Quantum Hamiltonian Identification With Classical Colored Measurement Noise

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Abstract—In this brief, we present a Hamiltonian-identification method for a closed quantum system whose time-trace observables are measured with colored measurement noise. The dynamics of the quantum system are described by a Liouville equation that can be converted into a coherence vector representation. Since the measurement process is disturbed by classical colored noise, we introduce an augmented system model to describe the total dynamics, where the classical colored noise is parameterized. Based on the augmented system model as well as the measurement data, we can find a realization of the quantum system with unknown parameters by employing an eigenstate-realization algorithm. The unknown parameters can be identified using a transfer-function-based technique. An example of a two-qubit system with colored measurement noise is shown to verify the effectiveness of our method.

Index Terms—Classical colored noise, closed quantum systems, coherence vector, Hamiltonian identification, time-trace observables.

I. INTRODUCTION

IN RECENT years, great progress has been achieved on quantum technologies, such as quantum computation [1], quantum communication [2], and quantum metrology [3]. Relying on the precise models of relevant quantum systems, these quantum-mechanics-based techniques can achieve better performance than the classical-mechanics-based counterparts. However, under some circumstances, some parameters in these models may not be known, which results in degraded performance [4]. For acquiring these parameters, a fundamental step is identification. In the classical system-identification theory, various methods have been proposed, such as wavelet cross spectrum analysis, least squares methods, or maximum-likelihood estimators [5], to estimate the unknown system parameters using the input and output data of a system.

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extended to open quantum systems [18]. Fourier analysis was also applied to quantum Hamiltonian identification. Cole et al. [19] adopted the Fourier transform of the measurement of one observable to identify the Hamiltonian of a closed two-level quantum system. Schirmer et al. [20] estimated the Hamiltonian of a two-level quantum system based on Fourier analysis, and Burgarth et al. [21] provided the solution for an N-level quantum system. In these previous works, the measurement process is assumed ideal or disturbed by Gaussian noise, which is convenient for the analysis and design of identification algorithms. However, in practice, we use classical devices in the measurement process that may cause classical colored noise [22], [23]. Ignoring the impact of colored noise may degrade the performance of identification algorithms.

In this brief, we propose an augmented system method to identify parameters in the Hamiltonian of a closed quantum system where the data of the measured time-trace observables carry classical colored noise. We consider a closed finite-level quantum system that can be represented in a coherence vector representation. Correspondingly, when the observable of the system is specified, the dynamics of the system can be described by a reduced equation of the coherence vector. To combine the colored noise into the model for identification, a spectral factorization method is used such that an augmented system model for quantum Hamiltonian identification can be obtained. Moreover, using the data of the time-trace observables, an eigenstate realization algorithm (ERA) is employed to find a realization of the augmented system. Equating the transfer function of both the original system with unknown parameters and the realization generated by the measurement data, we can obtain a set of nonlinear algebraic equations for the unknown parameters, which is usually difficult to be solved analytically. Numerically, these equations can be solved using a PHCpack [24]. Finally, we provide an example of a two-qubit system with the measurement data polluted by classical colored noise.

The contribution of our work is that we present an augmented system model for Hamiltonian identification under colored measurement noise that has not been considered before in the field of quantum system identification. The augmented system model is effective to deal with various kinds of colored measurement noises with a rational power spectral density (PSD). It can also be applied to model colored measurement noise with an irrational one by using Padé approximation. The augmented system model cooperated with an ERA can obtain a better performance than that in [17].

The remainder of this brief is organized as follows. Section II describes the model for the identification of finite-level quantum systems. In Section III, we develop a colored noise realization that is used to augment the original system model. The procedure to obtain identified Hamiltonian is presented in Section IV. In Section V, the effectiveness of our algorithm is verified in an example of a two-qubit system with classical colored measurement noise. Conclusions are drawn in Section VI.

II. DESCRIPTION OF FINITE-LEVEL QUANTUM SYSTEMS

In this brief, we consider a closed N-level quantum system. The system Hamiltonian $H$ satisfies $i H \in \mathfrak{su}(N)$, where the Lie algebra $\mathfrak{su}(N)$ can be represented by the $N \times N$ traceless skew-Hermitian matrices. The dimension of $\mathfrak{su}(N)$ over $\mathbb{R}$ is $N^2 - 1$. Therefore, we can expand the Hamiltonian as

$$H = \sum_{m=1}^{N^2-1} a_m X_m \tag{1}$$

where $\mathcal{X} = \{i X_m, m = 1, 2, \ldots, N^2 - 1\}$ is a set of orthogonal bases for $\mathfrak{su}(N)$ [17]. The commutation relations for the elements in $\mathcal{X}$ are $[X_j, X_k] = \sum_{l=1}^{N^2-1} C_{jkl} X_l$, where the commutator $[\cdot, \cdot]$ is calculated as $[X, Y] = XY - YX$ for the two operators $X$ and $Y$ and $C_{jkl}$ are the antisymmetric constants with respect to the interchange of any pair of indices [25]. This property indicates that $C_{jkl}$ is equal to zero with any two identical indices.

The Hamiltonian determines the dynamics of the density matrix $\rho(t)$ of the system as

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

which is the so-called Liouville equation [26]. The density matrix $\rho$ describes the probability distribution of the system states, which is an $N \times N$ Hermitian and positive semidefinite matrix with $\text{tr}(\rho) = 1$. We have assumed $\hbar = 1$.

The Liouville equation (2) can be transformed into a coherence vector representation [27], which is convenient for the design of an identification algorithm. In this representation, the state of the system is alternatively described by a coherence vector $x = [x_1, \ldots, x_{N^2-1}]^T$, where $x_j$ is the expectation value of $X_j$, i.e., $x_j = \text{tr}(X_j \rho)$. The corresponding dynamical equation is, thus, written as

$$\dot{x}_j(t) = i \sum_{l=1}^{N^2-1} \sum_{m=1}^{N^2-1} a_m C_{mlj} x_l(t), \quad j = 1, 2, \ldots, N^2 - 1. \tag{3}$$

To observe the quantum system, we can choose $L$ observables $O_1, O_2, \ldots, O_L$ and their expectations can be taken as the outputs of the system, that is

$$y(t) = [y_1(t), y_2(t), \ldots, y_L(t)]^T$$

where $y_j(t) = \langle O_j \rangle = \text{tr}(O_j \rho)$. An observable $O_i$ can be expanded in terms of the bases in $\mathcal{X}$ as $O_i = \sum_j o_i^{(j)} X_j$, where the corresponding bases $\mathcal{M} = \{X_{\mu_1}, X_{\mu_2}, \ldots, X_{\mu_p}\}$ span a minimal space containing the $L$ observables. Here, $\mu_j$ denotes the indices for the corresponding bases and the number of $\mu_j$ is $p$.

With respect to the bases in $\mathcal{M}$, an accessible set of $\mathcal{M}$ can be generated using a filtration process [17]. Denoting $\mathcal{F}_0 = \mathcal{M}$, an iterative procedure can be calculated $\mathcal{F}_i = \mathcal{F}_{i-1} \cup [\mathcal{F}_{i-1}, \mathcal{X}]$, where $[\mathcal{F}_{i-1}, \mathcal{X}] = \{X_j\text{tr}(X_j^\dagger g, h) \neq 0, g \in \mathcal{F}_{i-1}, h \in \mathcal{X}\}$, until $\mathcal{F}_i$ saturates. Supposing the final set is $\mathcal{F} = \{X_{\mu_1}, X_{\mu_2}, \ldots, X_{\mu_K}\}$ with a size $K$, the corresponding reduced coherence vector is $x = [x_{\mu_1}, x_{\mu_2}, \ldots, x_{\mu_K}]^T$. Therefore, the resulting reduced dynamical equation for the reduced
coherence vector can be written as
\[
\dot{x}(t) = Ax(t), \quad x(0) = x_0
\]
\[
y(t) = Cx(t)
\]  \hspace{1cm} (4)
with \( A \in \mathbb{R}^{K \times K}, \ C \in \mathbb{R}^{L \times K} \), where \( x_0 \) is the initial state, \( A_{ji} = -i \sum_{m=1}^{N-1} a_m C_{m,j}, \) and \( C \) are configured such that \( y(t) \) are the expectation values of our measured observables. Equation (4) affords the basic model for the system to be identified.

III. AUGMENTED MODEL FOR OUTPUTS DISTURBED BY CLASSICAL COLORED NOISE

In existing Hamiltonian-identification studies, ideal case or Gaussian noise-disturbing measurement results have been considered. However, in practice, measurement results may be polluted by the classical colored noise arising from the measurement devices. Hence, for the purpose of Hamiltonian identification, it is necessary to introduce the classical colored noise model to obtain a complete model.

A. Classical Colored Noise Model

In general, classical colored noise can be characterized by a shaped PSD \( S(\omega) \) describing the power distribution of the noise over all the frequency components [28]. Since the PSD and autocorrelation \( R(t) \) of the noise form a Fourier transform pair, the PSD can be calculated as
\[
S(\omega) = \int_{-\infty}^{\infty} e^{-i\omega t} R(t) dt.
\]  \hspace{1cm} (5)
The spectral factorization theorem tells that a positive, rational, and strictly proper PSD \( S(\omega) \) can be factorized as
\[
S(\omega) = \Gamma(s) \Gamma^T(-s)|_{s=i\omega}
\]  \hspace{1cm} (6)
where \( \Gamma(s) \) is a causal transfer function resulting from the internal dynamics of noises. Here, \( \Gamma(s) \) characterizes a mapping of a white noise input \( \eta(t) = \Gamma[\eta(t)] \) to a colored noise output \( v(s) = \mathcal{L}[v(t)] \). The operator \( \mathcal{L}[-] \) denotes Laplace transform, and \( \eta(t) \) and \( v(t) \) are the white noise input and the colored noise in the time domain, respectively. Note that the PSD of \( v(t) \) is \( S(\omega) \), which will reduce to a flat one when the output noise is white. In addition, for an irrational PSD, we can find its rational approximants using Padé approximation [29] and then a transfer function can be obtained by the factorization.

For a given transfer function \( \Gamma(s) \), it is easy to construct a corresponding minimal realization [30]. For the single-input–single-output (SISO) transfer function
\[
\Gamma(s) = \frac{\beta_1 s^{n-1} + \beta_2 s^{n-2} + \cdots + \beta_{n-1} s + \beta_n}{s^n + a_1 s^{n-1} + \cdots + a_{n-1} s + a_n}
\]  \hspace{1cm} (7)
which is strictly proper, we can write its realization in a controllable canonical form as
\[
\dot{\xi}(t) = E\xi(t) + F\eta(t)
\]
\[
v(t) = G\xi(t)
\]  \hspace{1cm} (8)
with
\[
E = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -a_{n} & -a_{n-1} & -a_{n-2} & \cdots & -a_1 \end{bmatrix}
\]
\[
F = \begin{bmatrix} 0 & 0 & \cdots & 0 \end{bmatrix}^T
\]
\[
G = [\beta_n \beta_{n-1} \beta_{n-2} \cdots \beta_1]^T
\]  \hspace{1cm} (9)
where \( \xi \in \mathbb{R}^n \) represents the internal state vector of the noise with an initial state \( \xi(0) = \xi_0 \). It is straightforward to obtain the dynamics of the expectation \( \bar{\xi}(t) \) of the internal mode \( \xi \) as
\[
\dot{\bar{\xi}}(t) = \bar{E}\xi(t), \quad \bar{\xi}(0) = \bar{\xi}_0
\]
\[
\bar{v}(t) = G\bar{\xi}(t)
\]  \hspace{1cm} (10)
where \( \bar{v}(t) \) is the expectation of the colored noise \( v(t) \) and the input term vanishes since \( \bar{\eta}(t) = 0 \).

B. Augmented System Model

The classical colored noise considered in this brief may arise from the measurement devices for measuring the time traces of the observables. Before measuring an observable, we generally initialize the measurement device in the same state. In addition, we can use the same device to measure the time traces for different observables. Hence, in the following derivation, we assume that different observables are disturbed by the same additive classical colored noise \( v(t) \). After averaging over the measurement results, the time traces for an observable can be obtained, where the expectation of the classical colored noise is taken, that is, the time trace of the \( i \)th observable \( O_i \) is disturbed by the classical colored noise. Hence, the polluted output can be expressed as
\[
\bar{y}_i(t) = y_i(t) + \bar{v}(t)
\]  \hspace{1cm} (11)
where \( y_i(t) \) is the original quantum output for the \( i \)th observable and \( \bar{y}_i(t) \) is the polluted one. Hence, the polluted output of the system can be written as
\[
\bar{y}(t) = \begin{bmatrix} y_1(t) + \bar{v}(t) \\ y_2(t) + \bar{v}(t) \\ \vdots \\ y_L(t) + \bar{v}(t) \end{bmatrix} = Cx(t) + \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \bar{v}(t).
\]  \hspace{1cm} (12)
Further, substituting the expression of \( \bar{v}(t) \) in (10) into (12) and denoting a new state vector \( \bar{x} \) as \( \bar{x} = [x(t)\bar{\xi}(t)]^T \), we can combine the original system with the noise model as
\[
\dot{\bar{x}}(t) = \bar{A}\bar{x}(t), \quad \bar{x}(0) = \bar{x}_0
\]
\[
\bar{y}(t) = \bar{C}\bar{x}(t)
\]  \hspace{1cm} (13)
with
\[
\bar{A} = \begin{bmatrix} A & E \\ 0 & \bar{E} \end{bmatrix}
\]
\[
\bar{C} = \begin{bmatrix} G \\ \vdots \\ G \end{bmatrix}
\]  \hspace{1cm} (14)
\[
G_L = \begin{bmatrix} G \\ \vdots \\ G \end{bmatrix}_{L \times n}
\]  \hspace{1cm} (15)
where $\mathbf{x} \in \mathbb{R}^d$, $\mathbf{A} \in \mathbb{R}^{d \times d}$, $\mathbf{C} \in \mathbb{R}^{L \times d}$, and the initial state of the augmented state is $\mathbf{x}_0 = [x_0^T \mathbf{0}_T]^T$. The order of the augmented model $\hat{n}$ is $\hat{n} = K + n$, where $K$ and $n$ are the orders of the quantum system model and the colored noise realization, respectively.

Now, we obtain an augmented system (13) of the finite-level quantum system whose output is disturbed by the classical colored noise. A similar model can be found in the design of Kalman filter under classical colored noise realization [31]. Note that both the dynamics of the quantum system and the classical colored noise contribute to the polluted outputs $\tilde{y}(t)$. However, it is difficult to distinguish the unpolluted quantum output $y(t)$ from the noise directly. A possible method is in demand for extracting the quantum information of the original system from the polluted output.

IV. HAMILTONIAN IDENTIFICATION WITH THE TIME-TRACE OBSERVABLES POLLUTED BY CLASSICAL COLORED NOISE

A. Problem Statement

In Section III, we have introduced the dynamics of the coherence vector for the finite-level quantum system and considered the measurement process disturbed by classical colored noise, which is represented by a linear system realization for a given spectrum density $S(o)$. Consequently, we have obtained a parameterized augmented system model for describing the total dynamics of the coherence vector and the internal modes of the noise. We aim to identify the unknown coefficients in $\{a_m \in \mathbb{R}, m = 1, 2, \ldots, M\}$ for a quantum system with the Hamiltonian (1) using the augmented model. Hence, we state our Hamiltonian-identification problem as follows.

Given the structure of the augmented system model (13) with an initial state $\mathbf{x}_0$, our identification problem is to estimate the unknown parameters $\{a_m \in \mathbb{R}, m = 1, 2, \ldots, M\}$ in the model using the disturbed measurements $\tilde{y}(t)$ of the time traces of the observables for the underlying system.

B. Measurement Process

To access the information of the quantum system, we measure the time-trace observables (4). We assume that we have a large number of copies of the system prepared in an identical initial state. We call a set of identical systems that we measure as an ensemble. Thus, we can measure an observable on an ensemble at a time and then obtain the expectation value of the observable. This is because in quantum mechanics, quantum measurement on an observable destroys the state of the measured quantum system. Moreover, since we cannot obtain the measurement results for the same system at different time instants from one ensemble, we need to measure different ensembles for different instants.

Concretely speaking, we sample the observables with an equal interval $\Delta t$. Denoting the measured value of $O_i$ of the $j$th copy at a time instant $k \Delta t$ as $y_i(j)(k)$, the measured value of $O_i$ accompanied by the colored noise $v_i(j)(k)$ can be expressed as $\tilde{y}_i(j)(k) = y_i(j)(k) + v_i(j)(k)$. Here, we have written $\{y_i(k \Delta t)\}$ as $\{y_i(k)\}$ for simplicity. After measuring many copies at different time instants, we can average over the measurement results and obtain (11). A schematic for the measurement process is shown in Fig. 1.

Note that when we consider multiobservable time traces, commutative observables can be measured simultaneously. However, due to the uncertainty principle in quantum mechanics [32], measurements on noncommutative observables should be carried out on different ensembles.

C. Identification With Measurement Data Carrying Classical Colored Noise

With respect to the given sampling interval $\Delta t$, we discretize the augmented system model as

$$\begin{align*}
\mathbf{x}(k + 1) &= \mathbf{A}_d \mathbf{x}(k), \quad \mathbf{x}(0) = \mathbf{x}_0 \\
\mathbf{y}(k) &= \mathbf{C} \mathbf{x}(k), \quad k = 0, 1, \ldots, N
\end{align*}$$

(17)

where $\mathbf{A}_d = e^{\mathbf{A} \Delta t} \in \mathbb{R}^{d \times d}$ and $N$ is the total time step. Hence, the output of (17) can be written as

$$\tilde{y}(k) = \mathbf{C} \mathbf{A}_d^k \mathbf{x}_0.$$  

(18)

It is difficult to solve $\{a_m\}$ from (18), since it is transcendental in $\{a_m\}$ and the system dimension of $\hat{n}$ is unknown. However, these difficulties can be overcome by combining a system realization method [17] and an ERA [33]. Using the ERA, the dimension $\hat{n}$ can be determined. In addition, a system realization can be constructed based on the measurement data such that the unknown parameters can be obtained by solving a set of nonlinear equations arising from the equivalence between the transfer functions of the original system and the realization. It should be mentioned that we calculate the realization using the measurement data disturbed by classical colored noise naturally, which results from both the dynamics of the quantum system and the noise.

The ERA begins with a generalized Hankel matrix [33]

$$H_s(k) = \begin{bmatrix}
\tilde{y}(k) & \tilde{y}(k + t_1) & \cdots & \tilde{y}(k + t_{s-1}) \\
\tilde{y}(k + j_1) & \tilde{y}(k + j_1 + t_1) & \cdots & \tilde{y}(k + j_1 + t_{s-1}) \\
\vdots & \vdots & \ddots & \vdots \\
\tilde{y}(k + j_{r-1}) & \tilde{y}(k + j_{r-1} + t_1) & \cdots & \tilde{y}(k + j_{r-1} + t_{s-1})
\end{bmatrix}$$

(19)

which is directly constructed from the measurement result. The indices $\{j_1, j_2, \ldots, j_{r-1}\}$ and $\{t_1, t_2, \ldots, t_{s-1}\}$ are the integers randomly taken from $\{1, 2, \ldots, r - 1\}$ and $\{1, 2, \ldots, s - 1\}$, respectively, satisfying $k + (r - 1) + (s - 1) \leq N$. 
The dimension of $H_r(k)$ is $rL \times s$. To determine $\hat{n}$ accurately, it is good to choose a sufficient number of measurement results, i.e., two large integers $r$ and $s$ are preferred. Substituting (18) into the Hankel matrix, we have

$$H_r(k) = V_r \bar{A}_d^k W_r$$  \hspace{1cm} (20)

with

$$V_r = \begin{bmatrix} \bar{C} \\ \bar{C} \bar{A}_d^1 \\ \vdots \\ \bar{C} \bar{A}_d^{r-1} \end{bmatrix} \in \mathbb{R}^{rL \times \hat{n}}$$

and

$$W_r = \begin{bmatrix} \bar{x}_0, \bar{A}_d^0 \bar{x}_0, \ldots, \bar{A}_d^{r-1} \bar{x}_0 \end{bmatrix} \in \mathbb{R}^{\hat{n} \times s}.$$  \hspace{1cm} (21)

Since the realization (17) is minimal, the matrix $V_r$ is of full-column rank $\hat{n}$. If the pair $(\bar{A}_d, \bar{x}_0)$ is reachable, $W_r$ can be of full row rank $\hat{n}$. Thus, there exists a matrix $\tilde{H}$ satisfying

$$W_r \tilde{H} V_r = I_{\hat{n}}.$$  \hspace{1cm} (22)

To find such a matrix $\tilde{H}$, we first choose the measurement results at the initial time, i.e., $k = 0$, and then, we have $H_r(0) = V_r W_r$, and rank$(H_r(0)) = \hat{n}$. The singular value decomposition of $H_r(0)$ can be written as

$$H_r(0) = P \begin{bmatrix} D & 0 \\ 0 & 0 \end{bmatrix} Q^T = \begin{bmatrix} P_1 & P_2 \end{bmatrix} \begin{bmatrix} D & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} Q_1^T \\ Q_2^T \end{bmatrix}$$  \hspace{1cm} (23)

where $P \in \mathbb{R}^{rL \times rL}$ and $Q \in \mathbb{R}^{r \times s}$ are the unitary matrices. They are partitioned into $P_1, P_2$ and $Q_1, Q_2$ with respect to the dimension of the diagonal square matrix $D$, which is $\hat{n}$ as the same as the rank of $H_r(0)$. Thus, the $rL \times \hat{n}$ matrix $P_1$ and the $s \times \hat{n}$ matrix $Q_1$ are the corresponding $\hat{n}$ columns of the unitary matrices.

Denoting $P_1 D$ as $P_d$, we have $V_r W_r = H_r(0) = P_d Q_1^T$, where we can solve $Q_1^T$ as

$$Q_1^T = TW_r$$  \hspace{1cm} (24)

with the $\hat{n} \times \hat{n}$ matrix $T = (P_d^T P_d)^{-1} P_d^T V_r$ of full rank.

Right multiplying both sides of (24) by $Q_1$, we have

$$I_{\hat{n}} = TW_r Q_1 = TU,$$  \hspace{1cm} (25)

where $U$ is of full rank. Since $T$ and $U$ are invertible square matrices, we have $UT = I_{\hat{n}}$, that is

$$W_r Q_1 (P_d^T P_d)^{-1} P_d^T V_r = I_{\hat{n}}.$$  \hspace{1cm} (26)

Hence, comparing (25) with (22), we have

$$\tilde{H} = Q_1 (P_d^T P_d)^{-1} P_d^T = Q_1 D^{-1} P_d^T = Q_1 \tilde{P}_d$$  \hspace{1cm} (27)

where the $\hat{n} \times rL$ matrix $\tilde{P}_d$ is of rank $\hat{n}$.

We define $e_1$ as the first column of $I$, and $E_d^r = \{I, 0_1, \ldots, 0_{rL}\}_{r \leq L}$, where the subscript of the identity matrix $I$ indicates its dimension. According to the Hankel matrix (19), we can express $\hat{y}(k)$ as

$$\hat{y}(k) = E_d^r H_r(k) e_1 = E_d^r V_r \bar{A}^k W_r e_1.$$  \hspace{1cm} (28)

Using (22) and (26), we have

$$\hat{y}(k) = E_d^r V_r W_r H_r(k) \bar{A}^k W_r e_1 = E_d^r H_r(0) \bar{P}_d V_r \bar{A}^k W_r Q \bar{P}_d H_r(0) e_1.$$  \hspace{1cm} (29)

Comparing this output-response equation with (18), we can establish a realization

$$\hat{x}(k+1) = \hat{A}_d \hat{x}(k), \quad \hat{y}(k) = \hat{C} \hat{x}(k)$$  \hspace{1cm} (30)

with $\hat{A}_d = D^{-1/2} P_d^T H_r(1) D^{-1/2}$, $\hat{C} = E_d^r P_d D^{1/2}$, and $\hat{x}_0 = D^{1/2} Q_1^T e_1$ [33]. It is clear that the order of this realization is exactly $\hat{n}$, equivalent to the dimension of uncertain model (17). Then, letting $\hat{A} = \log \hat{A}_d / \Delta t$, the pair $(\hat{A}, \hat{C}, \hat{x}_0)$ formulates a continuous-time realization, describing the dynamics of both the quantum system and the colored noise.

Thus far, we have completed the process of developing a numerical time-continuous realization from the measured data and also determined the system dimension $\hat{n}$. Moreover, we have built up an augmented model $(\hat{A}, \hat{C}, \hat{x}_0)$ in (13). The corresponding transfer functions from the initial states to the outputs of the two models should be equal [30], that is

$$\hat{C} (sI_{\hat{n}} - \hat{A})^{-1} \hat{x}_0 = \hat{C} (sI_{\hat{n}} - \hat{A})^{-1} \hat{x}_0.$$  \hspace{1cm} (31)

In fact, the coefficients of $s$ in different orders of $P(s), Q(s)$ are the polynomials of the unknown parameters $(\alpha_m)$, and the corresponding coefficients in the right-hand side are the numbers obtained through experiment. For these nonlinear or high-order equations, professional numerical tools PHCpack [24] can be used to obtain the solutions.

To this end, we have introduced the whole procedure to identify the unknown parameters in the Hamiltonian under measurements disturbed by classical colored noise.

V. EXAMPLE FOR A TWO-QUBIT SYSTEM

In this section, we consider a two-qubit system whose Hamiltonian is written as

$$H = \sum_{n=1}^{2} \alpha_n z^n + \delta_i (\sigma_+ \sigma_- + \sigma_- \sigma_+)^2$$  \hspace{1cm} (32)

with Pauli matrices

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$  \hspace{1cm} (33)

and the corresponding ladder operators

$$\sigma_+ = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \sigma_- = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}.$$  \hspace{1cm} (34)
Here, the superscripts in the Hamiltonian label the qubits. With the aim of identification, we measure the local observable $\sigma_1^\dagger$ of the first qubit, and thus, with the observable-induced accessible set and the Hamiltonian, a dynamical equation of the coherence vector of the two-qubit system can be written as

$$\begin{bmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \dot{x}_3(t) \\ \dot{x}_4(t) \end{bmatrix} = \begin{bmatrix} 0 & -\omega_1 & 0 & \delta_1 \\ \omega_1 & 0 & -\delta_1 & 0 \\ 0 & \delta_1 & 0 & -\omega_2 \\ -\delta_1 & 0 & \omega_2 & 0 \end{bmatrix} \begin{bmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \\ x_4(t) \end{bmatrix} + \begin{bmatrix} 0 \\ \omega_1 \\ 0 \\ 0 \end{bmatrix} x(t) \quad (35)$$

where $x_1(t) = \langle \sigma_1^\dagger(t) \rangle$, $x_2(t) = \langle \sigma_1^\dagger(t) \rangle$, $x_3(t) = \langle \sigma_1^\dagger \sigma_2^\dagger(t) \rangle$, and $x_4(t) = \langle \sigma_1^\dagger \sigma_2^\dagger(t) \rangle$. The initial state is set as $[x_1(0) \ x_2(0) \ x_3(0) \ x_4(0)]^T = [0 \ 0 \ 1 \ 0]^T$. To simulate the real dynamics of the quantum system, we set the real parameters as $\omega_1 = 1.3$ GHz, $\omega_2 = 2.4$ GHz, and $\delta_1 = 4.3$ GHz.

As for the classical colored noise $v(t)$ involved in the measurement process, we assume that its power spectrum density is expressed as

$$S(\omega) = \frac{10^{12} \omega^2 + 4 \times 10^{26}}{\omega^4 - 3.999 \times 10^{13} \omega^2 + 4 \times 10^{26}} \quad (36)$$

Factorizing the spectrum $S(\omega)$, we can obtain a transfer function $\Gamma(s)$ as follows:

$$\Gamma(s) = \frac{10^6 s - 2 \times 10^{13}}{s^2 + 10^5 s + 2 \times 10^{13}} \quad (37)$$

A realization in a controllable canonical form can be found as

$$\dot{\xi}(t) = \begin{bmatrix} 0 & -2 \times 10^{13} & 1 \times 10^{-5} \end{bmatrix} \xi(t) + \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \eta(t) \quad (38)$$

with a 2-D internal mode $\xi(t)$.

We verify the validity of this noise realization (38) by checking its PSD. First, imposing a white noise signal $\eta(t)$ on both the transfer function (37) and the noise realization (38) with an arbitrary initial state, we obtain two colored noise outputs. Then, we estimate the PSDs of the two outputs using Welch’s overlapped segment averaging estimator [34]. The two estimated PSD curves are compared with the theoretical PSD (36), as shown in Fig. 2. It can be seen that the three curves are of a similar tendency. In simulation, we can produce the expectation of colored noises using model (38) with an arbitrary initial state. Note that the disparity therein is due to the imperfect white noise and the error for estimating the PSD.

The parameters to be identified are $\omega_1, \omega_2,$ and $\delta_1$ as well as the matrices and the state in (10) for the classical colored noise. Before we analyze the measurement data, we may not know the order $n$ for the colored noise model. However, with the noise model, we can still write an augmented system model for the parameter identification as

$$\dot{x}(t) = \tilde{A}\tilde{x}(t)$$
$$\dot{y}(t) = \tilde{C}\tilde{x}(t) \quad (39)$$

with

$$\tilde{A} = \begin{bmatrix} 0 & -\omega_1 & 0 & \delta_1 \\ \omega_1 & 0 & -\delta_1 & 0 \\ 0 & \delta_1 & 0 & -\omega_2 \\ -\delta_1 & 0 & \omega_2 & 0 \end{bmatrix}$$
$$\tilde{C} = [1 \ 0 \ 0 \ 0 \ G]$$

$$\tilde{x}(0) = [0, 1, 0, 0, \xi(0)^T]^T$$

where the augmented state vector is $\tilde{x}(t) = [x_1(t), x_2(t), x_3(t), \tilde{\xi}(t)^T]^T$. Note that for the classical colored noise, there exist many realizations that are equivalent and related by a similarity transformation. Therefore, we can just fix the part elements of the matrices in the noise realization to reduce the parameters to be identified. In our simulation, we assume the output vector $G = [1, 1, \ldots, 1]_n$. Moreover, with the sampling time $\Delta t = 0.1 \mu s$ and the final time $T = 12 \mu s$, we sample the output of system (35) as the real expectation values $\langle \sigma_1^\dagger(k) \rangle$. By adding the observable expectation values with the output of the noisy system (38), we obtain measured data $\{\tilde{y}(k)\}$. The measurement and real results of the output $\langle \sigma_1^\dagger \rangle$ are plotted as the black-dotted and yellow-dotted lines, respectively, in Fig. 3, where the polluted measurement result has a discrepancy of the real expectation value. We use the measurement result $\{\tilde{y}(k)\}$ to construct the Hankel matrix $H_r(0),_{L \times s}$, where we let $r = 20, L = 1, s = 100$, and $r_t$ and $t_j$ are randomly chosen from $[1, 2, \ldots, 19]$ and $[1, 2, \ldots, 99]$. Consequently, we can obtain the corresponding singular value decomposition, where we plot the singular values of $H_r(0)$ in logarithmic scale in Fig. 4. We can easily find a huge gap between the dominant singular values and the other quite small ones. Therefore, we can determine the dimension of the augmented system (39) according to the number of the dominant singular values, and thus, the order of the colored noise realization can be determined. Hence, we have the dimension of the augmented system $\hat{n} = 6$ and the order of the noise realization $n = 2$.

Following the procedure of the ERA in Section IV, a realization $\tilde{A}, \tilde{C}, \tilde{x}(0)$ with the dimension $\hat{n}$ can be obtained and its transfer function is identical to that of (39), that is

$$\tilde{C}(sI - \tilde{A})^{-1}\tilde{x}_0 = \tilde{C}(sI - \hat{A})^{-1}\tilde{x}_0 \quad (40)$$
whose both sides are polynomials in $s$. Specifically, the left-hand side of (41) contains the parameters to be identified, while the right-hand side of (41) is numerically constructed by the measurement data. Equaling the coefficients of $s$ in the same order on the both sides, we can collect a polynomial equation set as

$$-0.3 = \zeta_{01} + \zeta_{02}$$

$$-0.48 = \omega_{1} + e_{11} \xi_{02} - e_{12} \xi_{02} - e_{12} \xi_{01} + e_{22} \xi_{01}$$

$$-13.459 = e_{11} \omega_{1} + e_{22} \omega_{2} + 2\delta_{1} \zeta_{01} + 2\delta_{1} \zeta_{02}$$

$$+\omega_{1} \xi_{01} + 2\delta_{1} \zeta_{02} + \omega_{2} \xi_{01} + \omega_{2} \xi_{02}$$

$$-89.9734 = \omega_{1} \omega_{2} - \delta_{2} \omega_{2} + e_{11} \omega_{1} \xi_{02} + e_{11} \omega_{2} \xi_{02}$$

$$-e_{12} \omega_{1} \xi_{02} - e_{12} \omega_{2} \xi_{02} - e_{12} \omega_{1} \xi_{01}$$

$$+e_{22} \omega_{1} \xi_{01} + e_{22} \omega_{2} \xi_{01} + e_{11} e_{22} \omega_{1}$$

$$-e_{12} e_{21} \omega_{1} + 2e_{11} \omega_{1} \xi_{02} - 2e_{12} \omega_{2} \xi_{02}$$

$$-2e_{21} \omega_{1} \xi_{01} + 2e_{22} \omega_{1} \xi_{01}$$

$$67.182 = e_{11} \omega_{1} \omega_{2} - \delta_{2} \omega_{2} - e_{12} \omega_{1} \xi_{02} - e_{12} \omega_{2} \xi_{02}$$

$$-e_{12} \omega_{1} \xi_{02} - e_{12} \omega_{2} \xi_{02} - e_{12} \omega_{1} \xi_{01}$$

$$+e_{22} \omega_{1} \xi_{01} + 2e_{22} \omega_{1} \xi_{01} + 2e_{22} \omega_{2} \xi_{01}$$

$$64.43 = 2\delta_{2} + \omega_{2} + 2 \delta_{2} \omega_{1} \xi_{02} + 2 \delta_{2} \omega_{1} \xi_{02}$$

$$-4.443 = 2e_{11} \omega_{2} + 2e_{22} \omega_{1} - e_{11} \omega_{1}^{2} + e_{11} \omega_{2}^{2}$$

$$+e_{22} \omega_{1} + e_{22} \omega_{2}$$

$$1124.837 = \delta_{1} + \omega_{1}^{2} + 2 \delta_{2} \omega_{1} \omega_{2} + 2 e_{11} e_{22} \delta_{1}^{2}$$

$$-2e_{12} e_{21} \delta_{1} + e_{11} e_{22} \omega_{1} - e_{12} e_{21} \omega_{1}$$

$$+e_{11} e_{22} \omega_{2} - e_{12} e_{21} \omega_{2}$$

where $e_{ij}$ is the element of $E$ in the $i$th row and $j$th column and $\xi_{0}$ is the $i$th element of $\xi_{0}$. A set of solutions can be obtained using the PHCpack [24].

In Table I, we compare our identification result with that obtained by using Zhang and Sarovar’s method (ZS method) [17], which is not specially designed for the colored noise case. Our method can precisely identify the real values of the parameters in the Hamiltonian, while the results obtained by the method in [17] are different from the real values.

Moreover, in our method, the estimates for the noise realization are $e_{11} = 10^{6}(-50.025 + 410.92i)$, $e_{12} = 10^{6}(-49.97 + 415.41i)$, $e_{21} = 10^{6}(49.94 - 406.43i)$, $e_{22} = 10^{6}(49.925 - 410.92i)$, $\zeta_{01} = 10^{6}(-4053.8 + 3692.7i)$, $\zeta_{02} = 10^{6}(4053.5 - 410.92i)$. After substituting the solution of our method back into the augmented system model (39) and the solution of the ZS method back into the quantum system model (35), the outputs produced by the two identified systems are compared with the real measurements in Fig. 5. It can be seen that our identification results coincide with the parameters of the real system, which shows that our method is effective for Hamiltonian identification in the case of measurement results polluted by the classical colored measurement noise.

| $\omega_{1} (\text{GHz})$ | $\omega_{2} (\text{GHz})$ | $\delta_{1} (\text{GHz})$ |
|------------------------|------------------------|------------------------|
| real values            | 1.3                    | 2.4                    | 4.3                    |
| ZS method in [17]      | 0.8746                 | 2.0601                 | 4.1211                 |
| our method             | 1.3                    | 2.4                    | 4.3                    |

VI. CONCLUSION

In this brief, we have presented a method for quantum Hamiltonian identification under classical colored measurement noise and have shown its performance in the example of two qubits. In our method, an augmented system model has been proposed for the whole system based on which the ERA and the transfer function technique can be applied to identify accurately the unknown parameters in closed quantum systems. In principle, our identification procedure is applicable to various colored noises in the measurement process and does not require any prior information (e.g., PSD) about noise.
Future research will focus on extending our method to Hamiltonian identification under quantum colored noises [35], [36].

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