

# Positivity-preserving non-Markovian master equation for open quantum system dynamics: Stochastic Schrödinger equation approach

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Positivity preservation is naturally guaranteed in exact non-Markovian master equations for open quantum system dynamics. However, in many approximated non-Markovian master equations, the positivity of the reduced density matrix is not guaranteed. In this paper we provide a general class of time-local, perturbative, and positivity-preserving non-Markovian master equations generated from stochastic Schrödinger equations, particularly quantum-state-diffusion equations. Our method has an expanded range of applicability for accommodating a variety of non-Markovian environments. We show the positivity-preserving master equation for a three-level system coupled to a dissipative bosonic environment as a particular example to exemplify our general approach. We illustrate the numerical simulations with an analysis explaining why the previous approximated non-Markovian master equations cannot guarantee positivity. Our work provides a consistent master equation for studying the non-Markovian dynamics in ultrafast quantum processes and strong-coupling systems.

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## I. INTRODUCTION

A density matrix of a quantum system is positive semidefinite, as its eigenvalues naturally are the probabilities of the associated eigenstates. For a closed system, the positivity of the density matrix is always preserved in the dynamical equations, e.g., the von Neumann equation. However, no quantum systems can be isolated from the surrounding environment. In the context of the theory of open quantum systems (OQSs), the state of the central quantum system is characterized by the reduced density matrix whose time evolution equation is the master equation (ME) instead [1,2]. Generally, it is extremely difficult to obtain the exact ME due to the infinite number of degrees of freedom of the environment. Several perturbation strategies have been developed in the past decades to obtain approximated MEs [3,4]. For instance, Lindblad-type [5] and Redfield-type [6] MEs based on the Born-Markov approximation effectively describe the Markovian dynamics of many physical processes [7–9]. However, among the two typical Markovian MEs, the former can preserve positivity, while the latter cannot [3,10–15]. It is a dilemma to preserve the positivity of MEs with perturbative methods beyond the original Lindblad (Davies) MEs.

Moreover, the theory of non-Markovian OQSs recently attracted great interest because Markovian approximations are not valid in certain ultrafast processes [16–21]. A comprised

solution is to use various *weaker* approximations to maintain certain non-Markovian features beyond the Lindblad-type ME. Usually, such changes would lead to the new ME, which cannot guarantee positivity preservation. Another feasible solution is the hierarchical equations of motion (HEOM) technique [22,23], which is a numerically exact approach to studying the evolution of a density matrix without the typical assumptions that conventional Lindblad- or Redfield-type MEs use. HEOM technique is applicable in computing expectation values of quantum observables at both zero and finite temperature. But HEOM is not a conventional ME, which is supposed to be a homogeneous equation of the reduced density matrix only. In studying the detailed balance breaking in open quantum systems [24], the numerically generated density matrix, in chronological order,  $\hat{\rho}_r(t)$  is often insufficient to compute the probability flow and analyze the flow's detailed components, while a conventional ME can interpret transition processes between arbitrary two states explicitly. As the result, it is crucial and necessary to obtain a self-consistent ME. And the consequent challenge is twofold: (1) obtaining exact non-Markovian MEs is extremely difficult because of the lack of mathematical tools [25–39] and (2) positivity preservation is not guaranteed in perturbative MEs when certain approximations are applied [40]. The purpose of this paper is to solve this long-standing problem.

We demonstrate our solution in Fig. 1. Due to the failure to guarantee positivity, the path of obtaining the consistent approximated ME from the exact ME is blocked. However, in contrast to the dynamics of mixed states of OQSs, the positivity preservation is always guaranteed in the pure state

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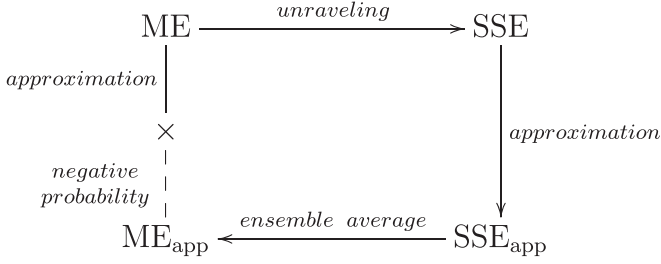


FIG. 1. Mind map of obtaining positivity-preserving MEs.

dynamics, even when approximations are applied ( $|\psi\rangle\langle\psi|$  is always positive-semidefinite; here the state  $|\psi\rangle$  does not have to be normalized). Additionally, the stochastic Schrödinger equation (SSE) approach has provided a rigorous method to obtain the associated ME by averaging an infinite number of stochastic pure-state trajectories in the Markov limit [41–47]. Thus, we propose a strategy to generate positivity-preserving non-Markovian MEs: (1) start with a formal exact non-Markovian SSE; (2) apply truncation and obtain the approximated SSE; and (3) recover the approximated ME from the approximated SSE rigorously. In the end we ensure that the generated approximated ME using the strategy can guarantee positivity as expected.

If we restrict the measurement on the environment to Bargmann coherent states, the evolution of the stochastic pure state can be characterized by the quantum-state-diffusion (QSD) equation [48–54], a time-evolution equation of a stochastic quantum trajectory  $|\psi_z\rangle \equiv \langle z|\Psi_{\text{tot}}\rangle$ , where  $\|z\rangle$  is the Bargmann coherent state of the environment and  $z$  represents a large number of complex Gaussian random variables. Consequently, the reduced density matrix can be recovered using  $\hat{\rho}_r = \text{Tr}_E[|\Psi_{\text{tot}}\rangle\langle\Psi_{\text{tot}}|]$ , which is equivalent to the ensemble average over all stochastic quantum trajectories  $\hat{\rho}_r = \mathcal{M}(|\psi_z\rangle\langle\psi_z|)$ . As shown in Fig. 1, the exact ME and SSE are equivalent. When some approximations have to be employed, the approximated SSE ( $\text{SSE}_{\text{app}}$ ) can numerically generate the positivity-preserving reduced density matrix  $\hat{\rho}_r(t)$  at any time. But the approximated ME, if derived in the same manner, is not positivity-preserving guaranteed. In this paper we develop a method to generate an approximated ME ( $\text{ME}_{\text{app}}$ ), which is positivity-preserving and has the same reduced density matrix as the ones numerically recovered from the corresponding approximated SSE at any time.

This paper is organized as follows. In Sec. II we briefly review the QSD approach and introduce our method to derive the positivity-preserving MEs. In Sec. III we study a dissipative three-level system and demonstrate how to derive the positivity-preserving ME explicitly. We close with a conclusion in Sec. IV.

## II. GENERAL METHODS

The theory of OQSs studies the dynamics of a quantum system coupled with an external quantum system or an environment. Generally the system's dynamics are significantly influenced by the environment, e.g., the quantum decoherence process and the quantum entanglement regeneration process. The total Hamiltonian of the combined system and

environment is usually written as

$$\hat{H}_{\text{tot}} = \hat{H}_S + \hat{H}_{\text{int}} + \hat{H}_E. \quad (1)$$

Here the environment Hamiltonian  $\hat{H}_E$  contains an infinite number of bosonic modes. The interaction Hamiltonian of the coupling between system and environment can be assumed and formally written as

$$\hat{H}_E = \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k,$$

$$\hat{H}_{\text{int}} = \hat{L} \sum_k g_k \hat{b}_k^\dagger + \text{H.c.},$$

where  $\hat{L}$  is the system's operator linearly coupled to the environment. We assume that the environment is at zero temperature and the initial state of the combined system and environment is a product state,  $|\Psi_{\text{tot}}(t=0)\rangle = |\psi_S(t=0)\rangle \otimes |0_E\rangle$ . As mentioned above, having restricted the measurement on the environment to Bargmann coherent states will lead to the quantum trajectory in the form of  $|\psi_z\rangle \equiv \langle z|\Psi_{\text{tot}}\rangle$ , where  $\|z\rangle \equiv \otimes_k \|z_k\rangle$  is the Bargmann coherent state of the entire environment, satisfying  $\hat{b}_k \|z\rangle = z_k \|z\rangle$ . The evolution of  $|\psi_z\rangle$  is governed by the QSD equation.

### A. Quantum-state-diffusion approach

In the environmental interaction picture, the interaction Hamiltonian reads

$$\hat{H}_{\text{int}}^I(t) = \hat{L} \sum_k g_k \hat{b}_k^\dagger e^{i\omega_k t} + \hat{L}^\dagger \sum_k g_k^* \hat{b}_k e^{-i\omega_k t}. \quad (2)$$

Using the identity resolution of Bargmann coherent states

$$\hat{1}_E = \int \frac{d^2z}{\pi} e^{-|z|^2} \|z\rangle\langle z|, \quad (3)$$

the reduced density operator of the system takes the form of  $\hat{\rho}_r(t) = \int d^2z \frac{e^{-|z|^2}}{\pi} \langle z|\Psi_{\text{tot}}(t)\rangle\langle\Psi_{\text{tot}}(t)|z\rangle = \int d^2z \frac{e^{-|z|^2}}{\pi} \langle z|\Psi_{\text{tot}}(t)\rangle\langle\Psi_{\text{tot}}(t)|z\rangle$ . When the term  $\frac{e^{-|z|^2}}{\pi} \langle z|\Psi_{\text{tot}}(t)\rangle\langle\Psi_{\text{tot}}(t)|z\rangle$  is considered as the outcome of a single shot measurement of the environment, the environmental variables  $\{z_k\}$  are interpreted as random numbers, and  $\int d^2z \frac{e^{-|z|^2}}{\pi} (\cdot)$  is the ensemble average. Consequently, the Schrödinger equation, regarding the evolution of the pure state of the composite system  $|\Psi_{\text{tot}}\rangle$ , can be rewritten in the Bargmann space representation (setting  $\hbar = 1$ ),

$$\begin{aligned} \partial_t \langle z|\Psi_{\text{tot}}\rangle &= -i \langle z|\left[\hat{H}_S + \hat{H}_{\text{int}}^I(t)\right]|\Psi_{\text{tot}}\rangle \\ &= -i \left( \hat{H}_S + \hat{L} \sum_k g_k z_k^* e^{i\omega_k t} \right) \langle z|\Psi_{\text{tot}}\rangle \\ &\quad - i \hat{L}^\dagger \sum_k g_k^* e^{-i\omega_k t} \frac{\partial}{\partial z_k^*} \langle z|\Psi_{\text{tot}}\rangle. \end{aligned} \quad (4)$$

Here we define a complex Gaussian process  $z_t^* \equiv -i \sum_k g_k z_k^* e^{i\omega_k t}$ , which satisfies the following relations:  $\mathcal{M}(z_t) = \mathcal{M}(z_t z_s) = 0$ , and  $\alpha(t, s) \equiv \mathcal{M}(z_t z_s^*) = \sum_k |g_k|^2 e^{-i\omega_k(t-s)}$ , where the ensemble average

$\mathcal{M}(\cdot) \equiv \int d^2z \frac{e^{-|z|^2}}{\pi}(\cdot)$ , and  $\alpha(t, s)$  is the correlation function of the complex Gaussian process  $z_t^*$ . Then, using the chain rule  $\frac{\partial(\cdot)}{\partial z_k^*} = \int_0^t ds \frac{\partial z_s^*}{\partial z_k^*} \frac{\delta(\cdot)}{\delta z_s^*}$ , Eq. (4) can lead to a formal linear non-Markovian QSD equation [55]:

$$\partial_t |\psi_z\rangle = \left[ -i\hat{H}_S + z_t^* \hat{L} - \hat{L}^\dagger \int_0^t ds \alpha(t, s) \delta_{z_s^*} \right] |\psi_z\rangle, \quad (5)$$

where  $\delta_{z_s^*}$  denotes the functional derivative with respect to the stochastic process at the time “s.” By taking the statistical mean over all trajectories, the reduced density matrix of the system can be recovered:

$$\hat{\rho}_r = \mathcal{M}(|\psi_z\rangle\langle\psi_z|). \quad (6)$$

The functional derivative term in Eq. (5) can be formally written using a to-be-determined operator  $\hat{O}$ , defined as

$$\hat{O}(t, s) |\psi_z\rangle \equiv \delta_{z_s^*} |\psi_z\rangle, \quad (7)$$

which can be solved through an operator evolution equation:

$$\partial_t \hat{O}(t, s) = -i[\hat{H}_{\text{eff}}, \hat{O}(t, s)] - i\delta_{z_s^*} \hat{H}_{\text{eff}}, \quad (8)$$

due to the consistency condition  $\partial_t \delta_{z_s^*} |\psi_z\rangle = \delta_{z_s^*} \partial_t |\psi_z\rangle$  [55]. Here  $\hat{H}_{\text{eff}}$  is the effective Hamiltonian in Eq. (5),

$$\hat{H}_{\text{eff}} \equiv \hat{H}_S + iz_t^* \hat{L} - i\hat{L}^\dagger \bar{O}, \quad (9)$$

and  $\bar{O}(t) \equiv \int_0^t ds \alpha(t, s) \hat{O}(t, s)$ . Therefore, the formal linear QSD equation reads

$$\partial_t |\psi_z\rangle = [-i\hat{H}_S + z_t^* \hat{L} - \hat{L}^\dagger \bar{O}(t)] |\psi_z\rangle. \quad (10)$$

Generally, the structure of the exact O-operator is complicated. Only a few models can be solved with the exact O-operator. A compromised solution to this difficulty is to replace the exact O-operator with an approximated one. One can drop certain terms of the O-operator to simplify the calculation, called a truncation operation. How to truncate the O-operator depends on the type of interaction and the size of the system. Without the loss of generality, the O-operator can be written as a sum of all component operators [56]:

$$\hat{O}(t, s, z^*) = \sum_n \hat{O}_n(t, s, z^*). \quad (11)$$

Note that the explicit form of  $\hat{O}_n(t, s, z^*)$  is not unique and depends on the method for sorting the O-operator. For instance, if sorting the O-operator by the noise order, then  $\hat{O}_n(t, s, z^*)$  represents the operator component with  $n$ th order of noise. And the approximated O-operator after the truncation is defined as

$$\hat{O}^N(t, s, z^*) \equiv \sum_{n=0}^N \hat{O}_n(t, s, z^*). \quad (12)$$

Consequently, the approximated QSD equation after the truncation reads

$$\partial_t |\psi_z^N\rangle = \left[ -i\hat{H}_S + z_t^* \hat{L} - \hat{L}^\dagger \int_0^t ds \alpha(t, s) \hat{O}^N \right] |\psi_z^N\rangle, \quad (13)$$

where the trajectory  $|\psi_z^N\rangle$  is the associated approximated trajectory.

One of the advantages of the non-Markovian QSD approach is that any reduced density operator recovered from

quantum trajectories  $\hat{\rho}_r = \mathcal{M}(|\psi_z\rangle\langle\psi_z|)$  is always positivity preserved, even if quantum trajectories are numerically generated by the approximated QSD equation (13),  $\hat{\rho}_r^N = \mathcal{M}(|\psi_z^N\rangle\langle\psi_z^N|)$ . For the single trajectory, we know that  $|\psi_z^N\rangle\langle\psi_z^N|$  must be positive semidefinite. The ensemble average  $\mathcal{M}(|\psi_z^N\rangle\langle\psi_z^N|)$  can be considered as a convex combination of  $|\psi_z^N\rangle\langle\psi_z^N|$ , therefore,  $\mathcal{M}(|\psi_z^N\rangle\langle\psi_z^N|)$  is also positive semidefinite. Principally, this is how we derive the positivity-preserving ME from the approximated QSD equation.

## B. Positivity-preserving ME

For a given exact QSD equation, the associated ME reads

$$\begin{aligned} \partial_t \hat{\rho}_r &= \mathcal{M} \left( \frac{\partial |\psi_z\rangle}{\partial t} \langle\psi_z| + |\psi_z\rangle \frac{\partial \langle\psi_z|}{\partial t} \right) \\ &= \mathcal{M}(-i\hat{H}_{\text{eff}} |\psi_z\rangle\langle\psi_z| + i|\psi_z\rangle\langle\psi_z| \hat{H}_{\text{eff}}^\dagger) \\ &= -i[\hat{H}_S, \hat{\rho}_r] + \hat{L} \mathcal{M}(z_t^* \hat{P}) + \mathcal{M}(z_t \hat{P}) \hat{L}^\dagger \\ &\quad - \hat{L}^\dagger \mathcal{M}(\bar{O} \hat{P}) - \mathcal{M}(\hat{P} \bar{O}^\dagger) \hat{L}, \end{aligned} \quad (14)$$

where  $\hat{P}$  denotes the stochastic operator  $\hat{P} \equiv |\psi_z\rangle\langle\psi_z|$ . Using the conclusions in Refs. [52,57,58], (see Appendix A), the two terms,  $\mathcal{M}(z_t^* \hat{P})$  and  $\mathcal{M}(z_t \hat{P})$ , in the above equation, can be estimated,

$$\mathcal{M}(z_t^* \hat{P}) = \int_0^t ds \mathcal{M}(z_t^* z_s) \mathcal{M}(\delta_{z_s} \hat{P}). \quad (15)$$

Using the definition of the  $\hat{O}$  operator in Eq. (7), we have  $\mathcal{M}(z_t^* \hat{P}) = \mathcal{M}(\hat{P} \bar{O}^\dagger)$  [52], then the formal ME is obtained,

$$\partial_t \hat{\rho}_r = -i[\hat{H}_S, \hat{\rho}_r] + [\hat{L}, \mathcal{M}(\hat{P} \bar{O}^\dagger)] - [\hat{L}^\dagger, \mathcal{M}(\bar{O} \hat{P})]. \quad (16)$$

The above-derived ME is positivity-preserving since the reduced density matrix  $\hat{\rho}_r$  is equivalent to the exact stochastic quantum trajectory governed by the QSD equation (5).

Next, we will demonstrate why the ME cannot guarantee positivity if all the four exact O-operators in Eq. (16) are replaced by the approximated one  $\hat{O}^N$ . Following the similar method of obtaining Eq. (16), the approximated ME for the perturbative reduced density matrix  $\hat{\rho}_r'$  reads

$$\partial_t \hat{\rho}_r' = -i[\hat{H}_S, \hat{\rho}_r'] + [\hat{L}, \mathcal{M}(\hat{P}'(\bar{O}^N)^\dagger)] - [\hat{L}^\dagger, \mathcal{M}(\bar{O}^N \hat{P}')]. \quad (17)$$

However, it is worth pointing out that the reduced density matrix  $\hat{\rho}_r'$  can violate positivity because the approximated ME can not be unraveled by the QSD equation (13). To clarify the difference between Eq. (17) and the approximated ME which is equivalent to the approximated QSD equation (13), we recover the ME starting from the identity  $\hat{\rho}_r^N = \mathcal{M}(|\psi_z^N\rangle\langle\psi_z^N|)$  and the QSD equation (13). The approximated ME reads

$$\begin{aligned} \partial_t \hat{\rho}_r^N &= -i[\hat{H}_S, \hat{\rho}_r^N] + \hat{L} \mathcal{M}(z_t^* \hat{P}^N) + \mathcal{M}(z_t \hat{P}^N) \hat{L}^\dagger \\ &\quad - \hat{L}^\dagger \mathcal{M}(\bar{O}^N \hat{P}^N) - \mathcal{M}(\hat{P}^N \bar{O}^N) \hat{L}, \end{aligned} \quad (18)$$

where  $\hat{P}^N \equiv |\psi_z^N\rangle\langle\psi_z^N|$ . After applying Eq. (15) to simplify the term of  $\mathcal{M}(z_t^* \hat{P}^N)$ , it is easy to verify that in the general case

$$\mathcal{M}(z_t^* \hat{P}^N) = \int_0^t ds \alpha^*(t, s) \mathcal{M}(\delta_{z_s} \hat{P}^N) \neq \mathcal{M}(\hat{P}^N \bar{O}^N)^\dagger.$$

This is why the above-mentioned approximated ME (17) cannot be unraveled by the QSD equation (13). To solve this problem, we need to know the exact value of  $\delta_{z_s} \hat{P}^N$ , therefore a new O-operators has to be introduced,

$$\hat{O}_d(t, s, z^*) |\psi_z^N\rangle \equiv \delta_{z_s^*} |\psi_z^N\rangle, \quad (19)$$

where the new operator  $\hat{O}_d(t, s, z^*)$  is determined by the consistency condition  $\partial_t \delta_{z_s^*} |\psi_z^N\rangle = \delta_{z_s^*} \partial_t |\psi_z^N\rangle$ . Substituting Eqs. (13) and (19) into the consistency condition, the evolution equation for the operator  $\hat{O}_d$  reads

$$\begin{aligned} \partial_t \hat{O}_d(t, s, z^*) &= [-i\hat{H}_S + z_r^* \hat{L} - \hat{L}^\dagger \bar{O}^N, \hat{O}_d(t, s, z^*)] \\ &\quad - \hat{L}^\dagger \delta_{z_s^*} \bar{O}^N, \end{aligned} \quad (20)$$

together with the initial condition,

$$\hat{O}_d(t = s, s, z^*) = \hat{L}. \quad (21)$$

The subtle difference between  $\hat{O}^N$  and  $\hat{O}_d$  is just the reason of positivity violation in the ME (17). Consequently, the result of applying Eq. (15) is revised to

$$\begin{aligned} \mathcal{M}(z_r^* \hat{P}^N) &= \int_0^t ds \alpha^*(t, s) \mathcal{M}(\delta_{z_s} \hat{P}^N) \\ &= \mathcal{M}(\hat{P}^N \bar{O}_d^\dagger), \end{aligned} \quad (22)$$

where  $\bar{O}_d^\dagger(t, z^*) \equiv \int_0^t ds \alpha^*(t, s) \hat{O}_d^\dagger(t, s, z^*)$ . By substituting Eq. (22) into Eq. (18), we obtain the formal positivity-preserving approximated ME,

$$\begin{aligned} \partial_t \hat{\rho}_r^N &= -i[\hat{H}_S, \hat{\rho}_r^N] + \hat{L} \mathcal{M}(\hat{P}^N \bar{O}_d^\dagger) - \mathcal{M}(\hat{P}^N \bar{O}^N) \hat{L} \\ &\quad - \hat{L}^\dagger \mathcal{M}(\bar{O}^N \hat{P}^N) + \mathcal{M}(\bar{O}_d \hat{P}^N) \hat{L}^\dagger. \end{aligned} \quad (23)$$

### III. MODELS AND RESULTS

In this section we consider a ladder-type three-level system coupled with a dissipative zero-temperature reservoir and use it to demonstrate how to obtain the positivity-preserving approximated ME. (Among models with exact O-operators, three-level systems are simple yet still capable of distinguishing between  $\hat{O}_d$  and a traditionally truncated  $\hat{O}$ .) The total Hamiltonian reads

$$\hat{H}_{\text{tot}} = \omega \hat{J}_z + \sum_k g_k (\hat{J}_+ \hat{b}_k + \hat{b}_k^\dagger \hat{J}_-) + \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k, \quad (24)$$

where  $g_k$  is the real coupling strength of the  $k$ th mode.  $\hat{J}_+$  ( $\hat{J}_-$ ) is the raising (lowering) operator of the three-level system, satisfying the commutation relation  $\hat{J}_z = \frac{1}{2}[\hat{J}_+, \hat{J}_-]$ . The three operators have the matrix form

$$\begin{aligned} \hat{J}_z &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad \hat{J}_+ = \sqrt{2} \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}, \\ \hat{J}_- &= \sqrt{2} \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}. \end{aligned}$$

#### A. ME for the three-level system

In Refs. [31,59] it has been proved that the exact O-operator of the dissipative three-level system contains noise

up to the first order. We use a noise-free operator  $\hat{O}^{(0)}$  to replace the exact  $\hat{O}$  in the QSD equation:

$$\partial_t |\psi_z^{(0)}\rangle = (-i\hat{H}_S + z_r^* \hat{L} - \hat{L}^\dagger \bar{O}^{(0)}) |\psi_z^{(0)}\rangle, \quad (25)$$

where  $\bar{O}^{(0)} \equiv \int_0^t ds \alpha(t, s) \hat{O}^{(0)}(t, s)$ , and the Lindblad operator  $\hat{L} = \hat{J}_-$ . By substituting the effective Hamiltonian in Eq. (25) into Eq. (8), the evolution equation of  $\hat{O}^{(0)}$  reads

$$\partial_t \hat{O}^{(0)}(t, s) = [-i\hat{H}_S - \hat{L}^\dagger \bar{O}^{(0)}, \hat{O}^{(0)}(t, s)], \quad (26)$$

with its initial condition

$$\hat{O}^{(0)}(t = s, s) = \hat{L}. \quad (27)$$

Practically, the ansatz of the operator  $\hat{O}^{(0)}$  has the form of

$$\hat{O}^{(0)}(t, s) \equiv f_1(t, s) \hat{J}_- + g_1(t, s) \hat{J}_z \hat{J}_-, \quad (28)$$

where  $f_1(t, s)$  and  $g_1(t, s)$  are two to-be-determined evolution coefficients [56,59]. By substituting the ansatz (28) into Eq. (26), the coefficients  $f_1$  and  $g_1$  can be determined by the following differential equations:

$$\begin{aligned} \partial_t f_1 &= (i\omega + 2G_1) f_1, \\ \partial_t g_1 &= (-2F_1 + 4G_1) f_1 + (i\omega + 2F_1 - 2G_1) g_1, \end{aligned} \quad (29)$$

associated with the initial conditions,

$$f_1(t = s, s) = 1, \quad g_1(t = s, s) = 0, \quad (30)$$

where  $F_1(t) \equiv \int_0^t ds \alpha(t, s) f_1(t, s)$ , and  $G_1(t) \equiv \int_0^t ds \alpha(t, s) g_1(t, s)$ . Subsequently, the time-evolution equation of the operator  $\hat{O}_d(t, s, z^*)$  reads

$$\partial_t \hat{O}_d = [-i\hat{H}_S + z_r^* \hat{L} - \hat{L}^\dagger \bar{O}^{(0)}, \hat{O}_d]. \quad (31)$$

Note that the last functional derivative term in Eq. (20) has been eliminated because  $\hat{O}^{(0)}$  is noise-free. Similarly, the ansatz of the operator  $\hat{O}_d$  reads

$$\begin{aligned} \hat{O}_d(t, s, z^*) &\equiv f_2(t, s) \hat{J}_- + g_2(t, s) \hat{J}_z \hat{J}_- \\ &\quad + \int_0^t ds' p_2(t, s, s') z_s^* \hat{J}_-^2. \end{aligned} \quad (32)$$

By substituting the ansatz (32) into Eq. (31), the new set of coefficients,  $f_2(t, s)$ ,  $g_2(t, s)$  and  $p_2(t, s, s')$ , are determined by

$$\begin{aligned} \partial_t f_2 &= (i\omega + 2G_1) f_2, \\ \partial_t g_2 &= (-2F_1 + 4G_1) f_2 + (i\omega + 2F_1 - 2G_1) g_2, \\ \partial_t p_2 &= (2i\omega + 2F_1) p_2, \end{aligned} \quad (33)$$

with the initial conditions

$$\begin{aligned} f_2(t = s, s) &= 1, \\ g_2(t = s, s) &= 0, \\ p_2(t = s', s, s') &= g_2(s', s). \end{aligned}$$

By comparing Eq. (29) and Eq. (33), it is clear that  $f_1 = f_2$  and  $g_1 = g_2$ , since they have the same evolution equations and the same initial conditions. As a result,  $f_1$  and  $g_1$ , in the rest of the paper, will be replaced by  $f_2$  and  $g_2$ , respectively.



After obtaining operators  $\hat{O}_d$  and  $\hat{O}^{(0)}$ , the formal ME (23) for the dissipative three-level model reads

$$\partial_t \hat{\rho}_r^{(0)} = -i[\hat{H}_S, \hat{\rho}_r^{(0)}] + \left\{ [(F_2 \hat{J}_- + G_2 \hat{J}_z \hat{J}_-) \hat{\rho}_r^{(0)}, \hat{J}_+] + \hat{J}_-^2 \int_0^t ds P_2(t, s) \mathcal{M}(z_s^* \hat{P}^{(0)}) \hat{J}_+ \right\} + \text{H.c.}, \quad (34)$$

where  $F_2(t)$ ,  $G_2(t)$ , and  $P_2(t, s')$  are defined as

$$\begin{aligned} F_2(t) &\equiv \int_0^t ds \alpha(t, s) f_2(t, s), \\ G_2(t) &\equiv \int_0^t ds \alpha(t, s) g_2(t, s), \\ P_2(t, s') &\equiv \int_0^t ds \alpha(t, s) p_2(t, s, s'). \end{aligned}$$

Applying Eqs. (15), (19), and the termination condition in Ref. [27], the term  $\hat{J}_-^2 \int_0^t ds P_2(t, s) \mathcal{M}(z_s^* \hat{P}^{(0)}) \hat{J}_+$  in the above ME can be further simplified to

$$\begin{aligned} \hat{J}_-^2 \mathcal{M}(z_s^* \hat{P}^{(0)}) \hat{J}_+ &= \int_0^t ds' \alpha^*(s, s') \hat{J}_-^2 \mathcal{M}(\hat{P}^{(0)}) \hat{O}_d^\dagger(t, s', z) \hat{J}_+ \\ &= \int_0^t ds' \alpha^*(s, s') f_2^*(t, s') \hat{J}_-^2 \hat{\rho}_r^{(0)} \hat{J}_+ \hat{J}_+. \end{aligned} \quad (35)$$

Here we observed that when substituting  $\hat{O}_d$  in Eq. (32) into  $\hat{O}_d^\dagger \hat{J}_+$ , certain terms are terminated:  $(g_2^*(t, s') \hat{J}_+ \hat{J}_z) \hat{J}_+ = 0$  and  $(\int_0^t ds'' p_2^*(t, s', s'') z_s'' \hat{J}_+^2) \hat{J}_+ = 0$ . Subsequently the approximated positivity-preserving ME reads

$$\begin{aligned} \partial_t \hat{\rho}_r^{(0)} &= -i[\hat{H}_S, \hat{\rho}_r^{(0)}] + \left\{ [(F_2 \hat{J}_- + G_2 \hat{J}_z \hat{J}_-) \hat{\rho}_r^{(0)}, \hat{J}_+] \right. \\ &\quad \left. + P_{f^*} \hat{J}_-^2 \hat{\rho}_r^{(0)} \hat{J}_+^2 \right\} + \text{H.c.}, \end{aligned} \quad (36)$$

where the coefficient  $P_{f^*}(t) \equiv \int_0^t \int_0^t ds ds' P_2(t, s) \alpha^*(s, s') f_2^*(t, s')$ . Note that  $\alpha(t, s)$  is the time correlation function, corresponding to a variety of spectra, white or colored. For simplicity, we assume the environment is described by an Ornstein-Uhlenbeck process. So its correlation function is  $\alpha(t, s) = a\gamma e^{-\gamma|t-s|} e^{-i\Omega(t-s)}$ , where  $1/\gamma$  is the scale of memory time and  $\Omega$  is the central frequency of the environment. As a result, the coefficients' evolution equations can be simplified from integrodifferential equations to differential equations that

$$\begin{aligned} \partial_t F_2 &= a\gamma + (i\omega - \gamma - i\Omega + 2G_2)F_2, \\ \partial_t G_2 &= -2F_2^2 + (i\omega - \gamma - i\Omega + 6F_2 - 2G_2)G_2, \\ \partial_t \tilde{P}_2 &= a\gamma G_2 + (2i\omega - 2\gamma - 2i\Omega + 2F_2)\tilde{P}_2, \\ \partial_t P_{f^*} &= (i\omega - \gamma - i\Omega + 2F_2 + 2G_2^*)P_{f^*} + \tilde{P}_2 + G_2 F_2^*, \end{aligned} \quad (37)$$

with the initial conditions,

$$F_2(t=0) = G_2(t=0) = \tilde{P}_2(t=0) = P_{f^*}(t=0) = 0,$$

where  $\tilde{P}_2(t) \equiv \int_0^t ds \alpha(t, s) P_2(t, s)$ .

In case some readers are not familiar with stochastic methods used in non-Markovian open quantum systems, we provide a brief explanation to show how our results in Eq. (36)

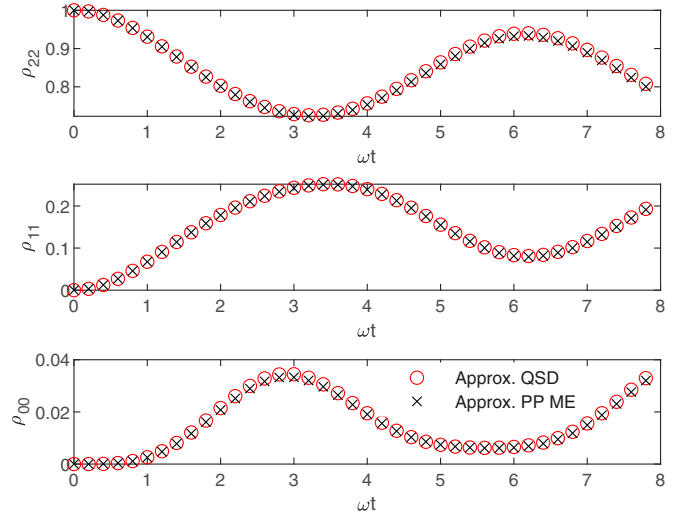


FIG. 2. Time evolution of the population of the dissipative three-level system,  $\rho_{00}$ ,  $\rho_{11}$ , and  $\rho_{22}$  are generated by two different methods: approximated linear QSD equation approach (red circle), and the derived positivity-preserving approximated ME (black cross). The parameters are  $\omega = 1$ ,  $a = 0.8$ ,  $\gamma = 0.05$ , and  $\Omega = 0$ . (The result of the approximated QSD equation approach is obtained by averaging over 5000 quantum trajectories.)

cover the Lindblad-type (Davies) MEs in the weak system-bath coupling regime. Our results contain several additional operator components,  $G_2[\hat{J}_z \hat{J}_- \hat{\rho}_r^{(0)}, \hat{J}_+]$ ,  $P_{f^*} \hat{J}_-^2 \hat{\rho}_r^{(0)} \hat{J}_+^2$ , and their Hermitian conjugates. In the Markov limit, with the evolution equations of the coefficients in Eq. (37) and the associated initial conditions, it is easy to estimate that  $G_2 \rightarrow 0$ ,  $P_{f^*} \rightarrow 0$ ,  $F_2 \rightarrow \Gamma(t)/2$ . Therefore, Eq. (36) can be simplified to resemble the Lindblad-type (Davies) MEs.

## B. Numerical results

In this section we compare the simulation results of the population of states of the three-level system using four different methods: (1) the exact ME,  $\hat{\rho}_r = \mathcal{M}(|\psi_z\rangle\langle\psi_z|)$  in Eq. (16); (2) the approximated positivity-preserving ME,  $\hat{\rho}_r^{(0)} = \mathcal{M}(|\psi_z^{(0)}\rangle\langle\psi_z^{(0)}|)$  in Eq. (23); (3) the approximated non-positivity-preserving ME,  $\hat{\rho}_r'$  in Eq. (17); and (4) the approximated QSD,  $|\psi_z^{(0)}\rangle$  in Eq. (25). (More details can be found in Appendix B.)

First of all, we plot the time evolution of the population of the dissipative three-level system,  $\rho_{00}$ ,  $\rho_{11}$ , and  $\rho_{22}$ , generated by the approximated QSD equation approach and the approximated positivity-preserving ME approach. The initial state of the system is prepared at an excited state:  $|\psi_z(t=0)\rangle = |2\rangle$ . [In the three-level ladder system, when we set the initial value of the density operator as  $\hat{\rho}_r(0) = |2\rangle\langle 2|$ , all the off-diagonal elements of the density operator remain zero throughout the evolution process. As a result, the three eigenvalues of  $\hat{\rho}_r(t)$  are  $\rho_{22}(t)$ ,  $\rho_{11}(t)$ , and  $\rho_{00}(t)$ .] We choose the frequency,  $\omega = 1$ , and the central frequency of the environment  $\Omega = 0$ . In a strong non-Markovian regime,  $\gamma = 0.05$ , the simulation results from two methods, as shown in Fig. 2, overlap each other. Since the reduced density matrix generated from the approximated QSD approach is naturally positivity-preserving,

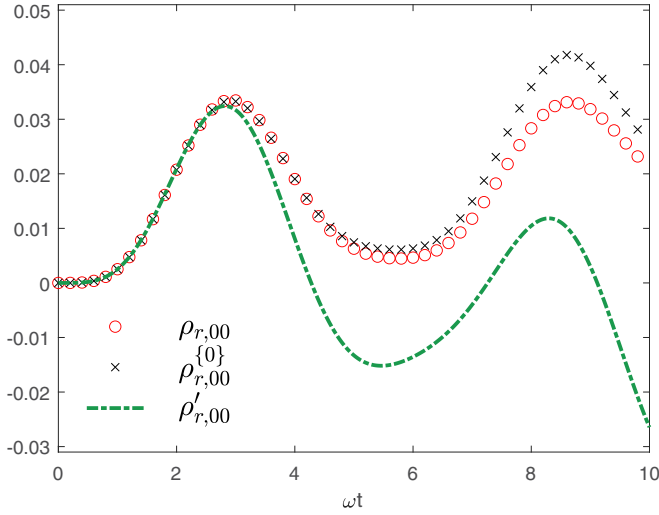


FIG. 3. Comparison of the time evolution of the population of the ground state, generated by three different ME approaches: exact ME ( $\rho_{r,00}$ , red circle), positivity-preserving approximated ME ( $\rho_{r,00}^{(0)}$ , black cross), and non-positivity-preserving approximated ME ( $\rho'_{r,00}$ , green dash-dotted line). The parameters are  $\omega = 1$ ,  $a = 0.8$ ,  $\gamma = 0.05$ , and  $\Omega = 0$ .

the matched dynamics prove that our approximated ME gives rise to the same degree of accuracy as the approximated QSD equation. It indicates that the approximated ME can guarantee positivity.

Next, we plot the time evolution of the population of the ground state using three different ME approaches in Fig. 3. Using the same parameters as Fig. 2, we observe that the exact ME and our approximated positivity-preserving ME both preserve the positivity. Meanwhile, the simulation result of the non-positivity-preserving ME leads to failure due to the appearance of negative probabilities in some time intervals. Furthermore, the magnitude of the negative probability increases with time up to infinity. Consequently, the probabilities of the other two levels also increase to infinity simultaneously. If one simply replaces the exact O-operator in the exact ME with the truncated operator  $\hat{O}^{(0)}$ , then Eq. (17) can be explicitly written as

$$\partial_t \hat{\rho}'_r = -i[\hat{H}_S, \hat{\rho}'_r] + ((F_2 \hat{J}_- + G_2 \hat{J}_z \hat{J}_-) \hat{\rho}'_r, \hat{J}_+) + \text{H.c.}).$$

It is clear that the above approximated ME does not preserve positivity in some parameter regions and may lead to meaningless physics.

To further demonstrate the importance of our method in studying non-Markovian dynamics, we plot Fig. 4, the time evolution of the population of the ground state in a *moderate* non-Markovian regime. When  $\gamma = 0.2$ , a shorter memory time compared with the parameter  $\gamma = 0.05$  used in Fig. 3, the dynamics simulated by the approximated non-positivity-preserving ME  $\rho'_{r,00}$  do not contain any negative probabilities. However, its distance from the results of the exact ME approach is significantly larger compared with the results of our positivity-preserving ME. Comparing Figs. 3 and 4, we show that the reduced density matrix  $\rho_r^{(0)}$  can guarantee positivity preservation from the Markovian to the strong non-Markovian regime. In contrast, the reduced density matrix  $\rho'_r$  cannot

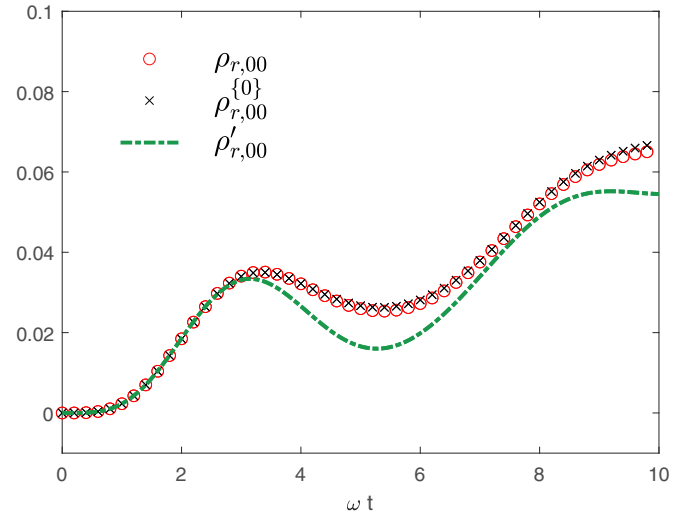


FIG. 4. Comparison of time evolution of the population of the ground state, generated by three different ME approaches: exact ME ( $\rho_{r,00}$ , red circle), positivity-preserving approximated ME ( $\rho_{r,00}^{(0)}$ , black cross), and non-positivity-preserving approximated ME ( $\rho'_{r,00}$ , green dash-dotted line) in a *moderate* non-Markovian regime. The parameters are  $\omega = 1$ ,  $a = 0.2$ ,  $\gamma = 0.2$ , and  $\Omega = 0$ .

offer such confidence. Moreover, for different models and interested parameter spaces, our method is flexible for different approximations. It provides a robust method to obtain positivity-preserving MEs for the analysis of non-Markovian dynamics.

#### IV. CONCLUSION

We have addressed a long-standing issue in OQSs on how to construct positivity-preserving approximated MEs in a general situation. Although several developed MEs, such as Lindblad- and Redfield-type MEs, can provide powerful and efficient mathematical tools, these approaches have common shortcomings since they are rooted in the Born-Markov approximation. In this study we start from the fact that a reduced density matrix must carry over positivity if recovered from the ensemble average over the stochastic pure states. Then we consider a class of linear approximated QSD equations, exploring the possibility of constructing MEs equivalent to QSD equations. A traditional solution is to utilize the approximation relationship  $\delta_{z^*} |\psi_z^N\rangle \approx \hat{O} |\psi_z^N\rangle \approx \hat{O}^N |\psi_z^N\rangle$  to obtain the approximated MEs [52]. However, this approximation could induce negative eigenvalues in the numerical simulations under certain conditions. In fact,  $\delta_{z^*} |\psi_z^N\rangle$  should be equal to  $\hat{O}_d |\psi_z^N\rangle$ , where  $\hat{O}_d$  is a newly defined operator. No matter how small the difference between the  $\hat{O}_d$  and the approximated  $\hat{O}^N$  is, replacing  $\hat{O}_d$  by  $\hat{O}^N$  in the derivation may lead to a violation of positivity of MEs. Consequently, it is necessary to introduce two different approximated  $\hat{O}$  to generate the positivity-preserving approximated ME. Generally, we explain why applying an approximation directly on the exact ME may violate positivity, while applying the same approximation on the exact SSE will not.

In the paper we propose a general class of positivity-preserving non-Markovian MEs generated from SSEs, in

particular, QSD equations. We explicitly derive the approximated positivity-preserving ME for a dissipative three-level system as a specific example of our general results. Moreover, our simulations also show that the negative probability generated by non-positivity-preserving MEs sometimes ends up with negative infinity, which is definitely not a trivial issue.

In summary, we have developed a systematic method to obtain a class of approximated but positivity-preserving non-Markovian MEs originating from approximated linear QSD equations. With such MEs, it is feasible to study nonequilibrium dynamics in living or biological systems, perform reliable error analysis for quantum engineering, and investigate dynamics and phase transitions in many-body systems.

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#### APPENDIX A: DERIVATION OF EQ. (15)

First, we recall several notations:

$$\mathcal{M}(\cdot) = \int \frac{d^2z}{\pi} e^{-|z|^2}(\cdot), \quad (\text{A1})$$

where  $\frac{d^2z}{\pi} \equiv \frac{d^2z_1}{\pi} \frac{d^2z_2}{\pi} \dots \frac{d^2z_k}{\pi} \dots$ ,  $|z|^2 \equiv \sum_k |z_k|^2$ ,  $\int d^2z_k \equiv \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx_k dy_k$ , and  $x_k \equiv \text{Re}(z_k)$ ,  $y_k \equiv \text{Im}(z_k)$ . In addition, the complex Gaussian process is defined as

$$z_t^* \equiv -i \sum_k g_k z_k^* e^{i\omega_k t}. \quad (\text{A2})$$

Consequently, the left-hand side of Eq. (15) can be explicitly expanded as

$$\begin{aligned} \mathcal{M}(z_t^* \hat{P}) &= \int \frac{d^2z}{\pi} e^{-|z|^2} z_t^* \hat{P} \\ &= \int \frac{d^2z}{\pi} e^{-|z|^2} \left( -i \sum_k g_k z_k^* e^{i\omega_k t} \right) \hat{P} \\ &= \int \frac{d^2z}{\pi} e^{-|z|^2} \left( -i \sum_k g_k (x_k - iy_k) e^{i\omega_k t} \right) \hat{P}. \end{aligned} \quad (\text{A3})$$

Using integration by parts for the  $k$ th mode, we have

$$\begin{aligned} &\int d^2z_k e^{-|z_k|^2} x_k \hat{P} \\ &= -\frac{1}{2} \int d^2z_k \frac{\partial}{\partial x_k} (e^{-|z_k|^2} \hat{P}) \\ &= -\frac{1}{2} \int dy_k (e^{-|z_k|^2} \hat{P})|_{x_k=-\infty}^{x_k=\infty} + \frac{1}{2} \int d^2z_k e^{-|z_k|^2} \partial_{x_k} \hat{P}. \end{aligned} \quad (\text{A4})$$

Usually, the boundary terms  $(e^{-|z_k|^2} \hat{P})|_{x_k \rightarrow \infty}$  and  $(e^{-|z_k|^2} \hat{P})|_{x_k \rightarrow -\infty}$  in the above equation converge to zero rapidly. Thus, we have

$$\int d^2z_k e^{-|z_k|^2} x_k \hat{P} = \frac{1}{2} \int d^2z_k e^{-|z_k|^2} \partial_{x_k} \hat{P}. \quad (\text{A5})$$

Similarly, we also have

$$\int d^2z_k e^{-|z_k|^2} y_k \hat{P} = \frac{1}{2} \int d^2z_k e^{-|z_k|^2} \partial_{y_k} \hat{P}. \quad (\text{A6})$$

According to the chain rule, we have

$$\begin{aligned} \begin{bmatrix} \partial_{x_k} \\ \partial_{y_k} \end{bmatrix} &= \begin{bmatrix} \partial z_k / \partial x_k & \partial z_k^* / \partial x_k \\ \partial z_k / \partial y_k & \partial z_k^* / \partial y_k \end{bmatrix} \begin{bmatrix} \partial_{z_k} \\ \partial_{z_k^*} \end{bmatrix} \\ &= \begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix} \begin{bmatrix} \partial_{z_k} \\ \partial_{z_k^*} \end{bmatrix}. \end{aligned} \quad (\text{A7})$$

By employing Eqs. (A5), (A6), and (A7), we obtain the conclusion:

$$\begin{aligned} \int d^2z_k e^{-|z_k|^2} z_k^* \hat{P} &= \int d^2z_k e^{-|z_k|^2} (x_k - iy_k) \hat{P} \\ &= \frac{1}{2} \int d^2z_k e^{-|z_k|^2} [1 \quad -i] \begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix} \begin{bmatrix} \partial_{z_k} \\ \partial_{z_k^*} \end{bmatrix} \hat{P} \\ &= \int d^2z_k e^{-|z_k|^2} \partial_{z_k} \hat{P}. \end{aligned} \quad (\text{A8})$$

Substituting Eq. (A8) into Eq. (A3), we obtain

$$\begin{aligned} \mathcal{M}(z_t^* \hat{P}) &= -i \sum_k g_k e^{i\omega_k t} \int \frac{d^2z}{\pi} e^{-|z|^2} \frac{\partial \hat{P}}{\partial z_k} \\ &= \sum_k \frac{\partial z_t^*}{\partial z_k^*} \int \frac{d^2z}{\pi} e^{-|z|^2} \frac{\partial \hat{P}}{\partial z_k}. \end{aligned} \quad (\text{A9})$$

Then we apply the chain rule,

$$\frac{\partial(\cdot)}{\partial z_k} = \int_0^t ds \frac{\partial z_s}{\partial z_k} \frac{\delta(\cdot)}{\delta z_s}, \quad (\text{A10})$$

and obtain Eq. (15) [52,57],

$$\begin{aligned} \mathcal{M}(z_t^* \hat{P}) &= \sum_k \frac{\partial z_t^*}{\partial z_k^*} \int \frac{d^2z}{\pi} e^{-|z|^2} \int_0^t ds \frac{\partial z_s}{\partial z_k} \frac{\delta \hat{P}}{\delta z_s} \\ &= \int \frac{d^2z}{\pi} e^{-|z|^2} \int_0^t ds \sum_k \left[ \frac{\partial z_t^*}{\partial z_k^*} \frac{\partial z_s}{\partial z_k} \right] \frac{\delta \hat{P}}{\delta z_s} \\ &= \int_0^t ds \mathcal{M}(z_t^* z_s) \mathcal{M} \left( \frac{\delta \hat{P}}{\delta z_s} \right), \end{aligned} \quad (\text{A11})$$

where we have utilized the property of the correlation function:  $\alpha^*(t, s) = \mathcal{M}(z_t^* z_s) = \sum_k \left[ \frac{\partial z_t^*}{\partial z_k^*} \frac{\partial z_s}{\partial z_k} \right]$ . Furthermore, the term  $\frac{\delta \hat{P}}{\delta z_s}$  can be formally expressed as  $\frac{\delta |\psi_z[z_t^*]\rangle}{\delta z_s} (\psi_z[z_t] + |\psi_z[z_t^*]\rangle \frac{\delta |\psi_z[z_t]\rangle}{\delta z_s})$ . Due to features of analytic functions, we have  $\frac{\delta |\psi_z[z_t^*]\rangle}{\delta z_s} = 0$ , as a result,  $\frac{\delta \hat{P}}{\delta z_s} = |\psi_z[z_t^*]\rangle \frac{\delta (\psi_z[z_t])}{\delta z_s} = \hat{P} \hat{O}^\dagger$ . Similarly, we can obtain the relations in Eq. (18).

## APPENDIX B: EXPLICIT FORMS OF THE EQUATIONS IN THE NUMERICAL SIMULATION

We have explicitly listed four equations used in numerical simulations. To maintain simplicity and improve readability, we assign the same notation to coefficients associated with the identical operators in different subsections, even though these coefficients differ from one another.

### 1. Exact ME

$$\begin{aligned} \partial_t \hat{\rho}_r = & -i[\hat{H}_S, \hat{\rho}_r] + \{(F\hat{J}_- + G\hat{J}_z\hat{J}_-)\hat{\rho}_r, \hat{J}_+\} \\ & + \{(P_{f^*}\hat{J}_-^2\hat{\rho}_r\hat{J}_+ + P_{g^*}\hat{J}_-^2\hat{\rho}_r\hat{J}_+\hat{J}_z), \hat{J}_+\} + \text{H.c.}, \end{aligned} \quad (\text{B1})$$

where the coefficients satisfy

$$\begin{aligned} \partial_t F = & a\gamma + (i(\omega - \Omega) - \gamma + 2G)F - 2\tilde{P}, \\ \partial_t G = & -2F^2 + (i(\omega - \Omega) - \gamma + 6F - 2G)G - 2\tilde{P}, \\ \partial_t \tilde{P} = & a\gamma G + (2i(\omega - \Omega) - 2\gamma - 2G + 4F)\tilde{P}, \\ \partial_t P_{f^*} = & (i(\omega - \Omega) - \gamma + 4F - 2G + 2G^*)P_{f^*} \\ & - 2P_{p^*} + GF^* + \tilde{P}, \\ \partial_t P_{g^*} = & (i(\omega - \Omega) - \gamma + 4F + 2F^* - 2G - 2G^*)P_{g^*} \\ & + (4G^* - 2F^*)P_{f^*} + |G|^2 - 2P_{p^*}, \\ \partial_t P_{p^*} = & (4F + 4F^* - 2G - 2G^* - 2\gamma)P_{p^*} + G^*\tilde{P} \\ & + G\tilde{P}^*, \end{aligned} \quad (\text{B2})$$

with the initial conditions  $F(0) = G(0) = \tilde{P}(0) = P_{f^*}(0) = P_{g^*}(0) = P_{p^*}(0) = 0$ .

### 2. Approximated positivity-preserving ME

$$\begin{aligned} \partial_t \hat{\rho}_r^{(0)} = & -i[\hat{H}_S, \hat{\rho}_r^{(0)}] + \{(F\hat{J}_- + G\hat{J}_z\hat{J}_-)\hat{\rho}_r^{(0)}, \hat{J}_+\} \\ & + P_{f^*}\hat{J}_-^2\hat{\rho}_r^{(0)}\hat{J}_+^2 + \text{H.c.}, \end{aligned} \quad (\text{B3})$$

where the coefficients satisfy

$$\begin{aligned} \partial_t F = & a\gamma + (i\omega - \gamma - i\Omega + 2G)F, \\ \partial_t G = & -2F^2 + (i\omega - \gamma - i\Omega + 6F - 2G)G, \\ \partial_t \tilde{P} = & a\gamma G + (2i\omega - 2\gamma - 2i\Omega + 2F)\tilde{P}, \\ \partial_t P_{f^*} = & (i\omega - \gamma - i\Omega + 2F + 2G^*)P_{f^*} + \tilde{P} + GF^*, \end{aligned} \quad (\text{B4})$$

with the initial conditions  $F(0) = G(0) = \tilde{P}(0) = P_{f^*}(0) = 0$ .

### 3. Approximated non-positivity-preserving ME

$$\partial_t \hat{\rho}'_r = -i[\hat{H}_S, \hat{\rho}'_r] + \{(F\hat{J}_- + G\hat{J}_z\hat{J}_-)\hat{\rho}'_r, \hat{J}_+\} + \text{H.c.}, \quad (\text{B5})$$

where the coefficients satisfy

$$\begin{aligned} \partial_t F = & a\gamma + (i\omega - \gamma - i\Omega + 2G)F, \\ \partial_t G = & -2F^2 + (i\omega - \gamma - i\Omega + 6F - 2G)G, \end{aligned} \quad (\text{B6})$$

with the initial conditions  $F(0) = G(0) = 0$ .

### 4. Approximated QSD equation

$$\partial_t |\psi_z^{(0)}\rangle = (-i\hat{H}_S + z_t^*\hat{J}_- - F\hat{J}_+\hat{J}_- - G\hat{J}_+\hat{J}_z\hat{J}_-)|\psi_z^{(0)}\rangle, \quad (\text{B7})$$

where the coefficients satisfy

$$\begin{aligned} \partial_t F = & a\gamma + (i\omega - \gamma - i\Omega + 2G)F, \\ \partial_t G = & -2F^2 + (i\omega - \gamma - i\Omega + 6F - 2G)G, \end{aligned} \quad (\text{B8})$$

with the initial conditions  $F(0) = G(0) = 0$ .

The stochastic process  $z_t^*$  can be generated using  $dz_t^* = (-\gamma + i\Omega)z_t^*dt + \gamma\sqrt{a\gamma}dW_t$ , where  $W_t$  is the complex Wiener process.

All the above equations of coefficients are based on the assumption that the correlation function is  $\alpha(t, s) = a\gamma e^{-\gamma|t-s| - i\Omega(t-s)}$ .

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