Quantum algorithm for the simulation of open-system dynamics and thermalization

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The quantum open-system simulation is an important category of quantum simulation. By simulating the thermalization process at zero temperature, we can solve the ground-state problem of quantum systems. To realize the open-system evolution on the quantum computer, we need to encode the environment using qubits. However, usually the environment is much larger than the system, i.e., numerous qubits are required if the environment is directly encoded. In this paper, we propose a way to simulate open-system dynamics by reproducing reservoir correlation functions using a minimized Hilbert space. In this way, we only need a small number of qubits to represent the environment. To simulate the nth-order expansion of the time-convolutionless master equation by reproducing up to n-time correlation functions, the number of qubits representing the environment is $\sim\lfloor\frac{n}{2}\rfloor\log_2(N_\omega N_\beta)$. Here, N_ω is the number of frequencies in the discretized environment spectrum, and N_β is the number of terms in the system-environment interaction. By reproducing two-time correlation functions, i.e., taking $n=2$, we can simulate the Markovian quantum master equation. In our algorithm, the environment on the quantum computer could be even smaller than the system.

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I. INTRODUCTION

The idea of quantum computation is motivated by quantum simulation. According to Feynman, "the physical world is quantum mechanical, and therefore the proper problem is the simulation of quantum physics" [1]. The physical world is not only *quantum* but also *open*. Many vital phenomena are attributed to open-system dynamics, e.g., thermalization [2,3]. Systems are influenced by their environments through external interactions. Therefore, by simulating the composite system, including the system and the environment, we can study an open system on a quantum computer [4–6]. However, the simulation of the environment is usually inefficient when the environment is big compared to the system. It is also a waste of resources. In many circumstances, we are only interested in the system, not the environment. The simulation of the environment making the most of computational resources may not give us any new knowledge, for instance, when the environment is modeled as an exactly solvable boson bath or spin bath. The dynamics of the system is determined by reservoir correlation functions. For example, in thermalization, transition rates between eigenstates are determined by two-time reservoir correlation functions [2]. Therefore, reproducing reservoir correlation functions is sufficient, and the full simulation of the environment is unnecessary.

An application of quantum computation is to compute the ground-state energy, which is an important problem in material science and chemistry [7–10]. Given an initial state with a finite probability in the ground state, we can use the quantum phase estimation algorithm to obtain the ground-state energy [7,8]. However, we do not have a universal algorithm that can prepare such an initial state [11,12]. Solving the ground-state problem for a general Hamiltonian is likely to be intractable even in quantum computation [13,14]. A related problem is preparing or sampling thermal states of a quantum system [15–20], and the ground state is the thermal state at zero temperature. If we only focus on systems in the real world, most of them reach the thermal state as a result of open-system dynamics. Therefore, for such real-world systems, simulating open-system dynamics is an efficient way to prepare thermal states, including the ground state. Although we have quantum algorithms that can implement semigroup dynamics (unitary or nonunitary) [4,21–31], they cannot be directly used for thermalization by simulating the corresponding Lindblad equation. Working out the Lindblad equation of thermalization requires the spectrum of the system [2], which is the information that we want to obtain in the computation. To computation the thermal state, we have to assume that the Lindblad equation is unknown. Therefore, we need an environment to simulate thermalization. In this paper, we propose a hardware-efficient quantum algorithm for the simulation of Markovian and non-Markovian open-system dynamics, which can be used for solving the thermalization and ground-state problems.

Qubits are valuable resources in the present and will continue to be in the future. They are similar to the classical computational resources we use today but more severe. Fault-tolerant quantum computation based on quantum error correction is the way to implement large-scale quantum computations, in which encoding one logical qubit may need thousands of physical qubits [32,33]. Therefore, reducing the number of logical qubits is essential. Variational quantum algorithms for solving the ground-state problem or simulating the real and imaginary time evolutions have been developed recently [34–37], which can avoid the enormous qubit cost and are suitable for near-term quantum computation. In this paper, our algorithm is in the category of conventional

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quantum algorithms demanding fault tolerance but does not rely on a good variational ansatz. We reduce the qubit cost by using a small environment to simulate open-system dynamics induced by a big environment. We achieve this by reproducing reservoir correlation functions of the big environment in the small environment.

Open-system dynamics is determined by reservoir correlation functions. According to the expansion of the time-convolutionless (TCL) master equation, the simulation of open-system dynamics is more accurate if higher-order correlation functions are reproduced. By reproducing two-time correlation functions, we can simulate the Redfield equation and, therefore, the Markovian quantum master equation when the Markov approximation is justified. From the Markovian quantum master equation, we can simulate thermalization.

Our algorithm is beyond two-time correlation functions. Any n-time correlation functions can be reproduced, therefore we can simulate the TCL master equation up to any nth-order expansion. Reservoir correlation functions can be reproduced using a tensor network, in which way the dimension of the environment increases exponentially with the number of terms in the system-environment coupling [38]. Our algorithm uses a different approach. By minimizing the Hilbert-space dimension for reproducing given correlation functions, the number of qubits required for representing the environment is $\sim\frac{n}{2}\log_2(N_\omega N_\beta)$, where N_ω is the number of frequencies in the discretized environment spectrum and N_β is the number of terms in the coupling. Reservoir correlation functions can be exactly reproduced up to the spectrum discretization, which usually converges polynomially with N_ω.

The theory of open-system dynamics is introduced in Sec. II. To simulate the open-system dynamics given by the Hamiltonian H and the environment state $\rho_{\rm E}$, instead, we implement the dynamics of the Hamiltonian $\widetilde{H}$ and the environment state $\widetilde{\rho}_{\rm E}$ on the quantum computer, as shown in Fig. 1. The overview of the algorithm is given in Sec. III, and details of the algorithm are discussed in Secs. IV–VI. In Sec. VII, we discuss how to reinitialize the environment in the simulation. In Sec. VIII, the circuit implementation, qubit cost, and gate-number cost are discussed. In Sec. IX, we give an illustrative example, and we numerically implement our algorithm on a classical computer to simulate the thermalization of a qubit.

Below, we will show how to choose $\widetilde{H}$ and $\widetilde{\rho}_{\rm E}$ such that reservoir correlation functions of H and $\rho_{\rm E}$ can be reproduced on the quantum computer. Because we want to minimize the number of qubits representing the environment, the state of the environment may significantly change with time. Therefore, we may need to reinitialize the environment state during the simulation. We also show how to implement the reinitialization without significantly modifying correlation functions.

II. DYNAMICS OF OPEN QUANTUM SYSTEMS WEAKLY COUPLED TO THE ENVIRONMENT

Given the Hamiltonian of the system and environment $H = H_{\rm S} + H_{\rm E} + \alpha H_{\rm I}$, where $H_{\rm S}$, $H_{\rm E}$, and $H_{\rm I}$, respectively, denote Hamiltonians of the system, environment, and interaction [see Fig. 1(a)], the evolution equation in the interaction picture is

$$\frac{\partial}{\partial t}\rho(t) = -i\alpha[H_{\rm I}(t), \rho(t)] \equiv \alpha\mathcal{L}(t)\rho(t). \tag{1}$$

Here, ρ is the state of the system and environment, α is a dimensionless coupling constant, and we have taken $\hbar = 1$. Derived from this evolution equation, the TCL equation [2] is

$$\frac{\partial}{\partial t}\mathcal{P}\rho(t) = \mathcal{K}(t)\mathcal{P}\rho(t) \tag{2}$$

for any initial state in the form $\rho(0) = \rho_{\rm S}(0)\otimes\rho_{\rm E}$, where $\mathcal{P}$ is a superoperator projection defined by $\mathcal{P}\rho \equiv {\rm Tr}_{\rm E}(\rho)\otimes\rho_{\rm E}$. We focus on the case that $\rho_{\rm E}$ is a stationary state of the environment, i.e., $[H_{\rm E}, \rho_{\rm E}] = 0$.

The TCL master equation is the evolution equation of the system state $\rho_{\rm S} = {\rm Tr}_{\rm E}(\rho)$, because $\mathcal{P}\rho(t) = \rho_{\rm S}(t)\otimes\rho_{\rm E}$, in which only the system state $\rho_{\rm S}(t)$ evolves with time, and the environment state $\rho_{\rm E}$ is constant.

When the coupling between the system and environment is weak, the expansion of TCL generator $\mathcal{K}(t)$ in powers of the coupling constant α provides a series of approximate evolution equations. The expansion reads $\mathcal{K}(t) = \sum_{n=1}^{\infty}\alpha^n\mathcal{K}_n(t)$, where $\mathcal{K}_n(t)$ does not depend on α. For example, up to the fourth order, we have $\mathcal{K}_1(t) = \mathcal{P}\mathcal{L}(t)\mathcal{P}$, $\mathcal{K}_2(t) = \int_0^t dt_1\mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{P}$, $\mathcal{K}_3(t) =$

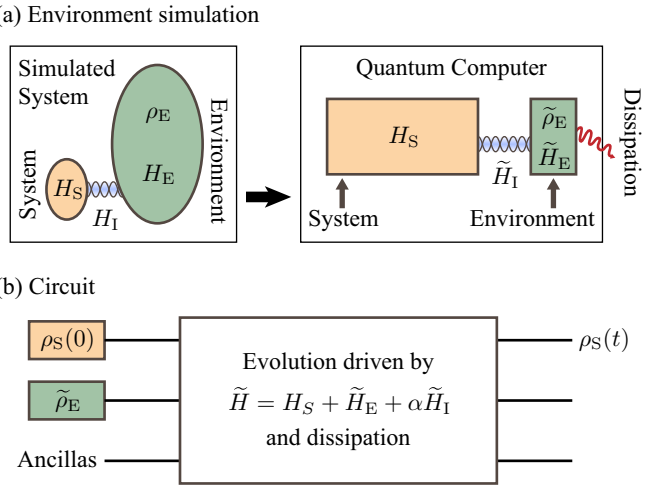

FIG. 1. (a) The simulated dynamics of the system is determined by the Hamiltonian $H = H_{\rm S} + H_{\rm E} + \alpha H_{\rm I}$ and the state of the environment $\rho_{\rm E}$. On the quantum computer, instead of directly simulating the environment, we use a Hilbert space with a much lower dimension to represent the environment and simulate the dynamics driven by the Hamiltonian $\widetilde{H} = H_{\rm S} + \widetilde{H}_{\rm E} + \alpha\widetilde{H}_{\rm I}$ and the environment state $\widetilde{\rho}_{\rm E}$. Because the environment on the quantum computer has a finite size, we may need to introduce dissipation in order to relax the environment. (b) The evolution driven by $\widetilde{H}$ and the dissipation is realized using a quantum circuit on the quantum computer. To obtain the final state of the system $\rho_{\rm S}(t)$, qubits representing the system are prepared in the initial state of the system $\rho_{\rm S}(0)$, qubits representing the environment are prepared in the initial state of the environment $\widetilde{\rho}_{\rm E}$, and then the evolution is implemented using computation operations, i.e., state preparation, quantum gates, and measurement operation. Ancillary qubits may be needed in the simulation, e.g., for implementing the dissipation.

$\int_0^t dt_1 \int_0^{t_1} dt_2 \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{L}(t_2)\mathcal{P}$, and

$$\mathcal{K}_4(t) = \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \times [\boldsymbol{\kappa}_4(t,t_1,t_2,t_3) - \boldsymbol{\kappa}_2(t,t_1)\boldsymbol{\kappa}_2(t_2,t_3) - \boldsymbol{\kappa}_2(t,t_2)\boldsymbol{\kappa}_2(t_1,t_3) - \boldsymbol{\kappa}_2(t,t_3)\boldsymbol{\kappa}_2(t_1,t_2)], \quad (3)$$

where

$$\boldsymbol{\kappa}_n(t,t_1,\ldots,t_{n-1}) = \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\cdots\mathcal{L}(t_{n-1})\mathcal{P}. \quad (4)$$

Without loss of generality, we have assumed $\mathcal{P}\mathcal{L}(t)\mathcal{P} = 0$ for simplification. In general, the nth-order TCL generator $\mathcal{K}_n(t)$ is determined by superoperators $\boldsymbol{\kappa}_m$ with $m \leqslant n$.

The TCL equation is the exact evolution equation of the system and, therefore, describes the non-Markovian dynamics of the system. By neglecting high-order terms and taking the approximation $\mathcal{K}_2(t) \simeq \mathcal{K}_2(\infty)$ under the assumption that the correlation time is short, we can get the Markovian quantum master equation $\frac{\partial}{\partial t}\mathcal{P}\rho(t) = \alpha^2\mathcal{K}_2(\infty)\mathcal{P}\rho(t)$.

Correlation functions of the environment

Open-system dynamics is determined by reservoir correlation functions. In general, the nth-order TCL generator $\mathcal{K}_n(t)$ is determined by up to the n-time correlations [2]. The interaction can always be expressed in the form $H_{\mathrm{I}} = \sum_\beta A_\beta \otimes B_\beta$, where A_β acts on the system, B_β acts on the environment, and they are both Hermitian. Expanding $\boldsymbol{\kappa}_n$ using the expression of H_{I}, we have

$$\boldsymbol{\kappa}_n(t,\ldots,t_{n-1})\rho = \sum_{\nu,\ldots,\nu_{n-1}} \sum_{\beta,\ldots,\beta_{n-1}} i^n(-1)^{\nu+\cdots+\nu_{n-1}} \times \mathrm{Tr}\big[\mathcal{B}_\beta(t,\nu)\cdots\mathcal{B}_{\beta_{n-1}}(t_{n-1},\nu_{n-1})\rho_{\mathrm{E}}\big] \times \mathcal{A}_\beta(t,\nu)\cdots\mathcal{A}_{\beta_{n-1}}(t_{n-1},\nu_{n-1})\mathcal{P}\rho. \quad (5)$$

Here, $\nu,\ldots,\nu_{n-1} = 0,1$ are binary numbers indicating on which side the Hamiltonian acts, we define superoperators $\mathcal{C}_\beta(\iota,\nu)\rho \equiv [C_\beta(\iota)]^\nu \rho [C_\beta(\iota)]^{1-\nu}$; $C = A, B$; and $\iota = t, \omega$ ($\iota = \omega$ will be used later). Therefore, the superoperator $\boldsymbol{\kappa}_n$ is determined by system operators A_β and n-time correlation functions of the environment. We note that reservoir correlation functions are time ordered, i.e., $t \geqslant \cdots \geqslant t_{n-1}$.

For the environment with a discretized spectrum, the environment Hamiltonian can be decomposed according to the spectrum as $H_{\mathrm{E}} = \sum_\varepsilon \varepsilon\Pi(\varepsilon)$, where $\Pi(\varepsilon)$ is the projection onto the eigenspace of the eigenenergy ε. We define operators $B_\beta(\omega) \equiv \sum_{\varepsilon'-\varepsilon=\omega}\Pi(\varepsilon)B_\beta\Pi(\varepsilon')$, then $B_\beta(t) = \sum_\omega e^{-i\omega t}B_\beta(\omega)$. We can find that $B_\beta^\dagger(\omega) = B_\beta(-\omega)$, because B_β is Hermitian.

Without loss of generality, we assume $\mathrm{Tr}(B_\beta\rho_{\mathrm{E}}) = 0$, i.e., $\mathcal{P}\mathcal{L}(t)\mathcal{P} = 0$. We note that ρ_{E} is a stationary state. If $\mathrm{Tr}(B_\beta\rho_{\mathrm{E}})$ is not zero, we can replace B_β with $B_\beta - \mathrm{Tr}(B_\beta\rho_{\mathrm{E}})\mathbb{1}$ and H_{S} with $H_{\mathrm{S}} + \sum_\beta \mathrm{Tr}(B_\beta\rho_{\mathrm{E}})A_\beta \otimes \mathbb{1}$, so that the total Hamiltonian is not changed but the assumption is satisfied.

Two distinct environments result in the same dynamics of the system if their correlation functions are the same and they are coupled to the system by the same set of operators A_β [see Fig. 1(a)].

Theorem 1. Let $\widetilde{H} = H_{\mathrm{S}} + \widetilde{H}_{\mathrm{E}} + \alpha\widetilde{H}_{\mathrm{I}}$ be the Hamiltonian of the system and a different environment, and $\widetilde{H}_I = \sum_\beta A_\beta \otimes \widetilde{B}_\beta$. The sufficient condition for the same dynamics of the system up to the nth order, i.e., $\sum_{m=1}^n \alpha^m\mathcal{K}_m(t) = \mathcal{P}\sum_{m=1}^n \alpha^m\widetilde{\mathcal{K}}_m(t)$, is that

$$\mathrm{Tr}\big[\widetilde{\mathcal{B}}_\beta(t,\nu)\cdots\widetilde{\mathcal{B}}_{\beta_{m-1}}(t_{m-1},\nu_{m-1})\widetilde{\rho}_{\mathrm{E}}\big] = \mathrm{Tr}\big[\mathcal{B}_\beta(t,\nu)\cdots\mathcal{B}_{\beta_{m-1}}(t_{m-1},\nu_{m-1})\rho_{\mathrm{E}}\big] \quad (6)$$

holds for all $m \leqslant n$.

III. OVERVIEW OF THE ALGORITHM

According to Theorem 1, in order to simulate the open-system dynamics driven by H up to the nth order, we can implement the evolution driven by $\widetilde{H}$ on the quantum computer. The algorithm has two stages. At the first stage, we compute correlation functions of the environment determined by H_{E} and $\{B_\beta\}$ and design the environment on the quantum computer, i.e., choose $\widetilde{H}_{\mathrm{E}}$, $\{\widetilde{B}_\beta\}$, and the dissipation of the environment to reproduce the same correlation functions. The purpose of our algorithm is to simulate the dynamics of an open quantum system and study the system rather than the environment. We assume that correlation functions of the environment are computable in classical computation. If correlation functions of the environment are classically intractable, we may need the quantum computer to study the dynamics of the environment, which is beyond the scope of this paper. On the quantum computer, we want to minimize the size of the environment, therefore dissipation of the environment may be required in order to relax the environment and suppress the finite-size effect. We will give the protocol for designing the environment on the quantum computer later. At the second stage, we use the quantum computer to realize the time evolution driven by $\widetilde{H}$ and the dissipation [see Fig. 1(b)]. Given the corresponding Lindblad equation in the explicit form, the evolution can be realized on the quantum computer using a quantum circuit [25–31].

IV. SIMULATION OF THE SECOND-ORDER EQUATION AND MARKOVIAN MASTER EQUATION

In this section, we consider the quantum simulation of the master equation with the second-order approximation. If $\mathcal{P}\mathcal{L}(t)\mathcal{P} = 0$ and higher-order contributions are neglected, the evolution equation of the system reads $\frac{\partial}{\partial t}\mathcal{P}\rho(t) = \alpha^2\mathcal{K}_2(t)\mathcal{P}\rho(t)$, which can also be expressed in the form

$$\frac{d\rho_{\mathrm{S}}}{dt} = -\alpha^2\int_0^t ds\,\mathrm{Tr}_{\mathrm{E}}[H_{\mathrm{I}}(t),[H_{\mathrm{I}}(t-s),\rho_{\mathrm{S}}\otimes\rho_{\mathrm{E}}]]. \quad (7)$$

This equation is determined by two-time correlation functions:

$$\langle B_\beta(t)B_{\beta'}(t-s)\rangle \equiv \mathrm{Tr}[B_\beta(t)B_{\beta'}(t-s)\rho_{\mathrm{E}}]. \quad (8)$$

In order to simulate the time evolution driven by Eq. (7), we reproduce such correlation functions on the quantum computer.

When the time scale over which reservoir correlation functions decay is negligible compared to the time scale over

which the system evolves significantly, the Markov approximation is justified. Then $\mathcal{K}_2(t) \simeq \mathcal{K}_2(\infty)$ and the upper limit t of the integral in Eq. (7) can be replaced by ∞. Our algorithm can simulate the open-system dynamics with a finite correlation time, i.e., the dynamics is non-Markovian, but we focus on the case that the correlation time is short although may not be negligible.

A. Algorithm for the second-order simulation

The correlation function of the environment can be expressed in the form

$$\langle B_\beta(t)B_{\beta'}(t-s)\rangle = \sum_\omega e^{-i\omega s}\gamma_{\beta,\beta'}(\omega), \tag{9}$$

where $\gamma_{\beta,\beta'}(\omega) = \mathrm{Tr}[B_\beta(\omega)B^\dagger_{\beta'}(\omega)\rho_\mathrm{E}]$. To choose the interaction operators $\{\widetilde{B}_\beta\}$ on the quantum computer, we diagonalize matrices $\gamma(\omega)$ on a classical computer. Matrices $\gamma(\omega)$ are Hermitian and positive. After the diagonalization, we obtain $\gamma(\omega) = U(\omega)\Lambda(\omega)U^\dagger(\omega)$, where $\Lambda(\omega)$ is the diagonalized matrix and $U(\omega)$ is unitary. Interaction operators $\{\widetilde{B}_\beta\}$ on the quantum computer depend on coefficients $g_{\beta,l}(\omega) = U_{\beta,l}(\omega)\sqrt{\Lambda_{l,l}(\omega)}$.

On the quantum computer, we use the Hilbert space $\widetilde{\mathcal{H}}_\mathrm{E} = \widetilde{\mathcal{H}}_v \oplus \bigoplus_\omega \widetilde{\mathcal{H}}_\omega$ to represent the environment. Here, $\widetilde{\mathcal{H}}_v$ is one dimensional and contains only one state $|v\rangle$ representing the vacuum, $\widetilde{\mathcal{H}}_\omega$ is d_ω dimensional and corresponds to the transition frequency ω, and $d_\omega = \mathrm{rank}[\gamma(\omega)]$. The orthonormal basis of $\widetilde{\mathcal{H}}_\omega$ is $\{|\omega, l\rangle\}$, where l corresponds to the lth eigenvalue of $\gamma(\omega)$. The dimension of the environment $\widetilde{\mathcal{H}}_\mathrm{E}$ is $d_\mathrm{E} = 1 + \sum_\omega d_\omega$, therefore we can use $N_\mathrm{E} = \lceil \log_2 d_\mathrm{E} \rceil$ qubits to simulate the environment. We have $d_\omega \leqslant N_\beta$ and $d_\mathrm{E} \leqslant 1 + N_\omega N_\beta$, where $N_\beta \equiv |\{\beta\}|$ is the number of terms in the interaction Hamiltonian, $N_\omega \equiv |\{\omega\}| \leqslant N_\varepsilon^2$ is the number of transition frequencies, and $N_\varepsilon \equiv |\{\varepsilon\}|$ is the number of eigenenergies in the discretized spectrum of the environment.

To simulate the environment, we take $\widetilde{\rho}_\mathrm{E} = |v\rangle\langle v|$,

$$\widetilde{H}_\mathrm{E} = \sum_{\omega,l} \omega\sigma_l^\dagger(\omega)\sigma_l(\omega), \tag{10}$$

$$\widetilde{B}_\beta = \sum_{\omega,l} g_{\beta,l}(\omega)\sigma_l(\omega) + \mathrm{H.c.}, \tag{11}$$

where $\sigma_l(\omega) \equiv |v\rangle\langle\omega, l|$. Then, correlations functions can be reproduced on the quantum computer. We note that $\mathrm{Tr}[\widetilde{B}_\beta(\omega)\widetilde{B}^\dagger_{\beta'}(\omega)\widetilde{\rho}_\mathrm{E}] = [U(\omega)\sqrt{\Lambda(\omega)}\sqrt{\Lambda(\omega)}U^\dagger(\omega)]_{\beta,\beta'} = \gamma_{\beta,\beta'}(\omega)$, where

$$\widetilde{B}_\beta(\omega) = \sum_l g_{\beta,l}(\omega)\sigma_l(\omega) + g^*_{\beta,l}(-\omega)\sigma_l^\dagger(-\omega). \tag{12}$$

Therefore, $\langle\widetilde{B}_\beta(t)\widetilde{B}_{\beta'}(t-s)\rangle = \langle B_\beta(t)B_{\beta'}(t-s)\rangle$, where $\langle\widetilde{B}_\beta(t)\widetilde{B}_{\beta'}(t-s)\rangle = \mathrm{Tr}[\widetilde{B}_\beta(t)\widetilde{B}_{\beta'}(t-s)\widetilde{\rho}_\mathrm{E}]$.

B. Discussion

In the algorithm, the initial state of the environment on the quantum computer is always the pure state $|v\rangle$, and the pure state is not the ground state, because the frequency ω can take negative values (see Fig. 2). The system can release energy into the environment via a transition from the state $|v\rangle$ to the state $|\omega, l\rangle$ with a positive ω. Similarly, the system can absorb energy from the environment via a transition from the state $|v\rangle$ to the state $|\omega, l\rangle$ with a negative ω. For a thermal bath with the temperature T, the γ matrix satisfies $\gamma_{\beta,\beta'}(-\omega) = \exp(-\hbar\omega/k_\mathrm{B}T)\gamma_{\beta',\beta}(\omega)$ [2]. If the temperature is zero, $\gamma(\omega) = 0$, i.e., $g_{\beta,l}(\omega) = 0$, for all negative ω. Then, states $|\omega, l\rangle$ with a negative ω are decoupled from the system. In this case, the state $|v\rangle$ is the effective ground state. If the temperature is finite, the system is coupled to not only positive-ω states but also negative-ω states. In this way, we can simulate a finite temperature environment using a pure state as the initial state of the environment.

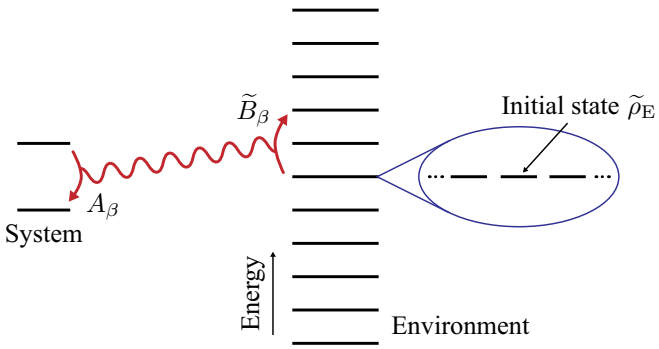

FIG. 2. Level scheme of the environment simulation. Each energy level of the environment represents a frequency with respect to the initial state of the environment. These levels are degenerate. The initial state is encoded as a pure state on the level with the frequency zero. The system can release energy into the environment or absorb energy from the environment via transitions between these energy levels. Transitions are caused by the interaction $\widetilde{H}_I = \sum_\beta A_\beta \otimes \widetilde{B}_\beta$.

V. STATE SPACE RELEVANT TO THE *n*TH-ORDER EXPANSION

We can generalize the algorithm in Sec. IV to simulate the TCL master equation up to the nth order. Before giving the general algorithm, we first analyze the space of relevant environment states. The dimension of the state space has an upper bound $d_{n,\max} = [(N_\omega N_\beta)^{\lfloor n/2\rfloor+1} - 1]/[N_\omega N_\beta - 1]$ as we explain in the next paragraph. Given the dimension of the state space, we can use a Hilbert space with the same dimension as the environment on the quantum computer to simulate the nth-order TCL master equation.

Now we explain the upper bound of the dimension. We can rewrite the m-time correlation function as

$$\begin{aligned}&\mathrm{Tr}\big[\mathcal{B}_\beta(t,\nu)\cdots\mathcal{B}_{\beta_{m-1}}(t_{m-1},\nu_{m-1})\rho_\mathrm{E}\big]\\ &= \sum_{\omega,\ldots,\omega_{m-1}} e^{-i(\omega t+\cdots+\omega_{m-1}t_{m-1})}\\ &\quad\times\mathrm{Tr}\big[\mathcal{B}_\beta(\omega,\nu)\cdots\mathcal{B}_{\beta_{m-1}}(\omega_{m-1},\nu_{m-1})\rho_\mathrm{E}\big].\end{aligned} \tag{13}$$

Let $|\psi\rangle$ be the purification of the state ρ_E, i.e., $|\psi\rangle$ is a state on the Hilbert space $\mathcal{H}_\mathrm{E}\otimes\mathcal{H}_\mathrm{a}$ satisfying $\mathrm{Tr}_\mathrm{a}(|\psi\rangle\langle\psi|) = \rho_\mathrm{E}$. Here, $\mathcal{H}_\mathrm{E}$ is the Hilbert space of the environment, and $\mathcal{H}_\mathrm{a}$ is the Hilbert space of an ancillary system with the minimum dimension $\mathrm{rank}(\rho_\mathrm{E})$. We define $b_\beta(\omega) \equiv B_\beta(\omega)\otimes\mathbb{1}_\mathrm{a}$, where $\mathbb{1}_\mathrm{a}$ is the identity operator of $\mathcal{H}_\mathrm{a}$. Expressing superoperators $\mathcal{B}$

using operators B, the last line of Eq. (13) can be expressed in the form

$$\mathrm{Tr}[(\text{some } B \text{ operators})\rho_{\mathrm{E}}(\text{some } B \text{ operators})],$$

and we can rewrite it as

$$\mathrm{Tr}[(\text{some } b \text{ operators})|\psi\rangle\langle\psi|(\text{some } b \text{ operators})].$$

Then using the cyclic property of the trace, we rewrite correlation functions in the form

$$\begin{aligned}&\mathrm{Tr}\big[\mathcal{B}_{\beta}(\omega,\nu)\cdots\mathcal{B}_{\beta_{m-1}}(\omega_{m-1},\nu_{m-1})\rho_{\mathrm{E}}\big]\\&=\langle\psi|\big[b_{\beta_{m-1}}(\omega_{m-1})\big]^{1-\nu_{m-1}}\cdots[b_{\beta}(\omega)]^{1-\nu}\\&\quad\times[b_{\beta}(\omega)]^{\nu}\cdots\big[b_{\beta_{m-1}}(\omega_{m-1})\big]^{\nu_{m-1}}|\psi\rangle.\end{aligned}\tag{14}$$

To simulate the nth-order TCL master equation, we only need to consider correlation functions with $m\leqslant n$. Therefore, the maximum number of b operators in the above equation is n. We introduce states

$$\begin{aligned}&|\phi_{\Omega,m}(\beta,\omega,\beta_1,\omega_1,\ldots,\beta_{m-1},\omega_{m-1})\rangle\\&\quad\equiv b_{\beta_{m-1}}(\omega_{m-1})\cdots b_{\beta_1}(\omega_1)b_{\beta}(\omega)|\psi\rangle,\end{aligned}\tag{15}$$

where $\Omega=\omega+\omega_1+\cdots+\omega_{m-1}$. Then, correlation functions can always be expressed in the form

$$\begin{aligned}&\mathrm{Tr}\big[\mathcal{B}_{\beta}(\omega,\nu)\cdots\mathcal{B}_{\beta_{m-1}}(\omega_{m-1},\nu_{m-1})\rho_{\mathrm{E}}\big]\\&=\big\langle\phi_{\Omega_{\mathrm{L}},m_{\mathrm{L}}}(\cdots)\big|\big[b_{\beta'}(\omega')\big]^{\nu'}\big|\phi_{\Omega_{\mathrm{R}},m_{\mathrm{R}}}(\cdots)\big\rangle,\end{aligned}\tag{16}$$

where two arguments of ϕ, β', ω', and ν' on the second line depend on β, ω, and ν on the first line. Here, we remark that $b_{\beta}^{\dagger}(\omega)=b_{\beta}(-\omega)$. Because the maximum number of b operators is n, all correlations can be expressed in the above form with $m_{\mathrm{L}},m_{\mathrm{R}}\leqslant\lfloor n/2\rfloor$. The number of states $|\phi_{\Omega,m}(\cdots)\rangle$ is $(N_{\omega}N_{\beta})^{m}$, because there are m operators b acting on $|\psi\rangle$, and each operator b has $N_{\omega}N_{\beta}$ options. Therefore, the total number of all relevant states $V_n=\{|\phi_{\Omega,m}(\cdots)\rangle\,|\,m\leqslant\lfloor n/2\rfloor\}$ is $1+N_{\omega}N_{\beta}+\cdots+(N_{\omega}N_{\beta})^{\lfloor n/2\rfloor}$, which is the upper bound of the space dimension.

We can decompose the space of relevant states according to the frequency. Because ρ_{E} is a stationary state, the correlation function in Eq. (16) is nonzero only if the summation of frequencies is zero, i.e., $\omega+\omega_1+\cdots+\omega_{m-1}=0$. Therefore, two states $|\phi_{\Omega_{\mathrm{R}},m_{\mathrm{R}}}(\cdots)\rangle$ and $|\phi_{\Omega_{\mathrm{L}},m_{\mathrm{L}}}(\cdots)\rangle$ are orthogonal if $\Omega_{\mathrm{R}}\neq\Omega_{\mathrm{L}}$. Then, the space of relevant states can be decomposed as $\mathcal{H}_{\mathrm{E}}^{\mathrm{r}}=\bigoplus_{\Omega}\mathcal{H}_{\Omega}$, where $\mathcal{H}_{\Omega}$ is the span of states $\{|\phi_{\Omega,m}(\cdots)\rangle\}$ with the frequency Ω.

VI. GENERAL ALGORITHM FOR SIMULATING THE ENVIRONMENT

The algorithm has two stages. At the first stage, we compute correlation functions of the environment and work out how to encode the environment on the quantum computer. At the second stage, we use the quantum computer to realize the time evolution driven by a Hamiltonian worked out at the first stage.

A. Classical computation

To simulate the dynamics of an open quantum system up to the nth-order expansion of the TCL equation, we compute correlation functions, $g_{\phi,\phi'}=\langle\phi|\phi'\rangle$ and $b_{\phi,\phi'}=\langle\phi|b|\phi'\rangle$, where $|\phi\rangle,|\phi'\rangle\in V_n$ and $b\in\{b_{\beta}(\omega)\}$. These correlations functions are all in the form of the last line in Eq. (16).

Using the Gram matrix $g_{\phi,\phi'}$ and Gram-Schmidt orthogonalization (see the Appendices), we can obtain a d_{E}-dimensional representation of states $|\phi\rangle$ and operators b, where $d_{\mathrm{E}}=\mathrm{rank}(g)\leqslant d_{n,\max}$ is the dimension of $\mathcal{H}_{\mathrm{E}}^{\mathrm{r}}$. Each state $|\phi\rangle\in V_n$ maps to a d_{E}-dimensional vector $|\widetilde{\phi}\rangle$, and each $b\in\{b_{\beta}(\omega)\}$ maps to a d_{E}-dimensional matrix $\widetilde{b}$. These d_{E}-dimensional vectors and matrices satisfy $\langle\widetilde{\phi}|\widetilde{\phi}'\rangle=g_{\phi,\phi'}$ and $\langle\widetilde{\phi}|\widetilde{b}|\widetilde{\phi}'\rangle=b_{\phi,\phi'}$. Then,

$$\langle\widetilde{\psi}|\widetilde{b}_m\cdots\widetilde{b}_2\widetilde{b}_1|\widetilde{\psi}\rangle=\langle\psi|b_m\cdots b_2b_1|\psi\rangle\tag{17}$$

holds for all mth-order correlation functions if $m\leqslant 2\lfloor n/2\rfloor+1$. Given $|\widetilde{\phi}\rangle$ and $\widetilde{b}$, we can simulate dynamics of the open quantum system on the quantum computer.

As with $\mathcal{H}_{\mathrm{E}}^{\mathrm{r}}$, the space of vectors $\{|\widetilde{\phi}\rangle\}$ can be decomposed in the form $\widetilde{\mathcal{H}}_{\mathrm{E}}=\bigoplus_{\Omega}\widetilde{\mathcal{H}}_{\Omega}$, where $\widetilde{\mathcal{H}}_{\Omega}$ is the span of states $\{|\widetilde{\phi}_{\Omega,m}(\cdots)\rangle\}$ with the frequency Ω, because $\langle\widetilde{\phi}_{\Omega_{\mathrm{L}},m_{\mathrm{L}}}(\cdots)|\widetilde{\phi}_{\Omega_{\mathrm{R}},m_{\mathrm{R}}}(\cdots)\rangle=0$ if $\Omega_{\mathrm{R}}\neq\Omega_{\mathrm{L}}$. We remark that $|\widetilde{\psi}\rangle$ is in the subspace $\widetilde{\mathcal{H}}_{\Omega=0}$.

B. Quantum computation

The simulation performed on the quantum computer is as follows. On the quantum computer, we use a d_{E}-dimensional Hilbert space $\widetilde{\mathcal{H}}_{\mathrm{E}}=\bigoplus_{\Omega}\widetilde{\mathcal{H}}_{\Omega}$, i.e., $N_{\mathrm{E}}=\lceil\log_2 d_{\mathrm{E}}\rceil$ qubits, to represent the environment, where $d_{\mathrm{E}}\leqslant d_{n,\max}$. We use $\widetilde{\Pi}_{\Omega}$ to denote the orthogonal projection on the subspace $\widetilde{\mathcal{H}}_{\Omega}$.

To simulate the environment, we take $\widetilde{\rho}_{\mathrm{E}}=|\widetilde{\psi}\rangle\langle\widetilde{\psi}|$,

$$\begin{aligned}\widetilde{H}_{\mathrm{E}}&=-\sum_{\Omega}\Omega\widetilde{\Pi}_{\Omega},\\\widetilde{B}_{\beta}&=\sum_{\omega}\widetilde{b}_{\beta}(\omega).\end{aligned}\tag{18}$$

On the quantum computer, we implement the time evolution with the Hamiltonian $\widetilde{H}=H_{\mathrm{S}}+\widetilde{H}_{\mathrm{E}}+\alpha\widetilde{H}_{\mathrm{I}}$ and the environment initial state $\widetilde{\rho}_{\mathrm{E}}$. Then the TCL generator of the system evolution on the quantum computer $\widetilde{\mathcal{K}}$ is the same as the generator of the dynamics to be simulated $\mathcal{K}$ up to the nth-order expansion, i.e., $\widetilde{\mathcal{K}}_m(t)=\widetilde{\mathcal{P}}\mathcal{K}_m(t)$ for all $m\leqslant n$, according to Theorem 1. The proof is given in the Appendices.

C. Discussion

We can understand the algorithm as follows. By introducing the ancillary Hilbert space $\mathcal{H}_{\mathrm{a}}$, we can write the purification of the initial state ρ_{E} as $|\psi\rangle=\sum_{\varepsilon}\sqrt{p_{\varepsilon}}|\Psi_{\varepsilon}\rangle_{\mathrm{E}}\otimes|\Phi_{\varepsilon}\rangle_{\mathrm{a}}$, where $|\Psi_{\varepsilon}\rangle_{\mathrm{E}}$ is the eigenstate of the environment with the energy ε, and both $\{|\Psi_{\varepsilon}\rangle_{\mathrm{E}}\}$ and $\{|\Phi_{\varepsilon}\rangle_{\mathrm{a}}\}$ are orthonormal. Here, we have used that ρ_{E} is a stationary state. Then, we can write the Hamiltonian of the system, environment, and ancillary system as $H'=H_{\mathrm{S}}+H_{\mathrm{E}}'+H_{\mathrm{I}}$, where $H_{\mathrm{E}}'=H_{\mathrm{E}}+H_{\mathrm{a}}$ and $H_{\mathrm{a}}=-\sum_{\varepsilon}\varepsilon|\Phi_{\varepsilon}\rangle\langle\Phi_{\varepsilon}|$. According to H', the ancillary system is decoupled from the system and environment, and $|\psi\rangle$ is an eigenstate of H_{E}' with the energy zero. Let Π_{E} be the orthogonal projection onto the relevant subspace $\mathcal{H}_{\mathrm{E}}^{\mathrm{r}}$, then $\widetilde{H}=\Pi_{\mathrm{E}}H'\Pi_{\mathrm{E}}$.

We would like to remark that the ancillary system discussed here has been included in the environment $\widetilde{H}_{\rm E}$ on the quantum computer, which are not the ancillary qubits used for realizing the evolution circuit shown in Fig. 1(b).

Similar to the second-order simulation, the initial state of the environment on the quantum computer is always a pure state, and the pure state is not the ground state, because the frequency Ω can take both positive and negative values (see Fig. 2).

VII. RELAXATION OF THE ENVIRONMENT ON THE QUANTUM COMPUTER

Usually, higher-order terms of the TCL equation are less significant, because of not only the weak coupling but also the huge energy and information capacity of the environment, i.e., the influence of the system on the environment is small. However, on the quantum computer, the environment always has a finite size. As a result, high-order terms may become significant when the evolution time is long enough, specifically when the system and the environment exchange multiple excitations and the environment becomes saturate. Therefore, in this case we need to introduce the relaxation of the environment, i.e., the dynamics implemented on the quantum computer is modified to $\frac{\partial}{\partial t}\rho(t) = -i[\widetilde{H}, \rho(t)] + \mathcal{L}_{\rm R}\rho(t)$, where the Lindblad superoperator $\mathcal{L}_{\rm R}$ acts on the environment and causes the relaxation. Evolution of such a Lindblad equation can also be implemented on the quantum computer [25–31]. In this section, we present three protocols for the environment relaxation.

Before we give relaxation protocols, we take the algorithm for the Markovian master equation simulation in Sec. IV as an example to show the impact of the finite environment. According to $\widetilde{H}$, we have $\widetilde{\mathcal{K}}_1(t) = \widetilde{\mathcal{K}}_3(t) = 0$, and $\widetilde{\mathcal{K}}_4(t)$ has four terms as shown in Eq. (3). The condition of the Markov approximation is the short correlation time $\tau_{\rm E}$ of the environment, i.e., $\langle B_\beta(t)B_{\beta'}(t-s)\rangle$ is insignificant if $s > \tau_{\rm E}$. Then, $\boldsymbol{\kappa}_2(t, t-s)$ is insignificant if $s > \tau_{\rm E}$. As a result, integrals of the last two terms in $\mathcal{K}_4(t)$ lead to $\mathcal{O}(\tau_{\rm E}^3)$. For example, the term $\boldsymbol{\kappa}_2(t,t_2)\boldsymbol{\kappa}_2(t_1,t_3)$ is significant only in the region defined by $t \geqslant t_1 \geqslant t_2, t \geqslant t_2 \geqslant t-\tau_{\rm E}$ and $t_2 \geqslant t_3 \geqslant t_1 - \tau_{\rm E}$. It is similar for $\boldsymbol{\kappa}_2(t,t_3)\boldsymbol{\kappa}_2(t_1,t_2)$. However, integrals of the second term result in $\mathcal{O}(\tau_{\rm E}^2 t)$, because $\boldsymbol{\kappa}_2(t,t_1)\boldsymbol{\kappa}_2(t_2,t_3)$ is significant if $t - t_1 \leqslant \tau_{\rm E}$, $t_2 - t_3 \leqslant \tau_{\rm E}$, but $t_1 - t_2$ can be any value. Therefore, $\mathcal{K}_4(t)$ is small only if the second term and the first term $\boldsymbol{\kappa}_4(t,t_1,t_2,t_3)$ cancel with each other, i.e., $\boldsymbol{\kappa}_4(t,t_1,t_2,t_3) \simeq \boldsymbol{\kappa}_2(t,t_1)\boldsymbol{\kappa}_2(t_2,t_3)$ when $t_1 - t_2 > \tau_{\rm E}$, which means that two excitations in the environment do not interfere with each other if they are separated by a time interval bigger than $\tau_{\rm E}$. However, in our algorithm for simulating the second-order equation, at most only one excitation can exist in the environment on the quantum computer, and the first excitation always prevents the second excitation, therefore $\widetilde{\mathcal{K}}_4(t) = \mathcal{O}(\tau_{\rm E}^2 t)$.

As an example, we consider one of 16 terms in $\widetilde{\boldsymbol{\kappa}}_4(t,t_1,t_2,t_3)$:

$$\begin{aligned}&{\rm Tr}\big[\widetilde{B}_\beta(t)\widetilde{B}_{\beta_3}(t_3)\widetilde{\rho}_{\rm E}\widetilde{B}_{\beta_2}(t_2)\widetilde{B}_{\beta_1}(t_1)\big]\\ &\quad\times A_\beta(t)A_{\beta_3}(t_3)\bullet A_{\beta_2}(t_2)A_{\beta_1}(t_1).\end{aligned}\tag{19}$$

Because at most only one excitation can exist in the environment, the contribution of the following components is nonzero [see Eq. (11)]: the $\sigma_l^\dagger(\omega)$ component of $\widetilde{B}_{\beta_3}$, the $\sigma_l(\omega)$ component of $\widetilde{B}_{\beta_2}$, the $\sigma_l^\dagger(\omega)$ component of $\widetilde{B}_{\beta_1}$ and the $\sigma_l(\omega)$ component of $\widetilde{B}_\beta$. As a result,

$$\begin{aligned}&{\rm Tr}\big[\widetilde{B}_\beta(t)\widetilde{B}_{\beta_3}(t_3)\widetilde{\rho}_{\rm E}\widetilde{B}_{\beta_2}(t_2)\widetilde{B}_{\beta_1}(t_1)\big]\\ &\quad= \big\langle B_\beta(t)B_{\beta_3}(t_3)\big\rangle \times \big\langle B_{\beta_1}(t_1)B_{\beta_2}(t_2)\big\rangle^*,\end{aligned}\tag{20}$$

which is significant if $t - t_3 \leqslant \tau_{\rm E}$. We remark that t_1 and t_2 are between t and t_3. The corresponding term in $\widetilde{\boldsymbol{\kappa}}_2(t,t_1)\widetilde{\boldsymbol{\kappa}}_2(t_2,t_3)$ is

$$\begin{aligned}&{\rm Tr}\big[\widetilde{B}_\beta(t)\widetilde{\rho}_{\rm E}\widetilde{B}_{\beta_1}(t_1)\big] \times {\rm Tr}\big[\widetilde{B}_{\beta_3}(t_3)\widetilde{\rho}_{\rm E}\widetilde{B}_{\beta_2}(t_2)\big]\\ &\quad\times A_\beta(t)A_{\beta_3}(t_3)\bullet A_{\beta_2}(t_2)A_{\beta_1}(t_1),\end{aligned}\tag{21}$$

where

$$\begin{aligned}&{\rm Tr}\big[\widetilde{B}_\beta(t)\widetilde{\rho}_{\rm E}\widetilde{B}_{\beta_1}(t_1)\big] \times {\rm Tr}\big[\widetilde{B}_{\beta_3}(t_3)\widetilde{\rho}_{\rm E}\widetilde{B}_{\beta_2}(t_2)\big]\\ &\quad= \big\langle B_\beta(t)B_{\beta_1}(t_1)\big\rangle^* \times \big\langle B_{\beta_2}(t_2)B_{\beta_3}(t_3)\big\rangle.\end{aligned}\tag{22}$$

For any value of $t_1 - t_2$, the corresponding term in $\widetilde{\boldsymbol{\kappa}}_2(t,t_1)\widetilde{\boldsymbol{\kappa}}_2(t_2,t_3)$ can be significant. Therefore, $\widetilde{\boldsymbol{\kappa}}_4(t,t_1,t_2,t_3) \simeq \widetilde{\boldsymbol{\kappa}}_2(t,t_1)\widetilde{\boldsymbol{\kappa}}_2(t_2,t_3)$ does not hold when $t_1 - t_2 > \tau_{\rm E}$.

Next, we show that $\widetilde{\mathcal{K}}_4(t)$ can be suppressed by introducing the environment relaxation.

A. Reinitialization protocol

A way to realize the environment relaxation is the periodic reinitialization of the environment state at time $j\tau$, where τ is the period and j is an integer [5,6]. In such a protocol, correlation functions on the quantum computer with $m \leqslant n$ are significantly modified by the relaxation and become

$$\begin{aligned}&{\rm Tr}\big[\widetilde{\mathcal{B}}_\beta(t,\nu)\cdots\widetilde{\mathcal{B}}_{\beta_{m-1}}(t_{m-1},\nu_{m-1})\widetilde{\rho}_{\rm E}\big]\\ &\quad= {\rm Tr}\big[\mathcal{B}_\beta(t,\nu)\mathcal{V}_1\cdots\mathcal{V}_{m-1}\mathcal{B}_{\beta_{m-1}}(t_{m-1},\nu_{m-1})\rho_{\rm E}\big],\end{aligned}\tag{23}$$

where $\mathcal{V}_i = [\mathbb{1}]$ if t_{i-1} ($t_0 = t$) and t_i are in the same period, i.e., $(j+1)\tau > t_{i-1} \geqslant t_i > j\tau$ for any integer j, otherwise $\mathcal{V}_i = \mathcal{P}$. Here, $\mathcal{P}$ is the projection onto the state $\rho_{\rm E}$, $\mathbb{1}$ is the identity operator, and $[U]\rho = U\rho U^\dagger$.

For two-time correlation functions, $\langle\widetilde{B}_\beta(t)\widetilde{B}_{\beta'}(s)\rangle = \langle B_\beta(t)B_{\beta'}(s)\rangle$ only if t and s are in the same period, otherwise it is zero. We note that even if t and s are close, the two-time correlation function is zero if they are in different periods. Because of the reinitialization, $\widetilde{\boldsymbol{\kappa}}_4(t,t_1,t_2,t_3) = \widetilde{\boldsymbol{\kappa}}_2(t,t_1)\widetilde{\boldsymbol{\kappa}}_2(t_2,t_3)$ if $t_1 - t_2 > \tau$, therefore the fourth-order term is suppressed to $\widetilde{\mathcal{K}}_4(t) = \mathcal{O}(\tau_{\rm E}^2\tau)$.

B. Projective dissipation protocol

We can implement the environment reinitialization stochastically at a constant rate of Γ, i.e., the corresponding Lindblad superoperator is $\mathcal{L}_{\rm R} = \Gamma(\widetilde{\mathcal{P}} - [\mathbb{1}])$. With such a relaxation term, correlation functions on the quantum computer with $m \leqslant n$ can also be expressed in the form of Eq. (23), but $\mathcal{V}_i = e^{-\Gamma s_i}[\mathbb{1}] + (1 - e^{-\Gamma s_i})\mathcal{P}$, where $s_i = t_{i-1} - t_i$. We remark that $\mathcal{L}_{\rm R}$ and the environment Hamiltonian $-i[\widetilde{H}_{\rm E}, \bullet]$ are commutative, because $\widetilde{\rho}_E$ is a stationary state.

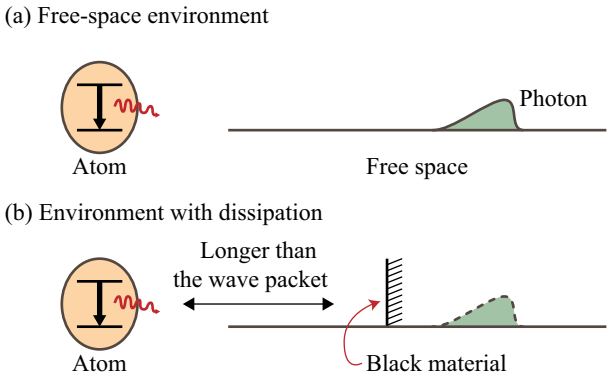

FIG. 3. An example of dissipation caused by the environment. (a) An atom coupled to the free space in the vacuum state. (b) A black material is placed at a distance from the atom and absorbs photons.

Using the projective dissipation protocol, two-time correlation functions become $\langle \widetilde{B}_\beta(t)\widetilde{B}_{\beta'}(s)\rangle = e^{-\Gamma(t-s)}\langle B_\beta(t)B_{\beta'}(s)\rangle$.

In some cases, correlation functions can be exactly reproduced on the quantum computer even with the presence of environment dissipation $\mathcal{L}_R$. For the second-order equation simulation, if Fourier transformations of $e^{\Gamma(t-s)}\langle B_\beta(t)B_{\beta'}(s)\rangle$ yield a set of positive matrices $\gamma(\omega)$, we can choose coefficients $g_{\beta,l}(\omega)$ according to $e^{\Gamma(t-s)}\langle B_\beta(t)B_{\beta'}(s)\rangle$, so that $\langle \widetilde{B}_\beta(t)\widetilde{B}_{\beta'}(s)\rangle = \langle B_\beta(t)B_{\beta'}(s)\rangle$ when the dissipation is introduced. It is similar for higher-order equation simulations.

If correlation functions cannot be exactly reproduced, we may need to take $\Gamma \ll \tau_E^{-1}$, so that correlation functions are not significantly modified. The relaxation time of the environment is Γ^{-1}. Therefore excitations in the environment do not interfere with each other if they are separated by a time interval bigger than Γ^{-1}, i.e., $\widetilde{\mathcal{K}}_4(t) = \mathcal{O}(\tau_E^2\Gamma^{-1})$ in the second-order equation simulation.

C. Conditional projective dissipation protocol

An optimal dissipation protocol relaxes the environment as soon as possible but does not modify correlations functions. Here we present such an environment dissipation protocol motivated by a typical open quantum system, an atom coupled to the free space in the vacuum state as shown in Fig. 3(a). The excited state of the atom decays into the ground state by emitting a photon into the free space. Because once the photon is emitted it leaves the atom and never comes back, the decay is irreversible. The correlation time depends on the length of the photon wave packet, because once the wave packet is out of the reach of the coupling the photon cannot affect the atom anymore. Therefore, if a black material is placed at a finite but sufficient distance from the atom and absorbs photons [see Fig. 3(b)], the black material does not affect the evolution of the atom (neglecting the radiation from the material). We are interested in cases that the correlation time is short compared with the coupling between the system and environment, so that the expansion of the TCL master equation is reasonable. We find that when the correlation time is short only a subspace of the correlation-relevant state space $\mathcal{H}_E^r$ effectively contributes to correlation functions. Therefore, we can let the environment evolve without dissipation within the subspace, i.e., the left side of the black material, and the environment dissipates once its state is out of the subspace, i.e., the right side of the black material.

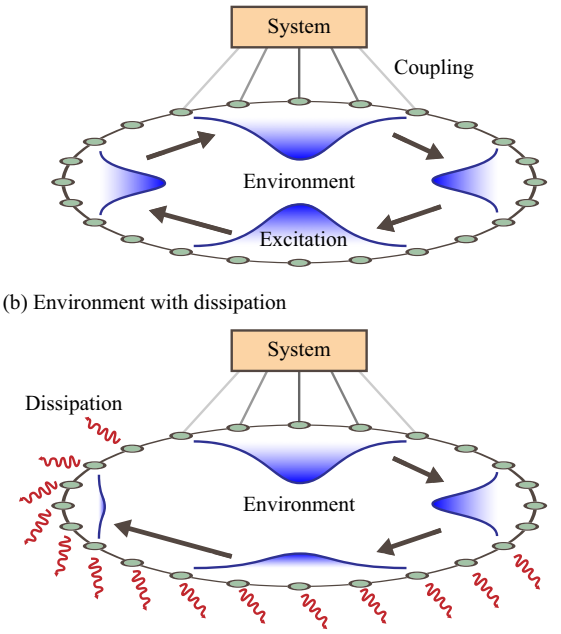

FIG. 4. Simulation of the second-order equation. (a) The system is coupled to the environment via local interaction. Without dissipation, an excitation in the environment leaves the interaction region but never disappears. (b) The dissipation is switched on in the region without interaction. The excitation disappears when it leaves the interaction region.

First, we consider the second-order equation simulation. We will generalize the protocol to higher-order equation simulations later. For the second-order equation simulation, we show that using the conditional dissipation protocol the environment relaxes in the time scale $\sim\tau_E$, but two-time correlation functions are only slightly modified.

Suppose that the environment spectrum is discretized with the uniform spacing $\delta\omega$, then each frequency ω corresponds to an integer k and $\omega = k\delta\omega$. We apply the Fourier transformation to states $|\omega, l\rangle$ and define $|x, l\rangle \equiv \frac{1}{\sqrt{N_\omega}}\sum_\omega e^{-i\frac{\omega x}{c}}|\omega, l\rangle$, where $c = \frac{N_\omega\delta_\omega}{2\pi}$ and $x = 0, \ldots, N_\omega - 1$. These states form a ring as shown in Fig. 4. For a wave packet in the form $\sum_x a_x|x, l\rangle$, the evolution driven by $\widetilde{H}_E$ transports the wave packet along the ring [see Fig. 4(a)], i.e., $e^{-i\widetilde{H}_E t}(\sum_x a_x|x, l\rangle) = \sum_x a_x|x + ct, l\rangle$ when ct is an integer. Here $|x + N_\omega\rangle \equiv |x\rangle$. Therefore, the evolution is periodic, and the period is $\frac{N_\omega}{c} = \frac{2\pi}{\delta\omega}$.

We would like to note that, using the uniformly discretized spectrum on the quantum computer, two-time correlation functions with $s = t - t_1$ in the interval $[0, \frac{2\pi}{\delta\omega}]$ are reproduced in the form of a Fourier series, which converges as $N_\omega \to \infty$. The optimal range of k depends on correlation functions. Without loss of generality, we suppose N_ω is odd, and we take $k = -\frac{N_\omega-1}{2}, \ldots, 0, 1, \ldots, \frac{N_\omega-1}{2}$.

In the x representation, we can reexpress interaction operators as

$$\widetilde{B}_\beta = \sum_{x,l} g_{\beta,l}(x)\sigma_l(x) + \text{H.c.}, \tag{24}$$

where $\sigma_l(x) \equiv |v\rangle\langle x, l|$ and

$$g_{\beta,l}(x) = \frac{1}{\sqrt{N_\omega}} \sum_\omega e^{-i\frac{2\pi kx}{N_\omega}} g_{\beta,l}(\omega). \tag{25}$$

Therefore, $\widetilde{B}_\beta|v\rangle = \sum_{x,l} g^*_{\beta,l}(x)|x, l\rangle$ is a wave packet in the x space. Without the dissipation, the correlation function

$$\langle \widetilde{B}_\beta(t)\widetilde{B}_{\beta'}(t-s)\rangle = \langle v|\widetilde{B}_\beta e^{-i\widetilde{H}_E s}\widetilde{B}_{\beta'}|v\rangle \tag{26}$$

is the overlap between two wave packets $\widetilde{B}_\beta|v\rangle$ and $e^{-i\widetilde{H}_E s}\widetilde{B}_{\beta'}|v\rangle$.

If $\beta = \beta'$, the correlation function is maximized at $s = 0$. The second wave packet moves in the x space with the speed c without dispersion. As a result, the correlation function decreases with the time s. The correlation function vanishes at $s \sim \tau_E$, which implies that the wave packet is localized in the x space with the width $x_E \equiv c\tau_E$. Because the wave packet is created by the coupling, the coupling strength $g_{\beta,l}(x)$ is also localized in the x space with the same width as shown in Fig. 4. The localized coupling means that the matrix $\gamma(\omega)$ varies slowly with the frequency ω. In the following, we assume that the coupling is localized in the region $0 \leqslant x \leqslant x_E$, which is reasonable when the system is coupled to the environment via local interactions.

The conditional dissipation protocol works as follows. In the region $0 \leqslant x \leqslant x_T$, where $x_T \geqslant x_E$, a wave packet propagates freely without dissipation, such that two-time correlation functions can be reproduced. We remark that two-time correlation functions are only determined by the wave packet in the region $0 \leqslant x \leqslant x_E$. In the region $x > x_T$, the excitation decays at the rate of Γ, and the environment is stochastically reinitialized to the state $|v\rangle$.

To implement the conditional dissipation, at the rate of Γ we perform a measurement to find out whether the environment is in states with $x > x_T$, i.e., the projection $\Pi = \sum_{x>x_T,l} \sigma_l(x)^\dagger\sigma_l(x)$. The environment reinitialization is implemented depending on the measurement outcome. The corresponding Lindblad superoperator reads $\mathcal{L}_R = \Gamma(\widetilde{\mathcal{P}}[\Pi] + [\mathbb{1} - \Pi] - [\mathbb{1}])$. Because of the dissipation, the wave packet disappears before the revival. When the wave packet disappears, the environment is reinitialized, and the next excitation can enter the environment.

The dissipation may cause quantum Zeno effect, which can prevent the wave packet from entering the dissipation region $x > x_T$. The propagation from $|x\rangle$ to $|x+1\rangle$ takes the time $c^{-1} = \frac{2\pi}{N_\omega\delta\omega}$. Therefore, the quantum Zeno effect is weak if $\Gamma \ll c$. Here, c^{-1} corresponds to the time resolution of the environment. When the time resolution is fine, we should have $\tau_E \gg c^{-1}$. In this case, we can take $\Gamma = \tau_E^{-1}$ and $x_T = x_E$, such that excitations in the environment do not interfere with each other if they are separated by a time interval bigger than τ_E, i.e., $\mathcal{K}_4(t) = \mathcal{O}(\tau_E^3)$.

As an example, let us consider a simple case that the interaction Hamiltonian of the system and environment consists of only one term, reading $\widetilde{H}_I = \alpha A \otimes \widetilde{B}$, with

$$\widetilde{B} = \sum_\omega [g(\omega)|\omega\rangle\langle v| + g^*(\omega)|v\rangle\langle\omega|], \tag{27}$$

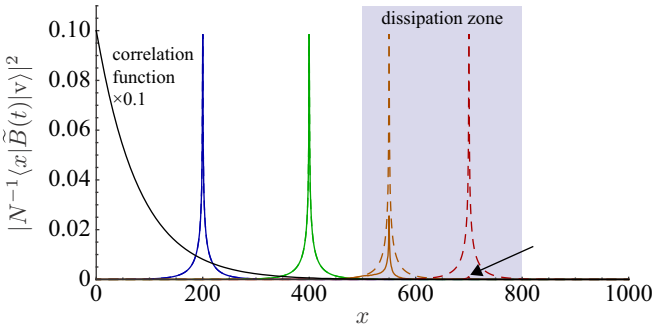

FIG. 5. Numerical results for the wave packet $N^{-1}\widetilde{B}(t)|v\rangle$, where $N = \|\widetilde{B}(0)|v\rangle\|$, i.e., the wave packet is normalized at $t = 0$. The probability in the state $|x\rangle$ is plotted. We take $N_\omega = 1001$, $\delta\omega = 0.001$, $\Gamma = 0.004$, and $\bar{\gamma} = 0.002$. The conditional dissipation is introduced between $x = 500$ and 800. The wave packet initializes at $x = 0$ when $t = 0$. From left to right, the blue, green, yellow, and red solid curves correspond to time $t = (200, 400, 550, 700) \times 2\pi/N_\omega\delta\omega$, respectively. The wave packet is computed using the quantum trajectory approach [39,40], and each curve is obtained with 1000 instances. For comparison, dashed curves denote the wave packet when the dissipation is turned off. The black curve represents the correlation function $e^{-\bar{\gamma}|s|}$ with $s = x/c$, which vanishes at about $x = 300$. Therefore, the wave packet centered at $x > 300$ does not contribute to the correlation function. The wave packet vanishes (see the arrow) after it enters the dissipation zone (marked in gray).

where the environment spectrum is discretized with the uniform spacing $\delta\omega$, and $g(\omega) = a\sqrt{\frac{2\bar{\gamma}}{\omega^2+\bar{\gamma}^2}\frac{\delta\omega}{2\pi}}$, where a and $\bar{\gamma}$ are constants with the dimensions of frequency. With such an environment, the reconstructed correlation function is $\langle\widetilde{B}(t)\widetilde{B}(t-s)\rangle = a^2e^{-\bar{\gamma}|s|}$ in the limit $N_\omega \to \infty$. In Fig. 5, we plot the wave packet $\widetilde{B}|v\rangle$ in the x space with the conditional dissipation. One can see that the wave packet travels freely from left to right, until it enters the dissipation zone in which it quickly diminishes.

D. Conditional reinitialization

To avoid the quantum Zeno effect, we can replace the continuous-time dissipation with periodic conditional reinitialization. The Lindblad superoperator becomes time dependent and reads $\mathcal{L}_R = \Gamma(t)(\widetilde{\mathcal{P}}[\Pi] + [\mathbb{1} - \Pi] - [\mathbb{1}])$, where $\Gamma(t) = +\infty$ when $t = jc^{-1}$, $\Gamma(t) = 0$ when $t \neq jc^{-1}$, and j is an integer. In other words, a wave packet can propagate freely in each time interval with the length c^{-1}, i.e., the wave packet can propagate by one site in the x space, and at each time $t = jc^{-1}$ the environment is conditionally reinitialized by implementing the operation $\widetilde{\mathcal{P}}[\Pi] + [\mathbb{1} - \Pi]$. In this way, without affecting the propagation of the wave packet in the region $x \leqslant x_E$, the environment relaxes in the time scale τ_E. Here we take $x_T = x_E$.

Generalization to the higher-order simulations

In this section, we discuss how to generalize the conditional dissipation (or reinitialization) protocol to higher-order simulations. For environments similar to the case in Fig. 3, the system only affects the part of the environment close to it, its influence (excitations) propagates in the environment, and

the part close to the system relaxes in the time scale $\tau_{\rm E}$, i.e., correlations

$$\Delta = {\rm Tr}\big[\cdots \mathcal{B}_{\beta_i}(t_i,\nu_i)\mathcal{B}_{\beta_{i+1}}(t_{i+1},\nu_{i+1})\cdots\rho_{\rm E}\big] - {\rm Tr}\big[\cdots \mathcal{B}_{\beta_i}(t_i,\nu_i)\mathcal{P}\mathcal{B}_{\beta_{i+1}}(t_{i+1},\nu_{i+1})\cdots\rho_{\rm E}\big] \quad (28)$$

are negligible when $t_i - t_{i+1} > \tau_{\rm E}$. We remark that because correlation functions are reproduced it is the same for the environment on the quantum computer. For such environments, the reinitialization operation $\mathcal{P}$ on $[e^{-iH_{\rm E}s}]\mathcal{B}_{\beta_{i+1}}(t_{i+1},\nu_{i+1})\cdots\rho_{\rm E}$ does not affect correlation functions. Here $s > \tau_{\rm E}$, and $[e^{-iH_{\rm E}s}]$ is the superoperator denoting the free evolution of the environment. To implement the condition dissipation, we need to find the proper projection Π representing the space of states in which the influence of the system has left the interaction region.

As an example, we consider the fourth-order simulation using the environment on the quantum computer given by

$$\widetilde{H}_{\rm E} = \sum_{\omega}\omega|\omega\rangle\langle\omega| + \sum_{\omega_1,\omega_2}(\omega_1+\omega_2)|\omega_1,\omega_2\rangle\langle\omega_1,\omega_2| \quad (29)$$

and

$$\widetilde{B}_\beta = \sum_{\omega} g_{\beta,\omega}|v\rangle\langle\omega| + \sum_{\omega,\omega_1,\omega_2} g_{\beta,\omega,\omega_1,\omega_2}|\omega\rangle\langle\omega_1,\omega_2| + {\rm H.c.} \quad (30)$$

Here, $|v\rangle$ denotes the vacuum state and the initial state of the environment, i.e., $\widetilde{\rho}_{\rm E} = |v\rangle\langle v|$, $|\omega\rangle$ denotes the state of one excitation with the frequency ω, and $|\omega_1,\omega_2\rangle$ denotes the state of two excitations with frequencies ω_1 and ω_2, respectively. By choosing coupling coefficients $g_{\beta,\omega}$ and $g_{\beta,\omega,\omega_1,\omega_2}$, we can reproduce some reservoir correlation functions (see the Appendices). The general algorithm for higher-order simulations is given in Sec. VI.

Correlation functions reproduced in the environment given by Eqs. (29) and (30) are

$$\langle v|\widetilde{B}_\beta(s)\widetilde{B}_{\beta_1}(s_1)|v\rangle = \sum_{\omega} e^{-i\omega(s-s_1)} g_{\beta,\omega}g^*_{\beta_1,\omega}, \quad (31)$$

$$\langle v|\widetilde{B}_\beta(s)\widetilde{B}_{\beta_1}(s_1)\widetilde{B}_{\beta_2}(s_2)|v\rangle = 0, \quad (32)$$

and

$$\langle v|\widetilde{B}_\beta(s)\widetilde{B}_{\beta_1}(s_1)\widetilde{B}_{\beta_2}(s_2)\widetilde{B}_{\beta_3}(s_3)|v\rangle = \langle v|\widetilde{B}_\beta(s)\widetilde{B}_{\beta_1}(s_1)|v\rangle\langle v|\widetilde{B}_{\beta_2}(s_2)\widetilde{B}_{\beta_3}(s_3)|v\rangle + \sum_{\omega,\omega',\omega_1,\omega_2} e^{-i\omega'(s-s_1)}e^{-i(\omega_1+\omega_2)(s_1-s_2)}e^{-i\omega(s_2-s_3)} \times g_{\beta,\omega'}g_{\beta_1,\omega',\omega_1,\omega_2}g^*_{\beta_2,\omega,\omega_1,\omega_2}g^*_{\beta_3,\omega}. \quad (33)$$

Similar to the second-order simulation, we suppose that the environment is discretized with the uniform spacing δ, i.e., $\omega,\omega_1,\omega_2 = k\delta\omega$ and $k = -\frac{N_\omega-1}{2},\ldots,0,1,\ldots,\frac{N_\omega-1}{2}$. Then, by applying the Fourier transformation, we have

$$|x\rangle \equiv \frac{1}{\sqrt{N_\omega}}\sum_{\omega} e^{-i\frac{2\pi\omega x}{N_\omega\delta\omega}}|\omega\rangle, \quad (34)$$

$$|x_1,x_2\rangle \equiv \frac{1}{N_\omega}\sum_{\omega_1,\omega_2} e^{-i\frac{2\pi(\omega_1x_1+\omega_2x_2)}{N_\omega\delta\omega}}|\omega_1,\omega_2\rangle. \quad (35)$$

In the x representation,

$$\widetilde{B}_\beta = \sum_x g_{\beta,x}|v\rangle\langle x| + \sum_{x,x_1,x_2} g_{\beta,x,x_1,x_2}|x\rangle\langle x_1,x_2| + {\rm H.c.}, \quad (36)$$

where

$$g_{\beta,x} = \frac{1}{\sqrt{N_\omega}}\sum_{\omega} e^{-i\frac{2\pi\omega x}{N_\omega\delta\omega}} g_{\beta,\omega},$$

$$g_{\beta,x,x_1,x_2} = \frac{1}{N_\omega^{\frac{3}{2}}}\sum_{\omega,\omega_1,\omega_2} e^{i\frac{2\pi(\omega x-\omega_1x_1-\omega_2x_2)}{N_\omega\delta\omega}} g_{\beta,\omega,\omega_1,\omega_2}. \quad (37)$$

If we only consider correlation functions at discretized times, i.e., cs, cs_1, cs_2, cs_3 are integers, two-time and four-time correlation functions are

$$\langle v|\widetilde{B}_\beta(s)\widetilde{B}_{\beta_1}(s_1)|v\rangle = \sum_x g_{\beta,x+c(s-s_1)}g^*_{\beta_1,x} \quad (38)$$

and

$$\langle v|\widetilde{B}_\beta(s)\widetilde{B}_{\beta_1}(s_1)\widetilde{B}_{\beta_2}(s_2)\widetilde{B}_{\beta_3}(s_3)|v\rangle = \langle v|\widetilde{B}_\beta(s)\widetilde{B}_{\beta_1}(s_1)|v\rangle\langle v|\widetilde{B}_{\beta_2}(s_2)\widetilde{B}_{\beta_3}(s_3)|v\rangle + \sum_{x,x',x_1,x_2} g_{\beta,x'+c(s-s_1)}g_{\beta_1,x',x_1+c(s_1-s_2),x_2+c(s_1-s_2)} \times g^*_{\beta_2,x+c(s_2-s_3),x_1,x_2}g^*_{\beta_3,x}. \quad (39)$$

Three-time correlation functions are zero.

Correlations in Eq. (28) are negligible if the system is only coupled to environment states $|x\rangle$ and $|x_1,x_2\rangle$ with $x,x_2 = 0,\ldots,x_{\rm E}$, where $x_{\rm E} = c\tau_{\rm E}$. We have $\Delta = 0$ if $g_{\beta,x} = 0$ when $x > x_{\rm E}$, $g_{\beta,x,x_1,x_2} = 0$ when $x_2 > x_{\rm E}$, and $g_{\beta,x,x_1,x_2} = \delta_{x,x_1}g_{\beta,x_2}$ when $x,x_1 > x_{\rm E}$. This is obvious for two-time correlation functions. For four-time correlation functions, considering values of ν [see Eq. (5)], there are 16 of them, but only four of them are independent, which are

$$\langle v|\widetilde{B}_\beta(t)\widetilde{B}_{\beta_1}(t_1)\widetilde{B}_{\beta_2}(t_2)\widetilde{B}_{\beta_3}(t_3)|v\rangle,$$
$$\langle v|\widetilde{B}_{\beta_1}(t_1)\widetilde{B}_\beta(t)\widetilde{B}_{\beta_2}(t_2)\widetilde{B}_{\beta_3}(t_3)|v\rangle,$$
$$\langle v|\widetilde{B}_{\beta_2}(t_2)\widetilde{B}_\beta(t)\widetilde{B}_{\beta_1}(t_1)\widetilde{B}_{\beta_3}(t_3)|v\rangle,$$
$$\langle v|\widetilde{B}_{\beta_2}(t_2)\widetilde{B}_{\beta_1}(t_1)\widetilde{B}_\beta(t)\widetilde{B}_{\beta_3}(t_3)|v\rangle, \quad (40)$$

where $t \geqslant t_1 \geqslant t_2 \geqslant t_3$. We can check that $\Delta = 0$ for all of them. Here, we have assumed that $N_\omega \gg x_{\rm E}$. Therefore, to implement the conditional dissipation, we can take the projection $\Pi = \sum_{x>x_{\rm E}}|x\rangle\langle x| + \sum_{x_1}\sum_{x_2>x_{\rm E}}|x_1,x_2\rangle\langle x_1,x_2|$.

VIII. CIRCUIT IMPLEMENTATION, TIME COST, AND HARDWARE RESOURCE REQUIREMENT

Given the Hamiltonian $\widetilde{H}$, an initial state of the system $\rho_{\rm S}(0)$, and the initial state of the environment $\widetilde{\rho}_{\rm E}$, we can implement the unitary dynamics $\rho(t) = e^{-i\widetilde{H}t}\rho_{\rm S}(0)\otimes\widetilde{\rho}_{\rm E}e^{i\widetilde{H}t}$ on the quantum computer. Then, $\rho(t)$ is a solution of the evolution equation $\frac{\partial}{\partial t}\widetilde{\mathcal{P}}\rho(t) = \widetilde{\mathcal{K}}(t)\widetilde{\mathcal{P}}\rho(t)$. According to discussions in the previous section, $\widetilde{\mathcal{K}}(t)$ and $\mathcal{K}(t)$ are the same up to the nth-order expansion.

We can implement the dynamics of $\widetilde{H}$ using the Trotterization algorithm [4]. Let $N_{\rm S}$ be the number of qubits

representing the system, then the total number of qubits used in the simulation is $N_{\rm S}+N_{\rm E}$. System operators can always be expanded using Pauli operators as $H_{\rm S}=\sum_{\sigma\in S_H} f_{H,\sigma}\sigma$ and $A_\beta=\sum_{\sigma\in S_\beta} f_{\beta,\sigma}\sigma$. Here, S_H and S_β are subsets of $N_{\rm S}$-qubit Pauli operators. Similarly, environment operators can also be expanded using Pauli operators as $\widetilde{H}_{\rm E}=\sum_{\sigma\in E_H} h_{H,\sigma}\sigma$ and $\widetilde{B}_\beta=\sum_{\sigma\in E_\beta} h_{\beta,\sigma}\sigma$. Here, E_H and E_β are subsets of $N_{\rm E}$-qubit Pauli operators. Expansion coefficients f and h are all real, because these expanded operators are all Hermitian. Using Trotterization, the evolution implemented on the quantum computer is

$$U_{N_{\rm T}}=\prod_{i=1}^{N_{\rm T}}\left[\left(\prod_{\sigma\in S_H} e^{-i\sigma\frac{f_{H,\sigma}t}{N_{\rm T}}}\right)\otimes\left(\prod_{\sigma'\in E_H} e^{-i\sigma'\frac{h_{H,\sigma'}t}{N_{\rm T}}}\right)\right]\times\left(\prod_{\beta}\prod_{\sigma\in S_\beta}\prod_{\sigma'\in E_\beta} e^{-i\sigma\otimes\sigma'\frac{\alpha f_{\beta,\sigma}h_{\beta,\sigma'}t}{N_{\rm T}}}\right),\tag{41}$$

where $N_{\rm T}$ is the number of Trotter steps, and each exponential of the k-qubit Pauli operator can be implemented on the quantum computer with up to $2(k-1)$ controlled-NOT gates and $2k+1$ single-qubit gates [41]. Therefore, the total number of gates $N_{\rm G}$ is less than $[(4N_{\rm S}-1)|S_H|+(4N_{\rm E}-1)|E_H|+(4N_{\rm S}+4N_{\rm E}-1)\sum_\beta|S_\beta||E_\beta|]N_{\rm T}$.

The Trotter-Suzuki decomposition is approximate, and the difference between $U_{N_{\rm T}}$ and $e^{-i\widetilde{H}}$ is

$$\epsilon_{\rm Trotter}=\left\|U_{N_{\rm T}}-e^{-i\widetilde{H}}\right\|\sim\frac{N_{\rm terms}\|\widetilde{H}\|^2t^2}{N_{\rm T}},\tag{42}$$

where $\|\bullet\|$ denotes the operator norm, and $N_{\rm terms}=|S_H|+|E_H|+\sum_\beta|S_\beta||E_\beta|$ is the number of terms in the Hamiltonian. We can prove that $\|\widetilde{B}_\beta\|\leqslant\|B_\beta\|$ (see the Appendices), therefore the norm of the Hamiltonian has the upper bound

$$\|\widetilde{H}\|\leqslant\|H_{\rm S}\|+n\times\max\{|\omega|\}+\alpha\sum_\beta\|A_\beta\|\|B_\beta\|.\tag{43}$$

Here, $\max\{|\omega|\}\sim\|H_{\rm E}\|$. However, usually it is sufficient to truncate the frequency at $\max\{|\omega|\}\sim\|H_{\rm S}\|$ when the coupling is weak.

Usually, for a Hamiltonian with local interactions, the number of terms in the Hamiltonian, i.e., each of $|S_H|$, $|S_\beta|$, and N_β, is a polynomial with respect to the system size $N_{\rm S}$.

The number of qubits required for simulating the environment is $N_{\rm E}\sim\lfloor\frac{n}{2}\rfloor\log_2(N_\omega N_\beta)$, because $d_{\rm E}\sim(N_\omega N_\beta)^{\lfloor\frac{n}{2}\rfloor}$. According to the maximum number of environment Pauli operators, we have $|E_H|,|E_\beta|\sim 4^{N_{\rm E}}\sim(N_\omega N_\beta)^n$.

To implement the conditional dissipation, we may need to introduce only one more qubit for the measurement of Π, i.e., we can use the state $|1\rangle$ of the qubit to indicate the subspace. Because the conditional dissipation operation is performed at a low rate, the cost of the gate number is small compared with the unitary evolution.

In summary, the simulation requires $N_{\rm E}\sim\lfloor\frac{n}{2}\rfloor\log_2(N_\omega N_\beta)$ qubits to simulate the environment. The number of terms in the Hamiltonian is $N_{\rm terms}=\mathcal{O}(N_\omega^n N_\beta^n)$. Then, we need the number of Trotter steps to be $N_{\rm T}\sim N_{\rm terms}\|\widetilde{H}\|^2t^2/\epsilon_{\rm Trotter}=\mathcal{O}(N_\omega^n N_\beta^{n+1})$. Therefore the total number of gates is $N_{\rm G}=\mathcal{O}(N_{\rm E}N_\omega^{2n}N_\beta^{2n+2})$. We note that a variety of methods have been developed to reduce the gate number in the Trotterization algorithm [22–24], which could be applied in our case.

In our algorithm, the system size can easily exceed the environment size. For example, to simulate the quantum master equation with $n=2$, considering an environment with 1×10^6 discretized frequencies ($N_\omega=10^6$) and 1000 interaction terms ($N_\beta=10^3$), we only need about 30 qubits for encoding the environment, which is even smaller than the system in a nontrivial quantum simulation problem (with above 50 qubits).

IX. THERMALIZATION OF A QUBIT ON A QUANTUM COMPUTER

Let us consider the thermalization of a qubit at zero temperature and finite temperature. The system Hamiltonian is $\widetilde{H}_{\rm S}=-\frac{\Delta}{2}\sigma^{\rm z}$. The system is coupled to the environment via only one term, i.e., $\widetilde{H}_{\rm I}=\alpha A\otimes\widetilde{B}$, where $A=\sigma^{\rm x}$, and $\widetilde{B}$ is the same as in Eq. (27), but coupling coefficients are [42]

$$g(\omega)=\begin{cases}\sqrt{a\bar{\gamma}\frac{|\omega|\bar{\gamma}}{\omega^2+\bar{\gamma}^2}}, & \omega\geqslant0,\\ \sqrt{a\bar{\gamma}\frac{|\omega|\bar{\gamma}e^{\beta\omega}}{\omega^2+\bar{\gamma}^2}}, & \omega<0.\end{cases}\tag{44}$$

Here, $\beta=1/k_{\rm B}T$ is the temperature, and a and $\bar{\gamma}$ are constants with the dimensions of frequency. We take $\rho_{\rm S}(0)=|+\rangle\langle+|$ as the initial state of the qubit, and $|+\rangle=\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)$.

In Fig. 6, we plot the probability in the ground state $p_{\rm g}=\langle0|\rho_{\rm S}(t)|0\rangle$, where $\rho_{\rm S}(t)$ is the state of the qubit at time t. When the simulated environment is at zero temperature, i.e., $\beta\to+\infty$, the qubit evolves into the ground state $|0\rangle$, i.e., $p_{\rm g}$ goes to 1. When the temperature is finite, the probability approaches a finite value and coincides with the thermal

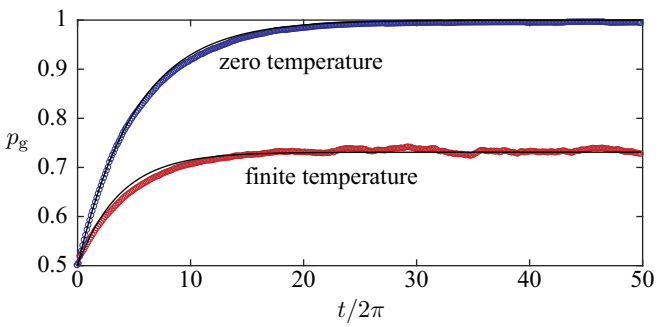

FIG. 6. Probability in the ground state, $p_{\rm g}$. We take $\Delta=1$, $\alpha\sqrt{a}=0.01$, $\bar{\gamma}=10$, $\delta\omega=0.02$, $N_\omega=401$. The dissipation of the environment is introduced using the condition reinitialization protocol (see the end of Sec. VII C). The probabilities $p_{\rm g}$ for zero temperature (blue circles) and finite temperature ($\beta=1$, red circles) are computed using the quantum trajectory approach [39,40]. We take 1000 instances for zero temperature and 5000 instances for finite temperature. The dissipation zone is $21\leqslant x\leqslant380$ for zero temperature; further moving the dissipation zone towards $x=0$ (e.g., taking the dissipation zone $11\leqslant x\leqslant390$) will change the correlation function. The dissipation zone is $3\leqslant x\leqslant398$ for finite temperature, which is chosen to obtain the best fit to the Lindblad equation of the thermalization. Black curves represent the result of the corresponding Lindblad equation of the thermalization.

distribution. For comparison, we also plotted the probability in the evolution driven by the corresponding Lindblad equation of thermalization [2]. The difference between the environment-simulation result and the Lindblad equation result is due to the discretization of the environment spectrum and approximations used to derive the Lindblad equation, including neglecting high-order terms in the TCL equation and the Markovian approximation.

X. CONCLUSIONS

In this paper, we propose a hardware-efficient quantum algorithm to simulate the TCL master equation up to any finite order. It is achieved by reproducing reservoir correlation functions using a minimized Hilbert space. The number of qubits representing the environment is $\sim\lfloor\frac{n}{2}\rfloor\log_2(N_\omega N_\beta)$ in the nth-order simulation. We remark that $n=2$ in the simulation of the Markovian quantum master equation and thermalization. In our algorithm, the system size can easily exceed the environment size, e.g., when the system has tens of qubits. Because the environment on the quantum computer is small, it needs to be reinitialized in the simulation of a long-time evolution. We also propose an efficient reinitialization protocol without significantly changing reservoir correlation functions. We illustrate our algorithm by using a classical computer and numerically simulate the thermalization of a qubit at zero and finite temperatures. Our results pave the way for practical quantum open-system simulation on a universal quantum computer.

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APPENDIX A: GRAM-SCHMIDT ORTHOGONALIZATION

In this section, we explicitly present the Gram-Schmidt orthogonalization process. We have $d_{n,\max}$ vectors $V_n=\{|\phi_{\Omega,m}(\cdots)\rangle\}$ in $\mathcal{H}_{\rm E}^{\rm r}$, where $m\leqslant\lfloor n/2\rfloor$. We label these vectors as $|\phi_1\rangle,\ldots,|\phi_{d_{n,\max}}\rangle$. Without loss of generality, we take $|\phi_1\rangle=|\psi\rangle$, which can simplify the preparation of the environment initial state on the quantum computer, and we assume that states from $|\phi_1\rangle$ to $|\phi_{d_{\rm E}}\rangle$ are linearly independent. We note that g is a $d_{n,\max}$-dimensional matrix with rank $d_{\rm E}$. The state $|\psi\rangle$ is normalized, therefore we take $|e_1\rangle=|\phi_1\rangle$. Then, we can obtain $d_{\rm E}$ orthonormal basis states by iterating

$$|e_i\rangle=\frac{|\phi_i\rangle-\sum_{j=1}^{i-1}|e_j\rangle\langle e_j|\phi_i\rangle}{\||\phi_i\rangle-\sum_{j=1}^{i-1}|e_j\rangle\langle e_j|\phi_i\rangle\|}. \tag{A1}$$

Given $|e_j\rangle=\sum_{\phi\in V_n}e_{j,\phi}|\phi\rangle$, we compute the overlap using $\langle e_j|\phi_i\rangle=\sum_{\phi\in V_n}e^*_{j,\phi}g_{\phi,\phi_i}$. The outcome of the Gram-Schmidt orthogonalization is the $d_{\rm E}\times d_{n,\max}$ matrix $e_{j,\phi}$.

Using the matrix $e_{j,\phi}$, we can express states $|\phi\rangle\in V_n$ and operators $b\in\{b_\beta(\omega)\}$ using the orthonormal basis of the subspace $\mathcal{H}_{\rm E}^{\rm r}=\mathrm{span}(V_n)$, i.e., $|\phi\rangle=\sum_i\langle e_i|\phi\rangle|e_i\rangle$ and $\Pi_{\rm E}b\Pi_{\rm E}=\sum_{i,j}\langle e_i|b|e_j\rangle|e_i\rangle\langle e_j|$, where $\Pi_{\rm E}=\sum_{i=1}^{d_{\rm E}}|e_i\rangle\langle e_i|$ is the projection onto the subspace, $\langle e_i|\phi\rangle=\sum_{\phi'\in V_n}e^*_{i,\phi'}g_{\phi',\phi}$, and $\langle e_i|b|e_j\rangle=\sum_{\phi',\phi\in V_n}e^*_{i,\phi'}g_{\phi',\phi}e_{j,\phi}$.

Let $\{|\widetilde{e}_i\rangle\,|\,i=1,\ldots,d_{\rm E}\}$ be $d_{\rm E}$-dimensional orthonormal states. Each $|\widetilde{e}_i\rangle$ is a state in $\widetilde{\mathcal{H}}_{\rm E}$ on the quantum computer. Then, for operators $b\in\{b_\beta(\omega)\}$, we define $\widetilde{b}\equiv\sum_{i,j}\langle e_i|b|e_j\rangle|\widetilde{e}_i\rangle\langle\widetilde{e}_j|$. Because $b^\dagger_\beta(\omega)=b_\beta(-\omega)$, $[\Pi_{\rm E}b_\beta(\omega)\Pi_{\rm E}]^\dagger=\Pi_{\rm E}b_\beta(-\omega)\Pi_{\rm E}$. Therefore, $\widetilde{b}^\dagger_\beta(\omega)=\widetilde{b}_\beta(-\omega)$.

For a state $|\varphi\rangle\in\mathrm{span}(V_n)$, we define $|\widetilde{\varphi}\rangle\equiv\sum_i\langle e_i|\varphi\rangle|\widetilde{e}_i\rangle$. Then,

$$\langle\widetilde{\varphi}|\widetilde{b}_m\cdots\widetilde{b}_2\widetilde{b}_1|\widetilde{\varphi}\rangle=\langle\varphi|b_m\Pi_{\rm E}\cdots\Pi_{\rm E}b_2\Pi_{\rm E}b_1|\varphi\rangle. \tag{A2}$$

We remark that $\Pi_{\rm E}|\varphi\rangle=|\varphi\rangle$.

Because $\Pi_{\rm E}b_m\Pi_{\rm E}\cdots\Pi_{\rm E}b_2\Pi_{\rm E}b_1|\psi\rangle=b_m\cdots b_2b_1|\psi\rangle\in V_n$ for all $m\leqslant\lfloor n/2\rfloor$, the following equation holds for all $m\leqslant 2\lfloor n/2\rfloor+1$:

$$\langle\psi|b_m\Pi_{\rm E}\cdots\Pi_{\rm E}b_2\Pi_{\rm E}b_1|\psi\rangle=\langle\psi|b_m\cdots b_2b_1|\psi\rangle. \tag{A3}$$

Therefore, Eq. (17) holds for all $m\leqslant 2\lfloor n/2\rfloor+1$.

APPENDIX B: PROOF OF THE ALGORITHM

Because $\langle\widetilde{\phi}_{\Omega_{\rm L},m_{\rm L}}(\cdots)|\widetilde{b}_\beta(\omega)|\widetilde{\phi}_{\Omega_{\rm R},m_{\rm R}}(\cdots)\rangle=0$ if $\omega\neq\Omega_{\rm L}-\Omega_{\rm R}$, we have $\widetilde{b}_\beta(\omega)=\sum_{\Omega_{\rm L}-\Omega_{\rm R}=\omega}\widetilde{\Pi}_{\Omega_{\rm L}}\widetilde{b}_\beta(\omega)\widetilde{\Pi}_{\Omega_{\rm R}}$, then $\widetilde{B}_\beta(t)=\sum_\omega e^{-i\omega t}\widetilde{b}_\beta(\omega)$. Therefore, $\widetilde{B}_\beta(\omega)=\widetilde{b}_\beta(\omega)$.

Correlation functions on the quantum computer can be expressed as

$$\begin{aligned}&\mathrm{Tr}\big[\widetilde{\mathcal{B}}_\beta(\omega,\nu)\cdots\widetilde{\mathcal{B}}_{\beta_{m-1}}(\omega_{m-1},\nu_{m-1})\widetilde{\rho}_{\rm E}\big]\\&=\langle\widetilde{\psi}|\big[\widetilde{b}_{\beta_{m-1}}(\omega_{m-1})\big]^{1-\nu_{m-1}}\cdots[\widetilde{b}_\beta(\omega)]^{1-\nu}\\&\quad\times[\widetilde{b}_\beta(\omega)]^{\nu}\cdots\big[\widetilde{b}_{\beta_{m-1}}(\omega_{m-1})\big]^{\nu_{m-1}}|\widetilde{\psi}\rangle.\end{aligned} \tag{B1}$$

Because of Eq. (17), the following equation holds for all $m\leqslant n$:

$$\begin{aligned}&\mathrm{Tr}\big[\widetilde{\mathcal{B}}_\beta(\omega,\nu)\cdots\widetilde{\mathcal{B}}_{\beta_{m-1}}(\omega_{m-1},\nu_{m-1})\widetilde{\rho}_{\rm E}\big]\\&=\langle\psi|\big[b_{\beta_{m-1}}(\omega_{m-1})\big]^{1-\nu_{m-1}}\cdots[b_\beta(\omega)]^{1-\nu}\\&\quad\times[b_\beta(\omega)]^{\nu}\cdots\big[b_{\beta_{m-1}}(\omega_{m-1})\big]^{\nu_{m-1}}|\psi\rangle\\&=\mathrm{Tr}\big[\mathcal{B}_\beta(\omega,\nu)\cdots\mathcal{B}_{\beta_{m-1}}(\omega_{m-1},\nu_{m-1})\rho_{\rm E}\big].\end{aligned} \tag{B2}$$

Therefore, Eq. (6) holds for all $m\leqslant n$.

APPENDIX C: NORM OF $\widetilde{B}_\beta$

For any state $|\widetilde{\varphi}\rangle\in\widetilde{\mathcal{H}}_{\rm E}$, we have

$$\|\widetilde{B}_\beta|\widetilde{\varphi}\rangle\|^2=\langle\varphi|b^\dagger_\beta\Pi_{\rm E}b_\beta|\varphi\rangle\leqslant\|b_\beta|\varphi\rangle\|^2\leqslant\|b_\beta\|^2\||\varphi\rangle\|^2, \tag{C1}$$

where $b_\beta=\sum_\omega b_\beta(\omega)=B_\beta\otimes\mathbb{1}_{\rm a}$. Notice that $\||\varphi\rangle\|=\||\widetilde{\varphi}\rangle\|$ and $\|b_\beta\|=\|B_\beta\|$, and we have $\|\widetilde{B}_\beta\|\leqslant\|B_\beta\|$.

APPENDIX D: CORRELATION FUNCTIONS REPRODUCED IN THE FOURTH-ORDER EXAMPLE

Correlation functions reproduced in the environment given by Eqs. (29) and (30) are

$$\langle v|\widetilde{B}_{\beta}(s)\widetilde{B}_{\beta_1}(s_1)|v\rangle = \sum_{\omega} e^{-i\omega(s-s_1)} g_{\beta,\omega} g^*_{\beta_1,\omega}, \tag{D1}$$

$$\langle v|\widetilde{B}_{\beta}(s)\widetilde{B}_{\beta_1}(s_1)\widetilde{B}_{\beta_2}(s_2)|v\rangle = 0, \tag{D2}$$

and

$$\begin{aligned}\langle v|\widetilde{B}_{\beta}(s)\widetilde{B}_{\beta_1}(s_1)\widetilde{B}_{\beta_2}(s_2)\widetilde{B}_{\beta_3}(s_3)|v\rangle &= \langle v|\widetilde{B}_{\beta}(s)\widetilde{B}_{\beta_1}(s_1)|v\rangle\langle v|\widetilde{B}_{\beta_2}(s_2)\widetilde{B}_{\beta_3}(s_3)|v\rangle \\ &+ \sum_{\omega,\omega',\omega_1,\omega_2} e^{-i\omega'(s-s_1)} e^{-i(\omega_1+\omega_2)(s_1-s_2)} e^{-i\omega(s_2-s_3)} \\ &\times g_{\beta,\omega'} g_{\beta_1,\omega',\omega_1,\omega_2} g^*_{\beta_2,\omega,\omega_1,\omega_2} g^*_{\beta_3,\omega}.\end{aligned} \tag{D3}$$

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