tilde{\mathbf{A}}$. However, the right hand side of this equation is a transcendental function of $a_m$'s, which makes it infeasible obtaining $a_m$'s.

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