Equation of motion for the process matrix: Hamiltonian identification and dynamical control of open quantum systems

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Equation of motion for the process matrix: Hamiltonian identification and dynamical control of open quantum systems

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We develop a general approach for monitoring and controlling evolution of open quantum systems. In contrast to the master equations describing time evolution of density operators, here, we formulate a dynamical equation for the evolution of the process matrix acting on a system. This equation is applicable to non-Markovian and/or strong-coupling regimes. We propose two distinct applications for this dynamical equation. We first demonstrate identification of quantum Hamiltonians generating dynamics of closed or open systems via performing process tomography. In particular, we argue how one can efficiently estimate certain classes of sparse Hamiltonians by performing partial tomography schemes. In addition, we introduce an optimal control theoretic setting for manipulating quantum dynamics of Hamiltonian systems, specifically for the task of decoherence suppression.

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I. INTRODUCTION

Characterization and control of quantum systems are among the most fundamental primitives in quantum physics and chemistry [1,2]. In particular, it is of paramount importance to identify and manipulate Hamiltonian systems which have unknown interactions with their embedding environment [3]. In the past decade, several methods have been developed for estimation of quantum dynamical processes within the context of quantum computation and quantum control [1,4–8]. These techniques are known as "quantum process tomography" (QPT) and originally were developed to estimate the parameters of a "superoperator" or "process matrix," which contains all information about the dynamics. This is usually achieved through an inversion of experimental data obtained from a complete set of state tomographies. QPT schemes are generally inefficient since for a complete process estimation the number of required experimental configurations and the amount of classical information processing grows exponentially with size of the system. Recently, alternative schemes for partial and efficient estimation of quantum maps have been developed [5–10] including efficient data processing for selective diagonal [7] and off-diagonal parameters of a process matrix [8]. However, it is not clear how the estimated elements of the process matrix could help us actually characterize the set of parameters for Hamiltonians generating such dynamics. These parameters of interest generally include the system free Hamiltonians and those coupling strengths of system-bath (SB) Hamiltonians. More importantly, it is not fully understood how the relevant information obtained from quantum process estimation experiments can be utilized for other applications such as optimal control of a quantum device.

In this work, we develop a theoretical framework for studying general dynamics of open quantum systems. In contrast to the usual approach of utilizing master equations for density operator of a quantum system, we introduce an equation of motion for the evolution of a process matrix acting on states of a system. This equation does not presume the Markovian or perturbative assumptions and hence provides a broad approach for analysis of quantum processes. We argue that the application of partial quantum estimation schemes [5–10] enables efficient estimation of sparse Hamiltonians. Furthermore, the dynamical equation for process matrices leads to alternative ways for controlling generic quantum Hamiltonian systems. In other words, one can utilize this equation to drive the dynamics of a(n) closed (open) quantum system to any desired target quantum operation. In particular, we apply quantum control theory to find the optimal fields to decouple a system from its environment, hence, "controlling decoherence."

II. DYNAMICAL EQUATION FOR OPEN QUANTUM SYSTEMS

In quantum theory, the evolution of a system—assuming separable initial state of the system and environment—can be described by a (complete-positive) quantum map $\mathcal{E}_t(\varrho)=\Sigma_i A_i(t)\varrho A_i^\dagger(t)$, where ϱ is the initial state of the system [11]. An alternative more useful expression is obtained by expanding $A_i(t)=\Sigma_m a_{im}(t)\sigma_m$ in $\{\sigma_k;k=0,1,\ldots,d^2-1\}$ (a fixed operator basis for the d-dimensional Hilbert space of the system) which leads to $\mathcal{E}_t(\varrho)=\Sigma_{mn=0}^{d^2-1}\chi_{mn}(t)\sigma_m\varrho\sigma_n^\dagger$. The positive-Hermitian process matrix $\boldsymbol{\chi}(t)=[\Sigma_i a_{im}(t)\bar{a}_{in}(t)]$ represents $\mathcal{E}_t$ in the $\{\sigma_k\}$ basis, where the bar denotes complex conjugation. The process matrix elements $\chi_{mn}(t)$, in any specific time t, can be experimentally measured by any QPT scheme [15].

In an open quantum system, the time-dependent Hamiltonian of the total SB has the general form $H(t)=H_S(t)+H_B(t)+H_{SB}(t)$, where $S(B)$ stands for the system (bath or the surrounding environment). We denote the evolution operator which is generated from this Hamiltonian, from time 0 to t, by $U(t)$. The Hamiltonian $H_{SB}(t)$ can be written as $H_{SB}(t)=\Sigma_k\lambda_k(t)\sigma_k\otimes B_k$, where $\lambda_k(t)$'s are the coupling strengths of the system-bath interaction and $\{B_k\}$ are some

bath operators. Now we describe the dynamics in the interaction picture by introducing the time evolution operators $U_0(t)$, $U_S(t)$, and $U_B(t)$ generated by $H_0=H_S\otimes I_B+I_S\otimes H_B$, H_S, and H_B, respectively.

The system-bath Hamiltonian in the interaction picture becomes $H_I(t)=U_0^\dagger(t)H_{SB}(t)U_0(t)$. By introducing $\tilde{\sigma}_k(t)=U_S^\dagger(t)\sigma_k U_S(t)\equiv\Sigma_l s_{kl}(t)\sigma_l$ and $\tilde{B}_k(t)=U_B^\dagger(t)B_k U_B(t)$ as the rotating operators under the evolution of the free Hamiltonian of the system and bath, we can rewrite $H_I(t)=\Sigma_k\lambda_k(t)\tilde{\sigma}_k(t)\otimes\tilde{B}_k(t)$. The Schrödinger equation in the interaction picture can be expressed as

$$id\mathbf{A}_i^I(t)/dt=\sum_k H'_{ik}(t)A_k^I(t), \tag{1}$$

where $U_I(t)=U_0^\dagger(t)U(t)$, $A_i^I(t)=_B\langle b_i|U_I(t)|b_0\rangle_B\equiv\Sigma_m a_{im}^I(t)\sigma_m$ are the Kraus operators at the interaction picture, $H'_{ij}(t)=\Sigma_{pq}\lambda_p s_{pq}\,{}_B\langle b_i|\tilde{B}_p|b_j\rangle_B\sigma_q$, and $\{|b_i\rangle\}$ is a basis for the bath Hilbert space. The interaction picture $\boldsymbol{\chi}$ matrix is defined as $\chi_{mn}^I(t)=\Sigma_i a_{im}^I(t)\bar{a}_{in}^I(t)$, which is related to the elements of the measured process matrix through $\chi_{mn}^I(t)=\Sigma_{m'n'}\chi_{m'n'}(t)\mathrm{Tr}[\sigma_m U_S^\dagger(t)\sigma_{m'}]\mathrm{Tr}[\sigma_n U_S^T(t)\sigma_{n'}]$. Thus, the time evolution of the a_m^I coefficients reads as

$$ida_{im}^I/dt=\sum_{klpq}a_{kl}^I\lambda_p s_{pq}\alpha_m^{qp}\,{}_B\langle b_i|\tilde{B}_p|b_k\rangle_B, \tag{2}$$

where $\alpha_m^{kl}=\mathrm{Tr}[\sigma_k\sigma_l\sigma_m^\dagger]$. From this equation, one can obtain the time evolution of $\boldsymbol{\chi}^I$ as follows:

$$id\boldsymbol{\chi}^I/dt=\tilde{\boldsymbol{H}}\mathbf{K}-\mathbf{K}^\dagger\tilde{\boldsymbol{H}}^\dagger, \tag{3}$$

where

$$[\tilde{\boldsymbol{H}}]_{n(imj)}=\sum_{pq}\lambda_p s_{pq}\alpha_n^{qp}\,{}_B\langle b_j|\tilde{B}_m|b_i\rangle_B, \tag{4}$$

$$[\mathbf{K}]_{(imj)n}=a_{im}^I\bar{a}_{jn}^I, \tag{5}$$

in which (imj) is considered as a new single index. The order of the pseudo-Hamiltonian $\tilde{\boldsymbol{H}}$ is $d^2\times d^6$, but number of independent parameters is $\leq d^2$, which is the maximum number of nonzero λ_p's. By using a generalized commutator notation $[A,B]^\star\equiv AB-B^\dagger A^\dagger$, Eq. (3) can be represented in the following form:

$$id\boldsymbol{\chi}^I/dt=[\tilde{\boldsymbol{H}},\mathbf{K}]^\star. \tag{6}$$

This is the (super)dynamical equation for open quantum systems, i.e., an equation for the time variation in quantum dynamics itself, in which no state of the system appears, in contrast to the existing master equations [11].

The knowledge of the $\boldsymbol{K}$ matrix is generally required for application of Eq. (6). The $\boldsymbol{\chi}^I$ matrix can be diagonalized by the unitary operator $\boldsymbol{V}$: $\boldsymbol{\chi}^I=\boldsymbol{V}\boldsymbol{D}\boldsymbol{V}^\dagger$, where $\boldsymbol{D}=\mathrm{diag}(D_i)$. Then, the Kraus operators in the interaction picture are $A_i^I(t)=\sqrt{D_i}\Sigma_m V_{mi}\sigma_m$ [1]. Hence, we obtain $a_{im}^I=\sqrt{D_i}V_{mi}$ and $K_{imjn}=\sqrt{D_i D_j}V_{mi}\bar{V}_{nj}$. Diagonalization of a sparse $\boldsymbol{\chi}^I$ matrix, hence construction of the $\boldsymbol{K}$ matrix, can be performed efficiently. The unknown parameters of Eq. (6) are elements of $\tilde{\boldsymbol{H}}$ matrix which contain the information about the system-bath coupling strengths λ_k.

For unitary evolutions, following a similar approach, the dynamical equation for the process matrix is obtained as

$$id\boldsymbol{\chi}/dt=[\tilde{\boldsymbol{H}},\boldsymbol{\chi}]^\star, \tag{7}$$

where $\tilde{\boldsymbol{H}}=[\tilde{h}_{ml}]$, $\tilde{h}_{mn}(t)\equiv\Sigma_k\alpha_m^{kn}h_k(t)$, and $h_l(t)$ are defined through $H(t)=\Sigma_l h_l(t)\sigma_l$. It should be noted that hermiticity of H implies only d^2 real independent parameters in $\tilde{\boldsymbol{H}}$, which can be estimated via QPT schemes.

III. HAMILTONIAN IDENTIFICATION

Consider a large ensemble of the identically prepared systems in the state ϱ, half of which are measured after duration t, and the rest are measured at $t+\Delta t$, where Δt is small relative to t. Thus, by performing any type of QPT strategy one can obtain the matrix elements $\chi_{mn}(t)$ and $\chi_{mn}(t+\Delta t)$, hence their derivatives $\dot{\chi}_{mn}(t)\approx[\chi_{mn}(t+\Delta t)-\chi_{mn}(t)]/\Delta t$ with accuracy Δt. Consequently, using Eq. (7) [Eq. (6)] one can in principle identify the free [system-bath] Hamiltonians for closed (open) quantum systems.

For unitary evolutions, a simple relation between the elements of the $\boldsymbol{\chi}$ matrix and the system Hamiltonian parameters is obtained, up to the second order in t and a global phase $\mathrm{Tr}[H]$ as $\chi_{00}(t)\approx 1-\frac{1}{2}t^2\Sigma_{ij}\alpha_0^{ij}h_i h_j+\bar{\alpha}_0^{ij}\bar{h}_i\bar{h}_j$, $\chi_{m0}(t)\approx ih_m t-\frac{1}{2}t^2\Sigma_{ij}\alpha_m^{ij}h_i h_j$, and

$$\chi_{mn}(t)\approx h_m\bar{h}_n t^2, \tag{8}$$

where $m,n\neq 0$. From Eq. (8), for a given short time t, we have $h_n=e^{i\varphi_n}\sqrt{\chi_{nn}}/t$, from which the relative errors satisfy $\mathrm{Re}[\delta h_n/h_n]=\delta\chi_{nn}/2\chi_{nn}$. According to the Chernoff bound [9,12], to estimate χ_{nn}'s with accuracy $\Delta\geq|\chi_{nn}-\bar{\chi}_{nn}|=\delta\chi_{nn}$—where $\bar{\chi}_{nn}$ is the average of the results of M repeated measurements—with success probability greater than $1-\epsilon$, one needs $M=O(|\log\epsilon/2|/\Delta^2)$. Information of the phases φ_n, up to a global phase, can be estimated by measuring χ_{mn}'s for $m\neq n$.

Using the above construction, next we discuss efficient Hamiltonian identification schemes via performing certain short-time scale QPTs. A precursor to this type of short-time expansion in order to efficiently obtain process matrix parameters can be found in Ref. [13]; however, its underlying models, the assumptions, and the identification method are more restrictive and generally incommensurable with ours.

In generic N-body physical systems (e.g., N qubits), interactions are L-local, where L is typically 2. That is, $H=\Sigma_k H_k$, where each H_k includes only interactions of L subsystems, with overall $O(N^L)$ independent parameters. This implies that in the $\{\sigma_k\}$ basis H has a sparse-matrix representation. Hence, the number of free parameters of the corresponding unitary or process matrix, unlike their exponential size, will be polylog(d) (i.e., a polynomial of N). Here, we mainly concentrate on controllable L-local Hamiltonians, which are of particular interest in the context of quantum information processing in order to generate a desired quantum operation. An important example of this class is the Heisenberg exchange Hamiltonian in a network of spins with nearest neighbor interactions. This two-local sparse Hamiltonian (in the Pauli basis) also generates a sparse process

matrix [10] and is computationally universal over a subspace of fixed angular momentum [14].

Let us consider a sparse Hamiltonian, $H(t)=\Sigma_m h_m(t)\sigma_m$, with polylog($d$) nonzero h_m's, where $\{\sigma_m\}$ is the nice error basis [6]. In the short-time limit, according to Eq. (8), if the Hamiltonian is sparse in the $\{\sigma_k\}$ basis, only polylog(d) of h_m's would be nonzero. Thus, number of nonzero elements in the $[t^2 h_m \bar{h}_n]_{m,n\neq 0}$ block would be also of the same order. *A priori* knowledge of the general form of a given sparse Hamiltonian leads to [up to $O(t^3)$] nonzero elements in the $[t^2 h_m \bar{h}_n]_{m,n\neq 0}$ block according to Eq. (8). Therefore, if we can efficiently determine all nonzero elements of this block, we would have polylog(d) quadratic equations from which we can estimate h_m's. In other words, by only *polynomial* experimental settings we would be able to extract relevant information about the Hamiltonian from a suitable QPT experiment [15]. In general, there are three distinct process estimation techniques, including standard quantum process tomography (SQPT) [1], direct characterization of quantum dynamics (DCQD) [5], and selective efficient quantum process tomography (SEQPT) [8]. The scaleup of physical resources varies among these process estimation strategies [9]. SQPT is inefficient by construction since we still need to measure an exponentially large number of observables in order to reconstruct the process matrix through a set of state tomographies. SEQPT can efficiently estimate quantum sparse Hamiltonians via selectively estimating a polynomial number of χ_{mn}'s associated to the Hamiltonian, within the context of short-time analysis. Using the DCQD scheme, in short-time limit, one can also efficiently estimate all the parameters of certain sparse Hamiltonians, specifically all the diagonal elements χ_{nn}—a detailed analysis thereof is beyond the discussion of this work and will be presented in another publication [16]. Note that in contrast to SQPT, both DCQD and SEQPT assume access to noise-free ancilla channels. However, recently a generalization of the DCQD scheme to certain cases of calibrated faulty preparation, measurement, and auxiliary systems has been developed [17].

We emphasize that, within the context of short-time analysis, the efficient estimation is only applicable to the Hamiltonians for which the location of nonzero elements in a given basis is known from general physical or engineering considerations, such as in the exchange Hamiltonian in solid-state quantum information processing [14]. The exchange Hamiltonian describes the underlying interactions for various systems, such as spin-coupled quantum dots [18], donor-atom nuclear/electron spins [19], semiconductor quantum dots [20], and superconducting flux qubits [21]. The anisotropic exchange Hamiltonian exists in quantum Hall systems [22], quantum dots/atoms in cavities [23], exciton-coupled quantum dots [24], electrons in liquid-Helium [25], and neutral atoms in optical lattices [26].

IV. APPLICATIONS TO QUANTUM DYNAMICAL CONTROL

An immediate application of any equation of motion, i.e., dynamical equation, for a quantum or classical system is to manipulate its state or dynamics toward a desired target. The ability to control quantum dynamics by certain external control fields is essential in many applications including physical realizations of quantum information devices. Due to environmental noise and device imperfections, it is generally difficult to maintain quantum coherence during dynamical evolution of quantum systems. Reducing or controlling decoherence, therefore, is an important objective in a control theoretic investigation of quantum systems.

Optimal control theory (OCT) [27] has been developed for finding control fields to guide a quantum system, subject to natural or engineering constraints, as close as possible to a particular target. For closed quantum system, OCT has been proposed for controlling states [27] and unitary dynamics [28]. In OCT, a quantum system is driven from an initial state or unitary operation to a final configuration, via applying external fields. This is achieved, for example, by modifying a free Hamiltonian H_0 as $H(t)=H_0-\mu\pi(t)$, where μ is a system operator (e.g., atomic or molecular dipole moment) and $\pi(t)$ is a shaped external field (e.g., laser pulse) [28]. The optimization is based on maximizing a yield functional $\tilde{\mathcal{Y}}$, e.g., fidelity of the final and target configurations, by a variational procedure ($\delta\tilde{\mathcal{Y}}/\delta\pi=0$) subject to a set of constraints.

Having an equation of motion implies how one can control dynamics of a system toward a target configuration. Thus, a method for controlling dynamics of *open* quantum systems can be developed by our equation of motion [Eq. (6)], specifically applicable to optimal decoherence control. For isolated systems we have $\lambda_k=0$ (hence $\tilde{\boldsymbol{H}}=0$), from which one can obtain $\chi^I_{mn}=\delta_{m0}\delta_{n0}\equiv[\boldsymbol{E}_{00}]_{mn}$. However, due to decoherence or other environmental effects, there might be some residual interaction $\tilde{\boldsymbol{H}}_0$ between the system and environment. Our objective, here, is to apply a control field $\pi(t)$ to modify the pseudo-Hamiltonian [Eq. (4)] in order to suppress the decohering interaction. Since $\tilde{\boldsymbol{H}}$ is linear in λ's, applying a control coupling field would affect $\tilde{\boldsymbol{H}}$ linearly. Thus, if we introduce an external controllable field $\pi(t)$, the pseudo-Hamiltonian $\tilde{\boldsymbol{H}}_0$ becomes $\tilde{\boldsymbol{H}}(t)=\tilde{\boldsymbol{H}}_0-\boldsymbol{\mu}\pi(t)$, where $\boldsymbol{\mu}$ is a system operator. The control strategy is to find the optimal $\pi(t)$ such that the constrained fidelity

$$\tilde{\mathcal{Y}}=\mathrm{Re}\left[\mathcal{Y}-\int_0^T dt\ \mathrm{Tr}\{\{d\boldsymbol{\chi}^I/dt+i[\tilde{\boldsymbol{H}}(t),\boldsymbol{K}(t)]^\star\}\boldsymbol{\Lambda}(t)\}\right]-\eta\int_0^T dt|\pi(t)|^2/f(t) \tag{9}$$

becomes maximal, where $\mathcal{Y}=\mathrm{Re}\{\mathrm{Tr}[\boldsymbol{\chi}^{I^\dagger}(T)\boldsymbol{E}_{00}]\}$ and $\boldsymbol{\Lambda}(t)(\eta)$ is an operator (scalar) Lagrange multiplier. The last term in Eq. (9) describes an "energy" constraint [28], in which $f(t)$ is a shape function for switching the control field on and off. In order to find the optimal field, we vary π, $\boldsymbol{\Lambda}$, and a^I_{im}, and set $\delta\tilde{\mathcal{Y}}=0$. By variation in the operator Lagrange multiplier $\boldsymbol{\Lambda}$, we obtain the original dynamical [Eq. (6)], and the variation in π yields

$$\pi(t)=-(f(t)/2\eta)\mathrm{Im}[\mathrm{Tr}\{[\boldsymbol{\mu},\boldsymbol{K}(t)]^\star\boldsymbol{\Lambda}(t)\}]. \tag{10}$$

This equation implies that the knowledge of $\boldsymbol{K}(t)$ and $\boldsymbol{\Lambda}(t)$ is necessary to specify the optimal control field. The superop-

erator $\boldsymbol{K}(t)$ can be constructed by process estimation techniques. To obtain the dynamics of $\boldsymbol{\Lambda}(t)$, we vary a^I_{im}, which in turn leads to variations in $\boldsymbol{\chi}^I$ and $\boldsymbol{K}$. Thus, the Lagrange operator satisfies

$$-i[\boldsymbol{K}(d\boldsymbol{\Lambda}/dt)]_{imim} = \sum_{njl} \Lambda_{ln}\tilde{H}_{nimj}K_{imjn} - \Lambda_{nm}\tilde{H}_{mjli}\bar{K}_{jlim}. \quad (11)$$

Equations (10) and (11), in principle, can be solved iteratively by the Krotov method [28,29] to find the optimal control field π for decoherence suppression. That is, one can effectively preserve coherence in dynamics of an open quantum system by applying external pulses to decouple it from the environment. This could provide an alternative method for an effective dynamical decoupling [30] in the language of process matrix evolution. One can devise a learning decoherence control strategy by estimating $\boldsymbol{K}(t)$, via certain QPT schemes on subensembles of identical systems, after each application of the optimal control field in a given time t. The information learned from the estimation is used through Eqs. (9)–(11) for a second round to find a new optimal π. This procedure can be repeated to enhance the decoherence suppression task.

V. CONCLUSION AND OUTLOOK

We have developed an alternative framework for monitoring and controlling dynamics of open quantum systems and have derived a dynamical equation for the time variation in process matrices. This nonperturbative approach can be applied to non-Markovian systems and systems or devices strongly interacting with their embedding environment. In addition, we have shown how the information gathered via partial process tomography schemes can be used to efficiently identify unknown parameters of certain classes of local Hamiltonians in short-time scales. Furthermore, we have proposed an optimal quantum control approach for the dynamics of open quantum systems. Specifically, we have suggested how this mechanism can be used for a generic decoherence suppression.

The approach presented here can be used for exploring new ways for dynamical open-loop or learning control of Hamiltonian systems [31]. One can utilize continuous weak measurements [32] for process tomography to develop a real-time dynamical closed-loop control for a quantum system. Our Hamiltonian identification scheme could be utilized for efficient verification of certain correlated errors for quantum computers and quantum communication networks [1]. Using our dynamical approach, one could explore the existence of certain symmetries in system-bath couplings which would lead to noiseless subspaces and subsystems. The dynamical equation developed here can also be applied to studying the energy transfer in multichoromophoric complexes in the non-Markovian and/or strong interaction regimes [33].

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