Identification of Non-Markovian Environments for Spin Chains

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Abstract— **Correlations of an environment are crucial for the dynamics of non-Markovian quantum systems, which may not be known in advance. In this brief, we propose a gradient algorithm for identifying the correlations in terms of the time-varying damping rate functions in a time-convolution-less master equation for spin chains. By measuring time trace observables of the system, the identification procedure can be formulated as an optimization problem. The gradient algorithm is designed based on a calculation of the derivative of an objective function with respect to the damping rate functions, whose effectiveness is shown in a comparison with a differential approach for a two-qubit spin chain.**

Index Terms— **Gradient methods, optimization, quantum mechanics, system identification.**

I. INTRODUCTION

TO EXACTLY process quantum information, accurate models, including parameters, structures, and descriptions of dynamics, for quantum information carriers are required. With these models, sophisticated feedback control strategies can be designed, for example, feedback stabilization of a number state in a cavity [1], preservation of quantum coherence and entanglement for qubit systems [2] and linear quantum systems [3], or coherent feedback rejection of quantum colored noise [4], [5].

However, in practice, an accurate model may not be obtainable since parts of the parameters, structures, or dynamics of the quantum system may not be well understood. This would lead to unexpected experimental results or degraded control performance of a quantum control system. For example, in a recent experiment on quantum dots [6], a calculation based on

the theoretical model has a discrepancy from the experimental data on the broadened resonator linewidth under suitable parameters, which means that some unknown dynamics of the system are not included in the model. Correspondingly, it is shown that the degraded estimation performance can be observed due to the ignorance of a noise model for a quantum system [7]. Hence, the problem of how to determine the unknown parameters, structures, or dynamics of a "dark" quantum system is an essential problem in quantum control theory, which is referred to quantum system identification.

A general identification methodology involves finding the unknown parts of a quantum system from measurement data (e.g., the spectrum of an output field or expectations of observables) extracted from the system under excitation [8]. The identification method was first explored to extract the Hamiltonian information for closed quantum systems [9]–[11]. Moreover, it is worth considering the identification problem for open quantum systems, where the quantum system is disturbed by the quantum noises arising from an environment. When the correlation function of the quantum noise is the Dirac delta function, i.e., the correlation time of the quantum noise is very short, the noise and the relevant quantum system refer to quantum white noise and a Markovian quantum system, respectively [12]. For Markovian quantum systems, a continuous-measurement-based method was proposed to identify unknown parameters in a cavity-atomic system [13] and unknown structures of a spin network [14]. In addition, a system-realization-theory-based method in [11] was extended to estimate unknown parameters in the Hamiltonian of a Markovian spin network from measurement time traces [15], whose identifiability was discussed in [16]. In addition, an identification method for the linear Markovian quantum systems was systematically discussed in [17].

In contrast to the Dirac correlation function of quantum white noise, correlation functions of quantum colored noise can be more complicated due to the memory effect of non-Markovian environments. A quantum system disturbed by the quantum colored noise is referred to as a non-Markovian quantum system, whose dynamics is quite different from that of the Markovian quantum systems [12]. To control the non-Markovian quantum systems, it is crucial to acquire the knowledge of the correlation functions of the non-Markovian environment beforehand. Wu *et al.* [8] proposed a frequency-domain approach to the identification of the environment spectrum for a superconducting single qubit at an optimal point. For the quantum dot system in [6], an augmented system model was presented to explore the structure of the non-Markovian environment [18]. In addition, a spectroscopic method was presented to explore the spectrum
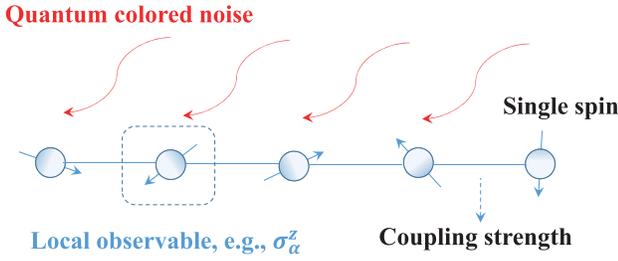
Fig. 1. Schematic of the spin chains in a non-Markovian environment.

of spin baths both theoretically [19] and experimentally [20], which involves high-energy dynamical decoupling pulses.

In this brief, we aim to extract the correlation functions of the non-Markovian environments for spin chains. The dynamics of the spin chains are described by a time-convolution-less master equation, in which the time-varying damping rate functions characterize the correlation functions of the non-Markovian environment. To identify the damping rate function, we measure the time trace for one local observable of the spin chains that correspond to dynamical variables in a coherence vector representation. Although this formulation for the coherence vector is similar to that in [15], the dynamical equation for the coherence vector is time-varying due to the damping rate functions. Thus, the method in [15] is invalid in our case. We alternatively formulate the identification problem for the damping rate function as an optimization problem. In addition, we design a gradient algorithm to iteratively recover the damping rate functions for the non-Markovian environment.

Our contribution in this brief is that we provide a systematic approach to acquire the unknown damping rate functions in a time-convolution-less master equation for the non-Markovian quantum systems. In principle, our gradient algorithm can achieve the damping rate function with a high fidelity, which would help to obtain an exact model of the spin chains in an experiment for quantum information processing. In addition, our method only requires measuring commutative observables of the spin chains, which is easy to be applied in an experiment, because it avoids measuring the noncommutative observables that cannot be accurately measured at the same time according to the uncertainty principle in quantum mechanics.

This brief is organized as follows. In Section II, we introduce the time-convolution-less master equation for the non-Markovian spin chains, whose corresponding coherence vector representation is also introduced. The identification problem formulation and the gradient algorithm are given in Section III. An example for two qubits in a non-Markovian environment is given in Section IV. Conclusions are drawn in Section V.

II. DESCRIPTION OF NON-MARKOVIAN SPIN CHAINS

A. Time-Convolution-Less Master Equation

The non-Markovian spin chain we consider in this brief is plotted in Fig. 1, where the nodes and the edges represent spin

components and their couplings, respectively. The components are disturbed by quantum colored noise arising from an unknown non-Markovian environment. Here, the time traces of local observables are measured, and the resulting data are to be processed for identification.

In this brief, the non-Markovian dynamics of spin chains are described by a time-convolution-less master equation [12]

$$\dot{\rho}(t) = \mathcal{L}_0 \rho(t) + \mathcal{L}_{\gamma(t)} \rho(t) \tag{1}$$

of the spin chains. The superoperator

$$\mathcal{L}_0 \rho(t) = -i[H, \rho(t)] \tag{2}$$

represents the internal dynamics of the spin chains, where the Hamiltonian of the spin chains H describes the internal energy of the system and their couplings. The commutator $[\cdot, \cdot]$ is calculated as $[A, B] = AB - BA$ for two matrices A and B with suitable dimensions. We let $\hbar = 1$, hereafter.

The Lindblad dissipative term induced by the non-Markovian environment is expressed as

$$\mathcal{L}_{\gamma(t)} \rho(t) = \frac{1}{2} \sum_{j,k=1}^{N^2-1} \gamma_{jk}(t)([L_j, \rho(t)L_k^\dagger] + [L_j\rho(t), L_k^\dagger]). \tag{3}$$

In contrast to the constant damping rates in the Markovian master equations, the damping rate functions $\gamma_{jk}(t)$ for characterizing the correlation of the non-Markovian environment are time-varying, which encapsules the coupling strengths between the system and the environment and the density state of the environment [12]. Here, we assume that $\gamma_{jk}(t)$ are complex functions, i.e., $\gamma_{jk}(t) = \text{Re}(\gamma_{jk}(t)) + i\,\text{Im}(\gamma_{jk}(t))$, where $\text{Re}(\cdot)$ and $\text{Im}(\cdot)$ represent the real and imaginary parts of a function, respectively.

In addition, the coupling operators L_k belong to a set $\mathcal{M} = \{L_k, k = 1, \ldots, M = N^2-1\}$, which are an orthonormal basis for the Lie algebra $\mathfrak{su}(N)$. Their commutation and anticommutation relations can be calculated as

$$[L_j, L_k] = i \sum_{l=1}^{M} C_{jkl} L_l \tag{4}$$

$$\{L_j, L_k\} = \frac{2}{N}\delta_{jk}I + \sum_{l=1}^{M} D_{jkl} L_l \tag{5}$$

respectively. The coefficients $C_{jkl}, D_{jkl} \in \mathbb{R}$ are the completely antisymmetric and symmetric structure constants of the Lie algebra $\mathfrak{su}(N)$, i.e., with respect to the interchange of any pair of indices [21]. Here, the anticommutator $\{\cdot, \cdot\}$ is calculated as $\{A, B\} = AB + BA$ for two matrices A and B with suitable dimensions, and δ is the Kronecker delta function.

Note that although the variation of the density matrix in the time-convolution-less master equation (1) only depends on the current density matrix mathematically, the time-varying damping rate functions enable (1) to describe a non-Markovian behavior physically, i.e., the energy exchanges between the system and the environment [12].

B. Dynamical Equations in a Coherence Vector Representation

Under the orthonormal basis in $\mathcal{M}$, we can expand the density matrix $\rho(t)$ and the Hamiltonian H as

$$\rho(t) = \frac{1}{N} I_N + \sum_{n=1}^{M} x_n(t) L_n$$

$$H = \sum_{m=1}^{M} h_m L_m \tag{6}$$

respectively, where $h_m = \mathrm{tr}(H L_m) \in \mathbb{R}$ and the coefficients $x_n(t)$ are the expectation values for the basis L_n, i.e., $x_n(t) = \mathrm{tr}(\rho(t) L_n) \in \mathbb{R}$. They constitute the so-called coherence vector $\mathbf{x}(t) = [x_1(t), \ldots, x_n(t), \ldots, x_M(t)]^T \in \mathbb{R}^M$. Here, I_N is an $N \times N$ identity matrix.

By using the relations (4)–(6), the time-convolution-less master equation (1) can be rewritten as a dynamical equation in the coherence vector representation as

$$\dot{\mathbf{x}}(t) = \mathbf{A}(t)\mathbf{x}(t) + \mathbf{b}(t), \quad x_n(0) = \mathrm{tr}(L_n \rho(0)) \tag{7}$$

where the initial value of the coherence vector $\mathbf{x}(0)$ is determined by the initial density matrix $\rho(0)$. The elements of the matrices $\mathbf{A}(t) \in \mathbb{R}^{M \times M}$ and $\mathbf{b}(t) \in \mathbb{R}^M$ can be calculated as $A_{np}(t) = Q_{np} + R_{np}(t)$ with $Q_{np} = \sum_{m=1}^{M} C_{mnp} h_m$, $R_{np}(t) = -(1/4) \sum_{l,j,k=1, l \leq m}^{M} (2 - \delta_{jk}) \mathrm{Re}(\gamma_{jk}(t)) \times (C_{jln} C_{klp} + C_{kln} C_{jlp}) + (1/2) \sum_{l,j,k=1, l \leq m}^{M} \mathrm{Im}(\gamma_{jk}(t)) \times (C_{kln} D_{jlp} - C_{jln} D_{klp})$, and $b_n(t) = -(2/N) \sum_{j,k=1, j < k}^{M} \mathrm{Im}(\gamma_{jk}(t)) C_{jkn}$, respectively. Here, the corresponding coefficients C and D are introduced in the calculation of the commutation and anticommutation relations (4) and (5) when transforming (1) into (7). Their indexes correspond to the labels of the orthonormal basis for $\mathfrak{su}(N)$ involved in the commutation and anticommutation relations.

Note that although (7) is in a similar form as the linear time-invariant (LTI) dynamical equation for a Markovian quantum system [15], it is a linear time-varying (LTV) dynamical equation due to the time-varying damping rate functions $\gamma_{jk}(t)$.

On the other hand, to extract information of $\gamma_{jk}(t)$, one can measure expectation values of S observables

$$\mathbf{y}(t) = [\langle O_1(t) \rangle, \langle O_2(t) \rangle, \ldots, \langle O_S(t) \rangle]^T \tag{8}$$

where $O_i(t)$ are local observables and the symbol $\langle \cdot \rangle = \mathrm{tr}[\cdot \rho(t)]$ represents the expectation of an observable. In addition, we can collect the data of $\mathbf{y}(t)$ as the output of the non-Markovian spin chains. In addition, these observables can be expanded under the orthonormal basis in $\mathcal{M}$ as $O_i = \sum_{n=1}^{M} o_n^{(i)} L_n$ with $o_n^{(i)} = \mathrm{tr}(O_i L_n)$, and thus, the output (8) can be reexpressed as

$$\mathbf{y}(t) = \mathbf{c}\mathbf{x}(t) \tag{9}$$

where $o_n^{(i)}$ is the ith row and nth column element of the matrix $\mathbf{c} \in \mathbb{R}^{S \times M}$.

Note that the measured operators in $\mathbf{y}(t)$ should be commutative since the uncertainty principle in quantum mechanics requires that the two noncommutative operators cannot be measured accurately at the same time. Hence, in general, the number of the measured observables S should be less than that of the orthonormal basis in $\mathcal{M}$, i.e., $S < M$.

It should be noted that the measurement of expectations of observables is applicable to the non-Markovian quantum systems. For example, in a superconducting non-Markovian single-qubit system, the measurement of average charge numbers is equivalent to measuring the z-component of the coherence vector for the single qubit. The procedure is to measure the same observable many times and then take the average of the results [8].

C. Reduced Dynamical Equation

Equation (7) describes the full dynamics of the non-Markovian spin chains. However, it is possible that not all the components in $\mathbf{x}(t)$ are relevant to the observables (8), i.e., the matrix $\mathbf{A}(t)$ would have a block-diagonalizable structure and a proper subblock corresponds to the observables. We can use a filtration procedure in [22] to find the *accessible set* which is related to the observables [15].

Thus, a reduced coherence vector $\tilde{\mathbf{x}}(t)$ corresponding to the observables (8) can be defined, and it obeys a reduced dynamical equation

$$\dot{\tilde{\mathbf{x}}}(t) = \tilde{\mathbf{A}}(t)\tilde{\mathbf{x}}(t) + \tilde{\mathbf{b}}(t)$$

$$\mathbf{y}(t) = \tilde{\mathbf{c}}\tilde{\mathbf{x}}(t) \tag{10}$$

where $\tilde{\mathbf{A}}(t)$, $\tilde{\mathbf{b}}(t)$, and $\tilde{\mathbf{c}}$ with suitable dimensions are the submatrices of $\mathbf{A}(t)$, $\mathbf{b}(t)$, and $\mathbf{c}$.

III. GRADIENT ALGORITHM FOR IDENTIFYING THE DAMPING RATE FUNCTION

A. Optimization Formulation for the Identification of the Damping Rate Function

The identification problem considered in this brief can be stated as follows. Considering the non-Markovian spin chains governed by the dynamical equation of the coherence vector (7), where all the information of the environment are encoded in the unknown damping rate functions, the environment identification problem is to identify the time-varying damping rate functions from the data of the time traces of the observables $\hat{\mathbf{y}}(t)$ (9).

Note that due to the interactions between the spin chains and the environment, in general, there is no decoherence-free subspace for a common non-Markovian system without control pulses, i.e., decoherence channels affect all the components in the coherence vector. Thus, the damping rate functions will be imprinted in the observables. Hence, the identification problem for the damping rate function should be solvable. In addition, since the time-varying damping rate functions $\gamma_{jk}(t)$ result in a LTV system (7), the identification method for the Markovian quantum systems in [15] cannot be applied in our case.

Generally, it is difficult to identify analytically a time-varying function in a dynamical system. Alternatively, we can numerically solve this problem by designing an algorithm. We consider that the system (7) evolves in a total time T

during which the observables are measured K times at equal time intervals Δt, i.e., $\Delta t = (T/K)$. Thus, a set of real measurement results $\hat{\mathbf{y}} = [\hat{\mathbf{y}}(0), \hat{\mathbf{y}}(1), \ldots, \hat{\mathbf{y}}(K-1)]$ can be obtained.

In addition, the time-varying damping rate functions $\gamma_{jk}(t)$ are discretized, and we assume that $\gamma_{jk}(t)$ in each time interval are constants $\gamma_{jk}(\kappa), \kappa = 0, 1, 2, \ldots, (K-2)$. Thus, in each time interval, we can consider the LTV system equation (7) as a LTI system and write the dynamical equation in a continuous-time form as

$$\dot{\mathbf{x}}(\tau) = \mathbf{A}(\gamma_{jk}(\tau))\mathbf{x}(\tau) + \mathbf{b}(\text{Im}(\gamma_{jk}(\tau))) \tag{11}$$
$$\mathbf{y}(\tau) = \mathbf{c}\mathbf{x}(\tau), \quad \tau \in [\kappa\Delta t, (\kappa+1)\Delta t] \tag{12}$$

where (11) can be solved as

$$\mathbf{x}(\kappa+1) = e^{\mathbf{A}(\gamma_{jk}(\kappa))\Delta t}\mathbf{x}(\kappa)$$
$$+ \int_{\kappa\Delta t}^{(\kappa+1)\Delta t} e^{\mathbf{A}(\gamma_{jk}(\kappa))((\kappa+1)\Delta t - \tau)}\mathbf{b}(\text{Im}(\gamma_{jk}(\kappa)))d\tau. \tag{13}$$

Here, we have written the initial coherence vector in the current and the next time intervals in an abbreviate form as $\mathbf{x}(\kappa)$ and $\mathbf{x}(\kappa+1)$, respectively.

For a given set of $\gamma_{jk}(\kappa), \kappa = 0, 1, 2, \ldots, (K-2)$, an output vector $\mathbf{y} = [\mathbf{y}(0), \mathbf{y}(1), \ldots, \mathbf{y}(K-1)]$ can be generated by using (12) and (13). A guessed set of $\gamma_{jk}(\kappa), \kappa = 0, 1, 2, \ldots, (K-2)$ may not be identical to the real damping rate function. Hence, the generated output $\mathbf{y}$ will be different from the real data $\hat{\mathbf{y}}$. Thus, we define an objective function

$$J = \frac{1}{2}\sum_{\kappa=0}^{K-1}(\mathbf{y}(\kappa) - \hat{\mathbf{y}}(\kappa))^2 \tag{14}$$

to evaluate the distance between the two vectors $\mathbf{y}$ and $\hat{\mathbf{y}}$.

Therefore, the identification problem for the damping rate functions $\gamma_{jk}(t)$ can be converted into an optimization problem as follows.

For real measurement results $\hat{\mathbf{y}}$, the optimization problem is to find a set of $\gamma_{jk}(\kappa), \kappa = 0, 1, 2, \ldots, (K-2)$, such that the objective function (14) is minimized, that is

$$\min_{\gamma_{jk}(\kappa)} J$$
$$\text{s. t. } (7), (9). \tag{15}$$

B. Gradient Algorithm for the Identification Problem

To design a gradient algorithm for the optimization problem (15), it is crucial to obtain the gradient of the objective J with respect to $\gamma_{jk}(\kappa)$ in each time interval. By using the chain rule, the gradient can be calculated as

$$\frac{dJ}{d\gamma_{jk}(\kappa)} = \frac{dJ}{d\mathbf{y}} \cdot \frac{d\mathbf{y}}{d\mathbf{x}} \cdot \frac{d\mathbf{x}}{d\gamma_{jk}(\kappa)}$$
$$= \sum_{\kappa'=0}^{K-1}(\mathbf{y}(\kappa') - \hat{\mathbf{y}}(\kappa')) \cdot \mathbf{c}\frac{d\mathbf{x}(\kappa')}{d\gamma_{jk}(\kappa)} \tag{16}$$

where

$$\frac{d\mathbf{x}(\kappa')}{d\gamma_{jk}(\kappa)} = \begin{cases} 0 & \kappa' < \kappa+1 \\ \dfrac{d\mathbf{x}(\kappa+1)}{d\gamma_{jk}(\kappa)} & \kappa' = \kappa+1 \\ \displaystyle\prod_{\kappa''=\kappa+1}^{\kappa'-1} e^{\mathbf{A}(\gamma_{jk}(\kappa''))\Delta t}\dfrac{d\mathbf{x}(\kappa+1)}{d\gamma_{jk}(\kappa)} & \kappa' > \kappa+1. \end{cases} \tag{17}$$

In the following, we will calculate the derivative of $\mathbf{x}$ with respect to the real and imaginary parts of $\gamma_{jk}(\kappa)$, respectively. By using a standard formula for derivative of a matrix exponential [23]

$$\frac{d}{dx}e^{(A+xB)t}|_{x=0} = e^{At}\int_0^t e^{A\tau}Be^{-A\tau}d\tau \tag{18}$$

with matrices A and B of suitable dimensions, we have

$$\frac{de^{\mathbf{A}(\gamma_{jk}(\kappa))\Delta t}}{d\text{Re}(\gamma_{jk}(\kappa))} = \Delta t e^{\mathbf{A}(\gamma_{jk}(\kappa))\Delta t}\tilde{\mathbf{E}}_R$$
$$\frac{de^{\mathbf{A}(\gamma_{jk}(\kappa))\Delta t}}{d\text{Im}(\gamma_{jk}(\kappa))} = \Delta t e^{\mathbf{A}(\gamma_{jk}(\kappa))\Delta t}\tilde{\mathbf{E}}_I \tag{19}$$

where $\tilde{\mathbf{E}}_R = \int_{\kappa\Delta t}^{(\kappa+1)\Delta t} e^{\mathbf{A}(\gamma_{jk}(\kappa))\tau}\mathbf{E}_R e^{-\mathbf{A}(\gamma_{jk}(\kappa))\tau}d\tau$ and $\tilde{\mathbf{E}}_I = \int_{\kappa\Delta t}^{(\kappa+1)\Delta t} e^{\mathbf{A}(\gamma_{jk}(\kappa))\tau}\mathbf{E}_I e^{-\mathbf{A}(\gamma_{jk}(\kappa))\tau}d\tau$. When the time interval Δt is small enough, such that $\Delta t \ll ||\mathbf{A}||^{-1}$, we have

$$\tilde{\mathbf{E}}_R = \mathbf{E}_R, \quad \tilde{\mathbf{E}}_I = \mathbf{E}_I \tag{20}$$

where the elements of $\mathbf{E}_R$ and $\mathbf{E}_I$ can be expressed as $E_{Rnp} = -(1/4)(2 - \delta_{jk})\sum_{l=1}^M (C_{jln}C_{klp} + C_{kln}C_{jlp})$ and $E_{Inp} = (1/2)\sum_{l=1}^M (C_{kln}D_{jlp} - C_{jln}D_{klp})$.

Thus, the derivative of $\mathbf{x}(\kappa+1)$ with respect to the real and imaginary parts of $\gamma_{jk}(\kappa)$ can be calculated as

$$\frac{d\mathbf{x}(\kappa+1)}{d\text{Re}(\gamma_{jk}(\kappa))}$$
$$= \Delta t e^{\mathbf{A}(\gamma_{jk}(\kappa))\Delta t}\mathbf{E}_R\mathbf{x}(\kappa)$$
$$+ \int_{\kappa\Delta t}^{(\kappa+1)\Delta t}((\kappa+1)\Delta t - \tau)e^{\mathbf{A}(\gamma_{jk}(\kappa))((\kappa+1)\Delta t - \tau)}$$
$$\times \mathbf{E}_R\mathbf{b}(\text{Im}\gamma_{jk}(\kappa))d\tau \tag{21}$$
$$\frac{d\mathbf{x}(\kappa+1)}{d\text{Im}(\gamma_{jk}(\kappa))}$$
$$= \Delta t e^{\mathbf{A}(\gamma_{jk}(\kappa))\Delta t}\mathbf{E}_I\mathbf{x}(\kappa)$$
$$+ \int_{\kappa\Delta t}^{(\kappa+1)\Delta t}((\kappa+1)\Delta t - \tau)e^{\mathbf{A}(\gamma_{jk}(\kappa))((\kappa+1)\Delta t - \tau)}$$
$$\times \mathbf{E}_I\mathbf{b}(\text{Im}\gamma_{jk}(\kappa))d\tau$$
$$+ \int_{\kappa\Delta t}^{(\kappa+1)\Delta t} e^{\mathbf{A}(\gamma_{jk}(\kappa))((\kappa+1)\Delta t - \tau)}\mathbf{F}d\tau \tag{22}$$

where the nth row element of the column vector $\mathbf{F}$ is $-\frac{2}{N}C_{jkn}$.

By combining (16), (17), (21), and (22), we obtain the gradient of the objective J with respect to γ_{jk}. Therefore, if we update γ_{jk} as

$$\text{Re}(\gamma_{jk}) \rightarrow \text{Re}(\gamma_{jk}) - \epsilon_R \cdot \frac{dJ}{d\text{Re}(\gamma_{jk})}$$
$$\text{Im}(\gamma_{jk}) \rightarrow \text{Im}(\gamma_{jk}) - \epsilon_I \cdot \frac{dJ}{d\text{Im}(\gamma_{jk})} \tag{23}$$

with small step sizes ϵ_R and ϵ_I, we can minimize the objective J. With the relation (23), our gradient algorithm for the identification problem can be summarized as follows.

Step 1: Choose and measure a set of observables $\hat{\mathbf{y}}(t)$, initialize the state of the system $\mathbf{x}(0)$, the output $\mathbf{y}(0)$, and the step sizes ϵ_R and ϵ_I, and guess the initial values of $\{\gamma_{jk}(\kappa)\}$.

Step 2: Calculate $\mathbf{x}(1)$ to $\mathbf{x}(K-1)$ and $\mathbf{y}(1)$ to $\mathbf{y}(K-1)$ with their initial values $\mathbf{x}(0)$ and $\mathbf{y}(0)$.

Step 3: Compute the gradient of the objective J with respect to $\gamma_{jk}(\kappa)$.

Step 4: Update $\gamma_{jk}(\kappa)$ by using the relation (23).

Step 5: When a termination condition is satisfied, stop the algorithm; otherwise, go to the step 2 and start a new iteration.

Note that this algorithm searches optimal solutions according to the gradient, and hence, it may stop at a local minimum point. Moreover, the final performance of the algorithm depends on the initial guessed solution $\{\gamma_{jk}(\kappa)\}$. When the initial guessed solution is closer to the optimal one, the algorithm will converge faster. The step size may also affect the performance of the algorithm. A small step size would result in a slow convergence process, and a large one would lead to an algorithm that saturates in the vicinity of a minimum. An adaptive step size can avoid the above problems. In addition, a proper termination condition can be the completion of a given number of iterations or the attainment of an accuracy of the objective J.

IV. PHYSICAL EXAMPLE

In the example, we consider two coupled qubits immersed in an unknown common environment, where the dissipative processes for the two qubits can be considered to be the same. Its non-Markovian dynamics can be described by a time-convolution-less master equation [12] as

$$\dot{\rho}_q(t) = -i[H_q, \rho_q(t)] + \frac{\gamma(t)}{2} \sum_{l=1}^{2} \left([\sigma_l^- \rho_q(t), \sigma_l^+] \right.$$
$$\left. + [\sigma_l^-, \rho_q(t)\sigma_l^+] \right) \quad (24)$$

where $\rho_q(t)$ is the density operator for the two qubits and the ladder operators are defined as $\sigma^+ = \frac{1}{2}(\sigma^x + i\sigma^y)$ and $\sigma^- = \frac{1}{2}(\sigma^x - i\sigma^y)$ with the Pauli matrices

$$\sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma^y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \quad (25)$$

Here, the label l is used to index the qubits. The two qubits are assumed to be coupled in an XY interaction form, and thus, the Hamiltonian of the two qubits is written as

$$H_q = \sum_{\alpha=1}^{2} \frac{\omega_\alpha}{2} \sigma_\alpha^z + \frac{g}{2}(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y) \quad (26)$$

where g is the coupling strength between two qubits and ω_α is the angular frequency for the αth qubit. In this time-convolution-less master equation (24), all the properties of the unknown environment are combined in the damping rate function $\gamma(t)$, which are the same with respect to each dissipative
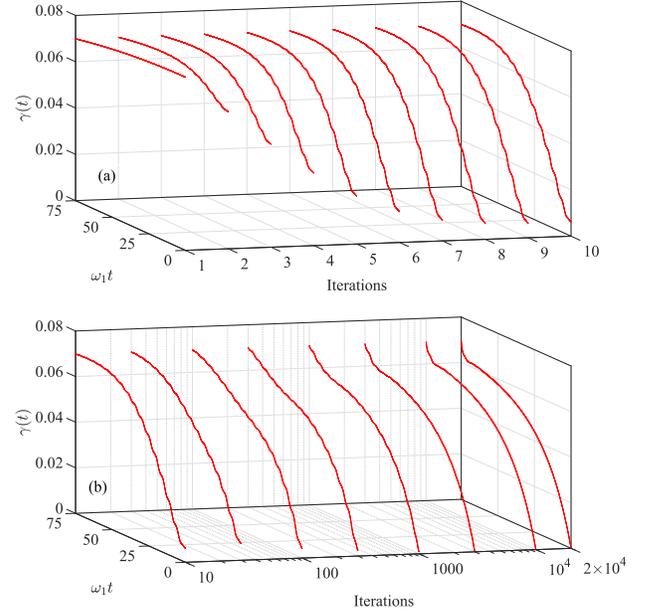

Fig. 2. Evolution of the identified damping rate function at specific iterations.

channel for the two qubits. Thus, the identification task is to recover the unknown damping rate function $\gamma(t)$. To simulate a real damping rate function induced by the non-Markovian environment, we assume that the real damping rate function is

$$\hat{\gamma}(t) = \frac{2h\lambda\sinh(dt/2)}{d\cosh(dt/2) + \lambda\sinh(dt/2)} \quad (27)$$

which results from a non-Markovian environment with a Lorentzian spectrum [12]. The values of the parameters h, λ, and d will be given in the following paragraph. This real damping rate function (27) is utilized to generate the real measurement results $\hat{\mathbf{y}}(t)$.

Furthermore, we measure the observable σ_1^z for the first qubit that induces the accessible set $\{\sigma_1^z, \sigma_2^z, \sigma_1^x\sigma_2^x, \sigma_1^x\sigma_2^y, \sigma_1^y\sigma_2^x, \sigma_1^y\sigma_2^y\}$. Due to the interactions between the two qubits, the accessible set also includes the operators for the second qubit. Hence, the reduced dynamical equation for the state vector $\tilde{\mathbf{x}}(t) = [\langle\sigma_1^z\rangle, \langle\sigma_2^z\rangle, \langle\sigma_1^x\sigma_2^x\rangle, \langle\sigma_1^x\sigma_2^y\rangle, \langle\sigma_1^y\sigma_2^x\rangle, \langle\sigma_1^y\sigma_2^y\rangle]^T$ is in the form of (10) with matrices

$$\tilde{\mathbf{A}}(t) = \begin{bmatrix} -\gamma(t) & 0 & 0 & -g & g & 0 \\ 0 & -\gamma(t) & 0 & g & -g & 0 \\ 0 & 0 & -\gamma(t) & -\omega_2 & -\omega_1 & 0 \\ g & -g & \omega_2 & -\gamma(t) & 0 & -\omega_1 \\ -g & g & \omega_1 & 0 & -\gamma(t) & -\omega_2 \\ 0 & 0 & 0 & \omega_1 & \omega_2 & -\gamma(t) \end{bmatrix}$$

$$\tilde{\mathbf{b}}(t) = \begin{bmatrix} -\gamma(t) & -\gamma(t) & 0 & 0 & 0 & 0 \end{bmatrix}^T.$$

In addition, the parameters of the system are chosen as follows. The angular frequencies of the two qubits are the same, i.e., $\omega_1 = \omega_2 = 1.5$ GHz. The coupling strength between the two qubits is $g = 1$ GHz. To simulate the real $\gamma(t)$, the parameters in (27) are chosen as $h = 0.05$ GHz, $d = 0.05$ GHz, and $\lambda = 0.1$ GHz. The gradient algorithm
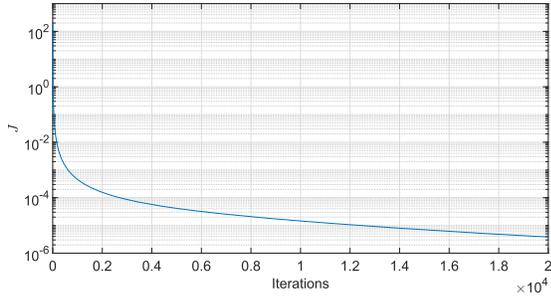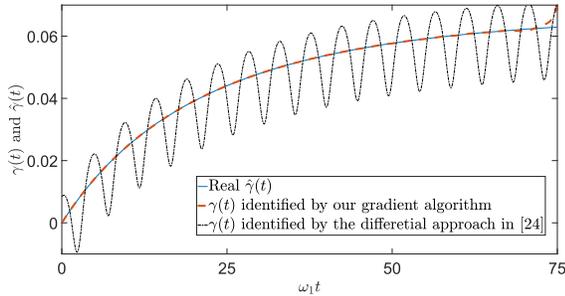
Fig. 3. Reduction of the objective function J.

Fig. 4. Comparison between the identified and real damping rate functions.

starts with a guessed damping rate function

$$\gamma_0(t) = 0.04 \cos(0.01t) + 0.0348 \qquad (28)$$

which is plotted as a red line at the first iteration in Fig. 2(a).

Both the step size in each iteration and the termination condition can affect the performance of the gradient algorithm. We choose the step size for updating the damping rate function as $\epsilon = 0.002$. Because a large step size would result in oscillations in the final stage for searching the minimum J, and a small one would lead to a slow convergence process. On the other hand, we choose to iterate the algorithm for 20 000 times as the terminal condition. Sufficient iteration times allow the algorithm to obtain a minimal objective J.

With these parameters, the evolution of the damping rate function from the initial guess to the identified one is given in Fig. 2. Initially, the gradient algorithm can significantly update the identified damping rate function, as shown in Fig. 2(a). After 10 iterations, the convergence rate of the identification process slows down, as shown in Fig. 2(b). This phenomenon also reflects in the reduction of the objective function J in Fig. 3. With 20 000 iterations, the objective function is down to about 10^{-5}, and we terminate the algorithm.

The final identified damping rate function is plotted as the red dashed line in Fig. 4. Compared with the real damping rate function represented as the blue solid line, our algorithm can identify the damping rate function well except at the final stage. This is because the measurement results at a final time interval contain limited information of the damping rate function, and thus, the resulting gradient provides very

small updates. We also make a comparison between our method and a differential approach in [24], whose identified result is plotted as the dashed dotted line in Fig. 4. Under the identical measurement result, our method obtains a better result than that by using the differential approach. This is because all the corresponding measured results are utilized to identify the unknown damping rate function in a sample time interval by using our method. However, the differential approach only uses the measurement results at the current and next times to estimate the damping rate function at the current time. Its identification result can be improved if we measure the observable densely.

V. Conclusion

In this brief, we have designed a gradient algorithm for identifying the damping rate function in the time-convolution-less master equation for the non-Markovian spin chains. We have formulated the identification problem as an optimization problem that can be solved iteratively by calculating the gradient of the objective with respect to the damping rate function in each time interval. The numerical example on a non-Markovian two-qubit system demonstrates the efficacy of our gradient algorithm. Compared with a differential approach, our method can identify the damping rate function with a high fidelity.

References

[1] C. Sayrin *et al.*, "Real-time quantum feedback prepares and stabilizes photon number states," *Nature*, vol. 477, pp. 73–77, Sep. 2011.

[2] J. Zhang, R.-B. Wu, C.-W. Li, and T. Tarn, "Protecting coherence and entanglement by quantum feedback controls," *IEEE Trans. Autom. Control*, vol. 55, no. 3, pp. 619–633, Mar. 2010.

[3] S. Xue, M. R. Hush, and I. R. Petersen, "Feedback tracking control of non-Markovian quantum systems," *IEEE Trans. Control Syst. Technol.*, vol. 25, no. 5, pp. 1552–1563, Sep. 2017.

[4] S. Xue, R. B. Wu, W. M. Zhang, J. Zhang, C. W. Li, and T. J. Tarn, "Decoherence suppression via non-Markovian coherent feedback control," *Phys. Rev. A, Gen. Phys.*, vol. 86, no. 5, p. 052304, 2012.

[5] S. Xue, R. Wu, M. R. Hush, and T.-J. Tarn, "Non-Markovian coherent feedback control of quantum dot systems," *Quantum Sci. Technol.*, vol. 2, no. 1, p. 014002, 2017.

[6] T. Frey *et al.*, "Dipole coupling of a double quantum dot to a microwave resonator," *Phys. Rev. Lett.*, vol. 108, p. 046807, Jan. 2012.

[7] S. Xue, M. R. James, V. Ugrinovskii, and I. R. Petersen, "LQG feedback control of a class of linear non-Markovian quantum systems," in *Proc. Amer. Control Conf.*, Boston, MA, USA, Jul. 2016, pp. 4775–4778.

[8] R. B. Wu *et al.*, "Spectral analysis and identification of noises in quantum systems," *Phys. Rev. A, Gen. Phys.*, vol. 87, p. 022324, Feb. 2013.

[9] J. M. Geremia and H. Rabitz, "Optimal identification of Hamiltonian information by closed-loop laser control of quantum systems," *Phys. Rev. Lett.*, vol. 89, no. 26, p. 263902, 2002.

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

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

[12] H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems*. Oxford, U.K.: Oxford Univ. Press, 2002.

[13] H. Mabuchi, "Dynamical identification of open quantum systems," *Quantum Semiclass. Opt.*, vol. 8, no. 6, pp. 1103–1108, 1996.

[14] Y. Kato and N. Yamamoto, "Structure identification and state initialization of spin networks with limited access," *New J. Phys.*, vol. 16, no. 2, p. 023024, 2014.

[15] J. Zhang and M. Sarovar, "Identification of open quantum systems from observable time traces," *Phys. Rev. A, Gen. Phys.*, vol. 91, p. 052121, May 2015.

[16] A. Sone and P. Cappellaro, "Hamiltonian identifiability assisted by a single-probe measurement," *Phys. Rev. A, Gen. Phys.*, vol. 95, p. 022335, Feb. 2017.

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

[18] S. Xue, T. Nguyen, M. R. James, A. Shabani, V. Ugrinovskii, and I. R. Petersen. (2017) "Modelling and filtering for non-Markovian quantum systems." [Online]. Available: https://arxiv.org/abs/1704.00986

[19] G. A. Paz-Silva, L. M. Norris, and L. Viola, "Multiqubit spectroscopy of Gaussian quantum noise," *Phys. Rev. A, Gen. Phys.*, vol. 95, p. 022121, Feb. 2017.

[20] F. K. Malinowski *et al.*, "Spectrum of the nuclear environment for GaAs spin qubits," *Phys. Rev. Lett.*, vol. 118, p. 177702, Apr. 2017.

[21] R. Alicki and K. Lendi, *Quantum Dynamical Semigroups and Applications* (Lecture Notes in Physics), vol. 717. Berlin, Germany: Springer, 2007.

[22] S. Sastry, *Nonlinear Systems*. New York, NY, USA: Springer, 1999.

[23] I. Najfeld and T. F. Havel, "Derivatives of the matrix exponential and their computation," *Adv. Appl. Math.*, vol. 16, no. 3, pp. 321–375, 1995.

[24] B. Bellomo, A. De Pasquale, G. Gualdi, and U. Marzolino, "Reconstruction of time-dependent coefficients: A check of approximation schemes for non-Markovian convolutionless dissipative generators," *Phys. Rev. A, Gen. Phys.*, vol. 82, p. 062104, Dec. 2010.