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Direct estimation of single- and two-qubit Hamiltonians and relaxation rates

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We provide a novel approach for characterization of quantum Hamiltonian systems via utilizing a single measurement device. Specifically, we demonstrate how external quantum correlations can be used for Hamiltonian identification tasks. We explicitly introduce experimental procedures for direct estimation of single- and two-qubit Hamiltonian parameters, and also for simultaneous estimation of transverse and longitudinal relaxation rates, using a single Bell-state analyzer. An advantage of our method over the earlier approaches is that it has a built-in feature which makes it suitable for partial characterization of Hamiltonian parameters.

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I. INTRODUCTION

Characterization of quantum dynamical systems is one of the most fundamental problems in quantum physics, and lies at the heart of quantum information processing [1] and coherent control [2]. There are a few known methods to achieve this goal, such as standard quantum process tomography [3], ancilla-assisted process tomography [4], and direct characterization of quantum dynamics (DCQD) [5, 8, 9]. Since the required physical resources grow exponentially with the number of degrees of freedom, all quantum process tomography schemes are in principle inefficient. However, in various physical situations a full characterization of the quantum dynamical superoperator is not always necessary, as sometimes the information about relevant physical quantities could be related to only a polynomial number of parameters in the system size [8]. This is indeed the case when: (i) important physical properties of a quantum system can be directly associated only to a subset of certain superoperator elements, (ii) a priori knowledge exists about general properties of quantum dynamics, and (iii) neglecting some elements will lead to small system characterization errors.

The task of Hamiltonian identification, as a characterization of quantum systems, is of paramount importance in quantum physics and chemistry. In particular, it is required for monitoring or controlling performance of noisy single- and two-qubit quantum gates/devices in quantum information processing [10, 11]. For various physical systems, a generic form of the Hamiltonian can be guessed from general physical/engineering considerations or observations. However, one still needs to estimate the Hamiltonian parameters for a given quantum system in order to study the internal dynamics of the system and also to investigate the exact form and the strength of a potential system-bath coupling.

Identification of time-independent (or piece-wise constant) Hamiltonians along with the estimation of errors have already been studied for both single-qubit and two-qubit cases [10, 11]. Characterization of a single-qubit Hamiltonian is achieved via determination of the measurement results using a single fixed readout process which is a periodic function of time. Through Fourier analysis of this signal and other related techniques, identification is reduced to finding the (relative) location of peaks and their heights of the Fourier spectrum [10]. Similarly, in the two-qubit case, Hamiltonian parameters are obtained through some entanglement measurements sampled in many time points, and then a Fourier analysis determines the parameters [11]. There are also more general Hamiltonian identification schemes which employ closed-loop learning control techniques along with efficient and improved global laboratory data inversion for identification [12]. These techniques are useful particularly when one has access to tailored control fields (e.g., shaped laser pulses) while the measurements are being performed. A fundamental relevant question is how one can exploit external quantum correlations in order to enhance identification of quantum Hamiltonian systems. This is the subject we address in this work.

In this paper, we introduce an analytical method for direct characterization of important classes of Hamiltonians. This method is based on a newly proposed DCQD scheme [5]. In particular, we demonstrate how to estimate all parameters of a general time-independent single-qubit Hamiltonian and two-qubit (isotropic or anisotropic) exchange Hamiltonian. A distinctive feature of our method is that, when only some partial knowledge about the system is requested, it does not require Fourier analysis of the experimental data. In principle, this obviates the need for long sampling times and in turn offers more controllability for the related estimation process. Our Hamiltonian identification method is applicable to quantum systems enabling two-body measurements, due to the fact that DCQD requires Bell-state measurements (BSMs). The required BSM can be in principle achieved in linear optical systems via postselections [13] or hyperentanglement [14], and also in trapped ions [15] (see Ref. [16] for a deterministic, programmed generation of “ultralong lifetime” Bell-states), and optical lattices [17]. In solid-state systems, several schemes for controllable two-body interactions have been proposed [8, 18, 19, 20, 21, 22, 23], with the state of the art experimental realization in semiconductor quantum dots [24] and superconducting flux qubits [25].

The evolution of a $d$-dimensional quantum system (open or closed) with initial state $ρ$ can, under some natural assumptions, be expressed in terms of a completely positive quantum dynamical map $ξ_t$, which can be represented as:
Bell-state measurement\[\chi\]

The positive matrix $\chi = [\chi_{mn}]$ encompasses all information about the dynamics, relative to the fixed operator basis $\{\sigma_m\}$, where $tr(\sigma_m^+ \sigma_n) = b \delta_{mn}$. The theory of DCQD determines elements of $\chi$ matrix [5] by relating them to measurement results more directly than the other existing schemes. The main idea of DCQD is based on quantum error detection theory in which by preparation of suitable states and measurement of their stabilizers and normalizers partial information about errors can be obtained. The required stabilizer and normalizer measurement can be physically realized with a single Bell-state analyzer. Table[1] summarizes the scheme for the single-qubit case.

II. IDENTIFICATION OF SINGLE-QUBIT HAMILTONIANS

Let us consider the cases that quantum dynamics is generated by a time-independent Hamiltonian, $\hat{E}(\rho) = \hat{U}(t)^\dagger \rho \hat{U}(t)$, where $\hat{U}(t) = e^{-i \hat{H}t} (\hbar \equiv 1)$, one obtains $\chi_{mn} = a_m a_n^\dagger$, where $\hat{U}(t) = \sum_m a_m(t) \sigma_m$ and $\hat{H}$ is the Hamiltonian of the system. Since an energy shift is always possible, we only consider traceless Hamiltonians. In the single-qubit case, where $\hat{H} = \vec{J} \cdot \sigma$, with the choice of $\{\sigma = (\sigma_x, \sigma_y, \sigma_z)\}$ as the operator basis, we have: $\chi_{00} = c^2, \chi_{0\alpha} = s^2 \hat{J}_{\alpha}, \chi_{\alpha 0} = ics \hat{J}_y, \chi_{\alpha \beta} = s^2 \hat{J}_{\alpha} \hat{J}_{\beta}$, in which $\hat{J} = J \hat{J}$ ($J = || \hat{J} ||$, $c = \cos(\hat{J}t)$, $s = \sin(\hat{J}t)$ and $\alpha, \beta = x, y, z$.

In order to find the real vector $J$, according to the DCQD theory, we can choose different experimental configurations (measurement settings) depending on our a priori information about the Hamiltonian. If the signs of the Hamiltonian parameters (i.e., the components of $J$) are already known, we can determine $J$ and the absolute values of the components, $|\hat{J}_\alpha|$, in a single experimental configuration. First, we prepare a maximally entangled state between the qubit of interest $A$, and an ancilla, $B$, as $|\Phi^+\rangle_{AB} = (|00\rangle + |11\rangle)/\sqrt{2}$. Next, the system evolves under $\hat{H}$ for a duration of time $t$. Finally, we perform a measurement by the four projection operators $P_{0+}$ and $P_{0-}$. The probabilities of obtaining these outcomes are found as $tr[\hat{P}_k \hat{E}_i(\rho)] = c^2$ and $tr[\hat{P}_k \hat{E}_i(\rho)] = s^2 \hat{J}_{\alpha}$, where the projection operators $P_x$ and $P_\alpha$ (for $\alpha = x, y, z$) correspond to the states $|\Phi^+\rangle, |\Psi^+\rangle, |\Psi^-\rangle$, and $|\Phi^-\rangle$, respectively. Thus, we have

$$\hat{J}_\alpha^2 = \frac{tr[P_\alpha \hat{E}_i(\rho)]}{(1 - tr[P_\alpha \hat{E}_i(\rho)])}.$$

The diagonal elements of the superoperator give the absolute values of the unknown parameters $J_\alpha$. Equation (1) bears this interesting result that measurements at a single time-point $t$ are in principle (ignoring the inherent issue of statistical errors)” enough to obtain $(|J_x|, |J_y|, |J_z|)$. When the relative signs are already known, this uniquely identifies the reference frame of the Hamiltonian.

In order to obtain $J$, we are required to estimate the frequency of the function $\cos^2(Jt) = tr[\hat{P}_f \hat{E}_i(\rho)]$. The theory of signal processing and discrete Fourier analysis state that one generally needs to perform many time samplings to obtain frequency. By the Nyquist criterion, the sampling frequency $f_s = 1/T \leq \frac{1}{2}f_s$ must be bounded below by half of the frequency of the original signal, i.e., $f_s > J$, to reduce the inherent aliasing [24]. In Refs. [10, 11] one can find more detailed analysis of these issues and how to read $J$ from experimental data. Specifically, in Ref. [11(b)] an interesting method of ensemble measurements in sample points has been introduced that can reduce the statistical error in inference.

In the more general case, to fully characterize the real vector $J$ we need to consider a different strategy and perform two measurements for the off-diagonal elements of $\chi$. According to DCQD, these two experimental configurations are sufficient to determine the diagonal of the superoperator, $\chi_{ii}$ for $i \in \{0, 1, 2, 3\}$, and four off-diagonal parameters $\operatorname{Im}(\chi_{0i})$ and $\operatorname{Re}(\chi_{jk})$, for any two sets of values of $\{i, j, k\}, \{i', j', k'\} \in \{1, 2, 3\}$ such that $i' \neq i$, $j \neq k \neq i$ and $j' \neq k' \neq j$'. For example, by preparation of a non-maximally entangled state $|\Phi_{xy}^+\rangle = \alpha|00\rangle + \beta|11\rangle$ (Table[1]) and performing a standard BSM, we can obtain the following equations:

$$\chi_{00} + \chi_{33} = P_+, \chi_{11} + \chi_{22} = P_{--},$$

$$a(\chi_{00} - \chi_{33}) + b \operatorname{Im}(\chi_{03}) = c_+,$$

$$a(\chi_{11} - \chi_{22}) - b \operatorname{Re}(\chi_{12}) = c_-,$$

with $p_{\pm} = tr[P_{\pm} \hat{E}_i(\rho)]$, $a = tr(\hat{N}_{\rho})$, $b = 2tr(\sigma_3 \hat{N}_{\rho})$, and $c_\pm = p_{\pm} tr(\hat{N}_{\rho} \pm 1)$, where $\rho = |\Phi_{xy}^+\rangle\langle \Phi_{xy}^+|$, $\hat{N} = \sigma_x^2 \sigma_y^2$, $P_{++} = P_{\Phi^+} + P_{\Phi^-}$, $P_{--} = P_{\Phi^+} + P_{\Phi^-}$, and $\rho_{\pm 1} = P_{\pm 1} \hat{E}_i(\rho) P_{\pm 1} / tr[P_{\pm 1} \hat{E}_i(\rho)]$. In the other experimental configuration, we prepare a non-maximally entangled state $|\Phi_{xy}^+\rangle_x$ and perform another standard BSM to obtain a similar set of equations in the $\{||\pm||\}$ basis (here and also for $\{||\pm||\}$ basis, $N = \sigma_x^2 \sigma_y^2$). Using these linearly independent equations we can determine diagonal elements of the superoperator, $\chi_{ii}$ (i = 0, 1, 2, 3) and four off-diagonal parameters $\operatorname{Im}(\chi_{03})$, $\operatorname{Im}(\chi_{01})$, $\operatorname{Re}(\chi_{12})$, and $\operatorname{Re}(\chi_{23})$. As we have shown above, the diagonal elements can be used to determine $J$ and the absolute values $|J_{\alpha}|$. The relative signs of $J_x, J_y$, and $J_z$ can be found from the off-diagonal parameters above; so, we can identify $J$ up to a global sign. This global sign is usually evident from the physical/engineered setup under consideration, e.g., from the direction of a global magnetic field for spin systems. In physical situations where this global sign cannot

### Table I: Input states and measurements for direct characterization of single-qubit $\chi$. Here $|\Phi_{xy}^+\rangle = \alpha|00\rangle + \beta|11\rangle$, $|\Phi_{xy}^+\rangle_{xy}(\alpha) = \alpha + +\chi(\alpha + \beta - \chi(\alpha)$ where $|\alpha| \neq |\beta| \neq 0$ and $\operatorname{Im}(\chi\alpha\beta \neq 0)$, and $\{||0||, |1\rangle\} \{||\pm\rangle\} \{||\pm\rangle\}$ are eigenstates of the Pauli operators $\sigma_x$, $\sigma_y$, and $\sigma_y$. $P_{\Phi^\pm}$ is the projector on the Bell state $|\Phi^\pm\rangle$, and similarly for the other projectors.

<table>
<thead>
<tr>
<th>input state</th>
<th>Bell-state measurement</th>
<th>output $\chi_{mn}$</th>
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<td>\Phi^+\rangle$</td>
<td>$P_{\Phi^+} = P_{\Phi^-}$</td>
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be deduced from general physical considerations, we need to perform a third measurement that corresponds to characterizing Im(χ_{02}) and Re(χ_{31}) which completes our knowledge about an arbitrary (time-independent) single-qubit Hamiltonian. The whole analysis is also applicable to the case of piece-wise constant Hamiltonians. In the following we discuss another important example of single-qubit dynamics, although non-Hamiltonian, that shows how the DCQD estimation may provide advantage in estimation of dynamical parameters in the Markovian regime.

III. SIMULTANEOUS DETERMINATION OF T₁ AND T₂

Let us consider the so-called quantum homogenization process acting on a single-qubit density matrix ρ(0) for time t, where ρ_{00}(0) = a and ρ_{01}(0) = b in the |0⟩, |1⟩ basis. This leads to the final state ρ(t) with ρ_{00}(t) = (a − a_{∞}) \exp(−t/T₁) + a_{∞} and ρ_{01}(t) = b \exp(−t/T₂), where a_{∞} characterizes the population of thermal equilibrium state, and the time-scales T₁ and T₂ (T₂ < 2T₁) are longitudinal and transverse relaxation time-scales of the system, respectively [1, 27]. The explicit form of χ_{ii} elements are as follows: χ_{00}(33) = [exp(−t/T₁) ± 2 exp(t/T₂)] / 2, χ_{11} = χ_{22} = [exp(t/T₁) + 1] / 2.

Now we demonstrate that both T₁ and T₂ can always be estimated in a single ensemble measurement by using the DCQD scheme for estimating diagonal elements of χ. We first prepare a Bell-state |Φ^+⟩_{AB}, and then let the qubit interact with a thermalizing environment for a given time t. The outcomes of a BSM yield the following relations for T₁ and T₂:

$$\frac{1}{T₁} = -\ln [2\text{tr}[P_{Φ^+}\mathcal{E}_i(ρ)] + 2\text{tr}[P_{Φ^-}\mathcal{E}_i(ρ)] - 1]/t,$$

$$\frac{1}{T₂} = -\ln [\text{tr}[P_{Φ^+}\mathcal{E}_i(ρ)] - \text{tr}[P_{Φ^-}\mathcal{E}_i(ρ)]]/t.$$ (2)

Ideally, these equations imply adequacy of single time-point measurements. This is, unlike the case of reading J, where time sampling is necessary and aliasing is inevitable, T₁ and T₂ can in principle be obtained through single time-point measurements. This feature could be utilized to reveal the non-Markovian nature of system-bath interaction; e.g., by observing time variations in the estimated relaxation and dephasing rates beyond the the natural deviation due to statistical errors. Moreover, due to orthogonality of BSM outcomes, it is easy to unambiguously distinguish T₁ from T₂, unlike the approach presented in Ref. [31]. Traditionally, in order to measure the longitudinal and transverse relaxation times, one needs to measure two non-commutative observables (e.g., Pauli operators σ_x and σ_z) on two subensembles of identical systems, corresponding to magnetization vectors M_z and M_y, parallel and perpendicular to a global magnetic field B_0. The number of repetitions in each measurement is determined by the desired accuracy in the time sampling estimation of the relaxation times associated with magnetizations M_z and M_y [32].

IV. IDENTIFICATION OF TWO-QUBIT EXCHANGE HAMILTONIANS

In solid-state systems, it is often the case that each pair of qubits (AB) interact directly or effectively through an exchange Hamiltonian \(H_x = \sum_{\alpha} J_{\alpha} \sigma_{\alpha}^x \sigma_{\alpha}^x\), where \(J_{\alpha}\) are the couplings of the two-qubit interaction (see also Ref. [17] for the exchange interaction between neutral atoms in optical lattices). The case of isotropic or Heisenberg interaction (\(J_x = J_y = J_z\)) is intrinsic to spin-coupled quantum dots, and donor atom nuclear-electron spins [18]. This interaction is also important in the context of universal fault-tolerant quantum computing [19]. The XY Hamiltonian (\(J_x = J_y\), \(J_z = 0\)) is available interaction in quantum Hall systems [20], quantum dots and exciton-coupled quantum dots [22]. The XXZ (\(J_x = J_y \neq J_z\)) interaction appears in the electrons in liquid Helium quantum computing proposals [23].

In the case of XYZ Hamiltonians, the \(\chi\) matrix has only 10 nonzero independent elements \(\chi_{m,n}\), for \(m, n = 0, 5, 10, 15\). Similar to the case of the general single-qubit Hamiltonian, these diagonal elements contain information only about the absolute values |\(J_{\alpha}\)|. In order to obtain information about the signs of \(J_{\alpha}\), we need to measure off-diagonal elements as well. However, in most physical/practical cases the signs of the terms in an exchange Hamiltonian are already known from some general properties of the system. For example, for many materials it is known whether below the phase transition point they become ferromagnetic or anti-ferromagnetic—alternatively this information can be obtained for a given material by measuring its linear response to an applied magnetic field. In these cases, the Hamiltonian can be completely determined with a single ensemble measurement corresponding to the diagonal elements of the superoperator.

Let us consider the important classes of isotropic and anisotropic exchange interactions. For these Hamiltonians the sign of \(J\) is known from the ferromagnetic property of the system. In fact, by definition \(J = E_S - E_T\) (where \(E_S\) and \(E_T\) are the energy of singlet and triplet states), is always negative for ferromagnetic materials. For example, for a two-electron system, the singlet state is the ground state of the system if \(J < 0\). On the contrary, for anti-ferromagnetic materials, \(J\) is always positive which indicates that in the ground state spins tend to arrange themselves in the same direction.

In order to determine the diagonal elements \(\chi_{ii}\) for Heisenberg interaction between two electrons \(A_1\) and \(A_2\), one can prepare a tensor product of maximally entangled states between each electron and a pair of ancilla electrons (\(B_1\) and \(B_2\)) such as \(|Φ^+⟩_{A_1B_1}|Φ^+⟩_{A_2B_2}\). Then, the unknown Hamiltonian \(H\) for the duration of \(t\) is applied, and a tensor product of BSMs acting on each pair \(A_iB_i\) is performed, where this operation can be represented by a tensor product of \(P_{Φ^+}, P_{Φ^-}, P_{Φ^0}, P_{Φ^±}\) for \(i = 1, 2\). The joint probability distributions of the BSMs are related to \(J\) through

\[\text{tr}[P_{Φ^+} P_{Φ^±} \mathcal{E}_i(ρ)] = e^6 + s^6\] and \[\text{tr}[P_{Φ^+} P_{Φ^-} \mathcal{E}_i(ρ)] = \text{tr}[P_{Φ^-} P_{Φ^±} \mathcal{E}_i(ρ)] = \text{tr}[P_{Φ^+} P_{Φ^0} \mathcal{E}_i(ρ)] = s^6 e^6.\] Therefore,
we have:

\[ \sin(2|J|t) = 2\sqrt{\text{tr}[P_{\Phi_1}^t P_{\Phi_2}^t \mathcal{E}_t(\rho)]}, \]  

(3)

and similar relations hold for \( P_{\Phi_1}^t P_{\Phi_2}^t \) and \( P_{\Phi_1}^t - P_{\Phi_2}^t \) as well.

In the case of anisotropic exchange interactions one can perform a similar Bell-state preparation and BSM as in the case of isotropic exchange, to obtain:

\[ \sin(2|J_x|t) = 2\sqrt{\text{tr}[P_{\Phi_1}^t P_{\Phi_2}^t \mathcal{E}_t(\rho)]}, \]  

(4)

\[ \cos(2|J_z|t) = \sqrt{(\text{tr}[P_{\Phi_1}^t P_{\Phi_2}^t \mathcal{E}_t(\rho)] - s_x^2)/(c_x^2 - s_x^2)}. \]  

(5)

To read \(|J_\alpha|\), one needs to have time samplings (i.e., ensemble measurements for many time-points) and follow the Fourier analysis based method sketched earlier. Therefore, having a priori knowledge about the ferromagnetic property of the system, one can identify the underlying exchange Hamiltonian.

Note that the energy spectrum of \( H_{\text{ex}} \) can be simply calculated using the above relations and knowing the fact that Bell-states are the eigenkets of the exchange Hamiltonian. Eigenvalues of \( H_{\text{ex}} \) can be written as \( E = \pm |J_\alpha| \pm |J_\beta - J_\gamma| \), where \( \alpha \neq \beta \neq \gamma \in \{x, y, z\} \). We have already shown how to estimate \(|J_\alpha|\) for \( \alpha = x, y, z \). In order to find relative signs of any two other components, such as \(|J_y - J_z|\), the DCQD algorithm can be utilized by performing a single ensemble measurement that corresponds to measuring the off-diagonal element \( \chi_{0.5} \). For full characterization of an exchange Hamiltonian without having any a priori knowledge about the signs of the coupling constants, one needs to measure the off-diagonal element \( \chi_{0.10} \) too. Therefore, with a total of three ensemble measurements, corresponding to \( \chi_{0.5}, \chi_{0.5}, \) and \( \chi_{0.10} \), full characterization of \( H_{\text{ex}} \) can be achieved.

V. REMARKS ON PRECISION

In a realistic estimation process, due to decoherence, limited measurement or preparation accuracies (because of specific device architecture or finite ensemble size), and other imperfections, some errors may occur (a generalization of the DCQD theory that addresses faulty preparations and measurements is underway and will be reported elsewhere [29]). These factors might affect the amount of physical resources required for a given accuracy of the estimation, hence some appealing features like sufficiency of single-time point measurements might be lost. For the case of ideal preparations/measurments scenario in which single time-point measurements are in principle sufficient, errors scale up as \( 1/\sqrt{N_E} \), where \( N_E \) is the number of repeated measurements. In the cases we need to perform time samplings, the error in the estimation of frequencies (and thus, Hamiltonian parameters) is governed by the Nyquist criterion and the quantum shot-noise limit [29]. Let us consider \( N_S \) samples, for each of which we perform \( N_E \) measurements. Therefore, according to the quantum shot-noise limit, \( \Delta f \sim 1/(N_S \tau_S \sqrt{N_E}) \), and the Nyquist criterion, \( f_S = 1/\tau_S \geq \Delta f/2 \), we get: \( \Delta f/\Delta f \sim 1/(N_S \sqrt{N_E}) \) (see Ref. [11]). That is, the average error in estimation of Hamiltonian parameters scales as \( 1/(N_S \sqrt{N_E}) \). In other words, for an error \( \epsilon \), or with the number of digits of precision \( \log(1/\epsilon) \), we need poly(1/\epsilon) more steps, which is common among all Fourier analysis based methods [30]. In this respect, our method does not provide an advantage over the one in Refs. [11]—both methods provide similar accuracy scaleup. However, the advantage of our method lies in the built-in ability of the method for partial characterization. That is, there is a level of independency in the way different sets of parameters are related to measurements results. For more general discussions on partial characterization by DCQD see Refs. [5] and for a very recent proof-of-principle experiment on this issue, using polarization and spatial degrees of freedom of a single photon, see Ref. [7]. Moreover, in our method some of the parameters are related more directly to the measurements data, hence obviating the need to (a full) inversion in the first place. E.g., in the single-qubit case, we obtain \(|J_x,y,z|\) just by a very simple algebraic manipulation of the data. This feature is not necessarily available in the methods of Refs. [11], because a Fourier analysis would be necessary even for extracting a partial information about the Hamiltonian.

VI. CONCLUSION AND DISCUSSION

We have presented a theoretical approach for utilizing auxiliary quantum correlations to perform Hamiltonian identification. In this method one can directly obtain full information about unknown parameters of time-independent of single- and two-qubit Hamiltonians without full quantum process tomography. In addition, we demonstrate that for a single qubit undergoing a generic Markovian homogenizing quantum map, both related relaxation times can be estimated simultaneously by utilizing a single Bell-state measurement. Furthermore, we illustrate how our prior knowledge about Hamiltonian systems can be exploited in order to reduce the required physical resources for identification tasks. In particular, we show that the required repeated measurements, associated to time sampling of data, can be reduced when we are interested in partial characterization of the Hamiltonian systems and also for estimating relaxation rates. With the recent advent of various methods for generation of controllable entanglement, our proposed method may have near-term application to a variety of quantum systems/devices, such as in trapped ions, liquid-state NMR, optical lattices, and entangled pairs of photons.

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