Creating dynamic leakage-free paths using coarse-graining techniques in the presence of decoherence

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We present a method aimed at protecting unitary dynamics in the presence of decoherence, by integrating leakage elimination operators (LEOs) into the system's evolution to create dynamical leakage-free paths. Deriving the dynamical equation for an open quantum system with general drives can be challenging. Our approach avoids the rotating wave approximation and instead uses the coarse-grained averaging technique to derive a quantum master equation for such systems. The combination of the coarse-graining approach and LEO operators appears suitable to study Markovian control methods. We show that employing LEO pulses in specific subspaces can reduce errors arising from undesired transitions due to decoherence. Notably, satisfactory final fidelity can still be achieved even when the reservoir is at a finite temperature. By looking into the dynamical equation governing the quantum state on the dynamical leakage-free path, we provide analytical insights into the effectiveness of the LEO method in suppressing decoherence effects.

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I. INTRODUCTION

The importance of precise control over quantum systems with high fidelity is widely recognized for advancing quantum science and technology. This approach finds broad applications in quantum technologies, such as quantum simulation [1,2] and computation [3,4]. However, a persistent challenge arises from the impact of dissipation and noise, which lead to decoherence and leakage. These factors gradually accumulate errors over time, consequently damaging the accuracy of control [5]. To address this challenge, various schemes have been proposed, including the decoherence-free subspace [6,7], shortcuts to adiabaticity [8–10], and dynamical decoupling [11,12].

These methods effectively shield quantum control processes from decoherence in a short time; however, they show a reduction in robustness when control timescales are long [13,14]. To enhance the performance of quantum control processes, a pivotal step involves redesigning the control strategy within the framework of the theory of open quantum systems. This redesign has been made to control schemes for open quantum systems [15-18], as well as to derive the Markovian master equation for driven quantum systems [19,20]. It has been demonstrated that under conditions where the environment is at an ultralow temperature and the rotating wave approximation (the secular approximation) is applicable, the time-dependent instantaneous steady state of the open system can be a pure state. This pure state serves as a promising candidate for executing quantum state engineering [19,21]. However, in scenarios where the rotating wave approximation is unavailable or the environment is at a finite temperature, the instantaneous steady state never becomes a

pure state. As a result, the quantum control task is destined to fail due to decoherence.

When the rotating wave approximation is no longer applicable, a promising method was proposed to derive a master equation, known as the coarse-graining master equation [22-25], which satisfies complete positivity and trace preservation and does not require the rotating wave approximation. The coarse-graining master equations are influenced by a parameter, the coarse-graining timescale. For short coarse-graining times that adaptively align with the physical time, the solution is designed to approximate the result of the Born approximation. For longer coarse-graining times and time-independent system Hamiltonians, the rotating wave approximation is reproduced. For all intermediate coarsegraining times, the Lindblad form of the resulting differential equations ensures a positive evolution of the system density matrix. If we choose the coarse-graining timescale to be the physical time, this timescale is referred to as the dynamical coarse-graining time [22,26], which has several advantages. Dynamical coarse graining can not only significantly decrease the computational effort required to solve the quantum master equation, but also can accommodate certain non-Markovian effects by incorporating memory functions or time-dependent rates, providing a more accurate description of systems where memory effects are significant.

Here, we combine the coarse-graining averaging technique and the leakage elimination operator (LEO) method, and show that this combination is beneficial to understand the effect of the dynamical decoupling pulse on the Markovian system. This approach operates independently of the rotating wave approximation and does not require an ultralow environmental temperature. The LEO method was first proposed in Ref. [27]. This method can suppress leakage from a subsystem encoding either a single logical qubit or a group of qubits into the broader framework of a multilevel Hilbert space [28-31] by employing unbounded fast and strong pulses, called "bang-bang" control [32], which originate from the spin-echo effect [33] applied for the first-order corrections of the evolution. The combination of the coarse-grained averaging technique and the LEO method allows us to examine the role of dynamical decoupling techniques in quantum control from a different perspective. By incorporating LEO operators into a set of time-dependent bases, we succeed in establishing dynamic leakage-free pathways in the presence of decoherence, including the tracking of eigenstates of a time-dependent Hamiltonian [34,35], even for open quantum systems [18]. While the LEO method has been extensively utilized in closed system dynamics, its theoretical framework for open quantum systems has rarely been thoroughly discussed.

In this paper, we combine the LEO operators method and dynamical equation for driven open quantum systems where the rotating wave approximation is inappropriate to protect unitary dynamics in the presence of decoherence. Although the Redfield master equation method can yield quite accurate results, especially the non-Markovian Redfield master equation which may outperform the coarse-graining master equation [36], To ensure the positivity of the driven open quantum system dynamics, we would like to focus on the coarse-graining master equation method. Therefore, we derive a coarse-graining master equation applicable to open quantum systems with an arbitrary time-dependent Hamiltonian at first. Through solving the Schrödinger equation of the system [37,38], we can explicitly determine the corresponding unitary operator for the system's free propagator [19]. This facilitates a concise and comprehensive formulation of our coarse-graining master equation, which incorporates explicit decoherence operators and their associated strengths. This formulation aids in visualizing the dynamics inherent in driven open quantum systems. Subsequently, we convert the coarse-graining master equation into a superoperator form. By deriving the one-component dynamical equation, we illustrate the remarkable effectiveness of the LEO method in protecting a dynamic leakage-free pathway during the system's interaction with its surroundings. Here, the quantum state shielded by the LEOs is referred to as the "dynamical leakage-free path" (DLFP). The one-component dynamical equation provides further insights into why the LEO pulse mitigates decoherence effects. It is noteworthy that the LEO pulse diminishes the impact of antirotating wave terms in the master equation by removing characteristic frequency degeneracy. Conversely, as the LEO pulse modifies the system's characteristic frequencies, it alleviates the influence of environmental temperature on the control process.

II. COARSE-GRAINING MASTER EQUATION FOR DRIVEN OPEN SYSTEMS

In this section, we initially introduce the general formulation and derivation of the coarse-graining master equation for driven quantum systems. Subsequently, we apply this general form to derive the coarse-graining master equation for the interaction between a driven system and a bosonic reservoir with finite temperature.

A. General formalism

As a first step, we employ the temporal coarse-graining approach [22,25] to derive a master equation for driven open quantum systems. We assume that the Hamiltonian of the total system can be expressed as

$$H(t) = H_{\rm S}(t) + H_{\rm B} + H_{\rm I}(t).$$

Here, $H_{\rm S}(t)$ represents the system Hamiltonian with timedependent drives, and $H_{\rm B}$ denotes the reservoir Hamiltonian. The interaction Hamiltonian takes the form

$$H_{\rm I}(t) = \lambda \sum_{k} A_k(t) \otimes B_k(t),$$

where λ is a dimensionless coupling parameter, and $A_k(t)$ and $B_k(t)$ are the Hermitian system and reservoir operators, respectively. Here, we do not restrict the interaction Hamiltonian to be time independent. By dynamically altering the coupling between the system and the environment, the interaction Hamiltonian can depend on time and can indirectly influence the evolution of the system, thereby enabling incoherent control. For instance, being able to smoothly turn on and off couplings to the reservoir is meaningful to quantum thermodynamics, such as finite stroke quantum heat engines.

The evolution of the total system follows the von Neumann equation

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

Here, we set $\hbar = 1$, and denote operators in the interaction picture by tilde symbols. The density operator and the interaction Hamiltonian in the interaction picture are expressed as

$$\begin{split} \tilde{\rho}(t) &= U_{\rm S}^{\dagger}(t)U_{B}^{\dagger}(t)\rho(t)U_{B}(t)U_{S}(t),\\ \tilde{H}_{\rm I}(t) &= \lambda \sum_{k} [U_{S}^{\dagger}(t)A_{k}(t)U_{S}(t)] \otimes [U_{B}^{\dagger}(t)B_{k}(t)U_{B}(t)]\\ &\equiv \lambda \sum_{k} \tilde{A}_{k}(t) \otimes \tilde{B}_{k}(t) \end{split}$$

with the free evolution operators of the system and reservoir

$$U_{\rm S}(t) = \mathcal{T}_{\leftarrow} \exp\left(-i\int_0^t d\tau H_{\rm S}(\tau)\right), \ U_{\rm B}(t) = \exp\left(-iH_{\rm B}t\right).$$

By following the standard derivation process of the coarsegraining master equation, the general form of the coarsegraining master equation can be written as

$$\begin{split} \tilde{\rho}_{\mathrm{S}}(t) &= -i[\langle S \rangle_{\Delta t}, \, \tilde{\rho}_{\mathrm{S}}(t)] \\ &+ \frac{\lambda^2 \Delta t}{2\pi} \sum_{i,j} \int_{-\infty}^{+\infty} d\omega \gamma_{ij}(\omega) \bigg(\langle \tilde{A}_j^{\omega} \rangle_{\Delta t} \tilde{\rho}_{\mathrm{S}}(t) \langle \tilde{A}_i^{\omega} \rangle_{\Delta t}^{\dagger} \\ &- \frac{1}{2} \big\{ \langle \tilde{A}_i^{\omega} \rangle_{\Delta t}^{\dagger} \langle \tilde{A}_j^{\omega} \rangle_{\Delta t}, \, \tilde{\rho}_{\mathrm{S}}(t) \big\} \bigg), \end{split}$$

where the coarse-graining decoherence operators are given by

$$\left\langle \tilde{A}_{i}^{\omega} \right\rangle_{\Delta t} = \frac{1}{\Delta t} \int_{t}^{t+\Delta t} \tilde{A}_{i}(\tau) e^{i\omega\tau} d\tau$$
 (1)

and the Lamb shift operator is

$$\langle \tilde{S} \rangle_{\Delta t} = \frac{\lambda^2 \Delta t}{4\pi i} \sum_{i,j} \int_{-\infty}^{+\infty} d\omega \sigma_{ij}(\omega) \langle \tilde{A}_i^{\omega} \rangle_{\Delta t}^{\dagger} \langle \tilde{A}_j^{\omega} \rangle_{\Delta t}.$$

The details of the derivation of the above coarse-graining master equation can be found in the Appendix.

Obtaining an explicit coarse-graining master equation of driven quantum systems crucially hinges on specifying the forms of the decoherence operators and Lamb shifts in the interaction picture. In the following sections, the coarse-graining decoherence operators $\langle \tilde{A}_i^{\omega} \rangle_{\Delta t}$ are identified by defining the DLFPs. First, we select an arbitrary complete basis set of the system Hilbert space at t = 0, denoted as $\{|\psi_n(0)\rangle\}$. For instance, the initial basis can be chosen as the eigenstates of the initial Hamiltonian. Then, by applying the free unitary evolution operator $U_S(t)$ to the initial basis, we can define a time-dependent basis of the system Hilbert space, termed as the dynamical leakage-free paths, which satisfy

$$U_{\rm S}(t)|\psi_n(0)\rangle = \exp[i\alpha_n(t)]|\psi_n(t)\rangle.$$
(2)

Here, $\alpha_n(t)$ is a global phase appearing in the *n*th basis. Thus, the formal solution of the system unitary evolution operator is

$$U_{\rm S}(t) = \sum_{n} \exp\left[i\alpha_n(t)\right] |\psi_n(t)\rangle \langle \psi_n(0)|. \tag{3}$$

Since $U_{\rm S}(t)$ satisfies $\dot{U}_{\rm S}(t) = -iH_{\rm S}(t)U_{\rm S}(t)$, we can identify the global phase $\alpha_n(t)$ by substituting Eq. (3) into it, i.e.,

$$\alpha_n(t) = \int_0^t \langle \psi_n(\tau) | [i\partial_\tau - H_S(\tau)] | \psi_n(\tau) \rangle \, d\tau.$$
 (4)

All of the DLFPs $\{|\psi_n(t)\rangle\}$ are orthogonal and satisfy the Schrödinger equation

$$|\dot{\psi}_n(t)\rangle = -i[H_{\rm S}(t) + \dot{\alpha}_n(t)]|\psi_n(t)\rangle,\tag{5}$$

which can be solved using both numerical and analytical methods [37,38]. It is evident that by introducing a new time variable *s* such that $t = st_f$ with $s \in [0, 1]$, we obtain

$$\frac{1}{t_f}\partial_s|\psi_n(s)\rangle = -i[H_{\rm S}(s) - E_n(s)]|\psi_n(s)\rangle,$$

where t_f represents the total evolution time and $E_n(s) \equiv -\dot{\alpha}_n(s)$. If the system's evolution satisfies the adiabatic condition, the first term in the above equation can be omitted, which leads to

$$H_{\rm S}(s)|\psi_n(s)\rangle = E_n(s)|\psi_n(s)\rangle.$$

This implies that $\{|\psi_n(s)\rangle\}$ are the eigenstates of the system Hamiltonian. Therefore, the adiabatic coarse-graining master equation can be straightforwardly obtained using our results when the system's evolution is adiabatic.

Based on the formal solution of the free evolution operator $U_{\rm S}(t)$, the system operator in the interaction picture reads as follows:

$$\tilde{A}_{i}(t) = U_{\rm S}^{\dagger}(t)A_{i}U_{\rm S}(t) = \sum_{n,m} e^{i\theta_{mn}^{i}(t)}\xi_{mn}^{i}(t)\tilde{F}_{mn}, \qquad (6)$$

where

$$\theta_{mn}^{i}(t) = \alpha_{n}(t) - \alpha_{m}(t) + \operatorname{Arg}(\langle \psi_{m}(t) | A_{i} | \psi_{n}(t) \rangle)$$
(7)

and $\xi_{mn}^{i}(t) = |\langle \psi_m(t)|A_i|\psi_n(t)\rangle|$. The time-independent operators $F_{mn} = |\psi_m(0)\rangle\langle\psi_n(0)|$ denote decoherence operators in the interaction picture. It can be observed that $\theta_{mn}^{i}(t)$ and $\xi_{mn}^{i}(t)$ are real numbers, and $\xi_{mn}^{i}(t) > 0$. Taking the Hermitian conjugate of Eq. (6), it yields

$$\tilde{A}_{i}^{\dagger}(t) = \sum_{n',m'} e^{-i\theta_{m'n'}^{i}(t)} \xi_{m'n'}^{i}(t) \tilde{F}_{m'n'}^{\dagger}.$$
(8)

Thus, according to Eq. (1), the coarse-graining decoherence operators can be obtained as

$$\left\langle \tilde{A}_{i}^{\omega} \right\rangle_{\Delta t} = \sum_{n,m} \left\langle c_{mn}^{i,\omega,t} \right\rangle_{\Delta t} e^{i\omega t} \tilde{F}_{mn}$$

with time-dependent coefficients

$$\langle c_{mn}^{i,\omega,t} \rangle_{\Delta t} = \frac{1}{\Delta t} \int_0^{\Delta t} e^{i(\theta_{mn}^i(t+\tau')+\omega\tau')} \xi_{mn}^i(t+\tau')d\tau',$$

where τ has been replaced by $t + \tau'$. Here, we assume that the driving rate is much smaller than the inverse of the reservoir correlation time. In other words, the reservoir correlation time τ_B is much shorter than the timescale τ_d defined as [20]

$$\tau_d \equiv \operatorname{Min}_{m,n,i,t} \left\{ \frac{\partial_t \theta_{mn}^i(t)}{\partial_t^2 \theta_{mn}^i(t)} \right\}$$

For τ' in the interval $[0, \Delta t]$ and $\tau' \ll t$, $\theta_{mn}^i(t + \tau')$ can be approximated by a polynomial expansion in orders of τ' as follows:

$$\theta_{mn}^{i}(t+\tau') \approx \theta_{mn}^{i}(t) + \partial_{t}\theta_{mn}^{i}(t)\tau' \equiv \theta_{mn}^{i}(t) + \alpha_{mn}^{i}(t)\tau',$$
(9)

where $\alpha_{mn}^{i}(t) = \partial_{t}\theta_{mn}^{i}(t+s)|_{s=0}$ represents an instantaneous frequency. In such a case, the first order is the dominant contribution to the dynamics. Furthermore, we assume that the first orders of expansion on $\xi_{mn}^{i}(t+\tau')$ are negligible relative to $\xi_{mn}^{i}(t)$, i.e., $\xi_{mn}^{i}(t+\tau') \approx \xi_{mn}^{i}(t)$. Under these assumptions, we have

$$\langle c_{mn}^{i,\omega,t} \rangle_{\Delta t} = \xi_{mn}^{i}(t) e^{i \{\theta_{mn}^{i}(t) + [\omega + \alpha_{mn}^{i}(t)] \Delta t/2\}} \\ \times \operatorname{sinc} \left[\frac{[\omega + \alpha_{mn}^{i}(t)] \Delta t}{2} \right],$$

where sinc(x) = sin(x)/x, and the following relation has been used:

$$\int_{0}^{\Delta t} e^{i\alpha\tau'} d\tau' = \Delta t e^{i\alpha\Delta t/2} \operatorname{sinc}\left(\frac{\alpha\Delta t}{2}\right).$$

Taking the conjugate on $\langle c_{mn}^{i,\omega,t} \rangle_{\Delta t}$, it yields

$$\left[c_{m'n'}^{i,\omega,t} \right]_{\Delta t}^{*} = \xi_{m'n'}^{i}(t) e^{-i\left\{ \theta_{m'n'}^{i}(t) + \left[\omega + \alpha_{m'n'}^{i}(t) \right] \Delta t/2 \right]} \\ \times \operatorname{sinc} \left[\frac{\left[\omega + \alpha_{m'n'}^{i}(t) \right] \Delta t}{2} \right],$$

resulting in

$$\left\langle \tilde{A}_{j}^{\omega}\right\rangle _{\Delta t}^{\dagger}=\sum_{n^{\prime},m^{\prime}}\left\langle c_{m^{\prime}n^{\prime}}^{j,\omega,t}\right\rangle _{\Delta t}^{*}e^{-i\omega t}\tilde{F}_{m^{\prime}n^{\prime}}^{\dagger}$$

$$\dot{\tilde{\rho}}_{S}(t) = -i[\langle \tilde{S} \rangle_{\Delta t}, \tilde{\rho}_{S}(t)] + \sum_{n,m,n',m'} \Gamma^{\Delta t}_{mn,m'n'}(t) \\ \times \left(\tilde{F}_{mn} \tilde{\rho}_{S}(t) \tilde{F}^{\dagger}_{m'n'} - \frac{1}{2} \{ \tilde{F}^{\dagger}_{m'n'} \tilde{F}_{mn}, \tilde{\rho}_{S}(t) \} \right)$$
(10)

with the decoherence rates

$$\begin{split} \Gamma^{\Delta t}_{mn,m'n'}(t) &= \frac{\lambda^2 \Delta t}{2\pi} \sum_{i,j} \xi^j_{m'n'}(t) \xi^i_{mn}(t) \\ &\times e^{i \left[\theta^i_{mn}(t) - \theta^j_{m'n'}(t)\right]} e^{i \left[\alpha^i_{mn}(t) - \alpha^j_{m'n'}(t)\right] \Delta t/2} \\ &\times \int_{-\infty}^{+\infty} \gamma_{ij}(\omega) \text{sinc} \left[\frac{\left[\omega + \alpha^j_{m'n'}(t)\right] \Delta t}{2} \right] \\ &\times \text{sinc} \left[\frac{\left[\omega + \alpha^i_{mn}(t)\right] \Delta t}{2} \right] d\omega. \end{split}$$

The Lamb shift operator can be written as

$$\langle \tilde{S} \rangle_{\Delta t} = \sum_{n,n',m} S^{\Delta t}_{mn,mn'}(t) \tilde{F}^{\dagger}_{mn'} \tilde{F}_{mn},$$

with

$$S_{mn,mn'}^{\Delta t}(t) = \frac{\lambda^2 \Delta t}{4\pi i} \sum_{i,j} \xi_{mn'}^j(t) \xi_{mn}^i(t)$$
$$\times e^{i[\theta_{mn}^i(t) - \theta_{m'n'}^j(t)]} e^{i[\alpha_{mn}^i(t) - \alpha_{m'n'}^j(t)]\Delta t/2}$$
$$\times \int_{-\infty}^{+\infty} \sigma_{ij}(\omega) \operatorname{sinc}\left[\frac{\left[\omega + \alpha_{mn'}^j(t)\right]\Delta t}{2}\right]$$
$$\times \operatorname{sinc}\left[\frac{\left[\omega + \alpha_{mn}^i(t)\right]\Delta t}{2}\right] d\omega.$$

B. Coarse-graining master equation for a driven two-level system

As an example, let us consider the driven two-level system in the laser-adapted interaction picture with the following Hamiltonian:

$$H_S^0 = \Delta(t)\sigma_z + \Omega(t)\sigma_x. \tag{11}$$

Here, $\Delta(t) = \omega_0(t) - \omega_L$ represents the time-dependent detuning, with $\omega_0(t)$ as the time-dependent Rabi frequency, and ω_L as the constant laser frequency. The driven field is represented by $\Omega(t)$. The formal solution also follows the pattern for the two-level system [39,40]:

$$\begin{aligned} |\psi_1(t)\rangle &= \cos\eta(t) \, e^{i\zeta(t)} |1\rangle + \sin\eta(t) |0\rangle, \\ |\psi_2(t)\rangle &= \sin\eta(t) \, e^{i\zeta(t)} |1\rangle - \cos\eta(t) |0\rangle, \end{aligned} \tag{12}$$

which are the general solutions of the Schrodinger equation. Here, $|1\rangle$ and $|0\rangle$ satisfy $\sigma_z |1\rangle = |1\rangle$ and $\sigma_z |0\rangle = -|0\rangle$. The coefficients in the formal solution (12) are related to the Hamiltonian (5), in such a way that

$$\partial_t \eta = \Omega \sin \zeta, \quad \sin 2\eta (2\Delta + \partial_t \zeta) = 2\Omega \cos 2\eta \cos \zeta.$$
 (13)

According to Eq. (4), the global phases of the DLFPs are

$$\alpha_1 = \int_0^t d\tau (-\partial_\tau \zeta \cos^2 \eta - \Delta \cos 2\eta - \Omega \cos \zeta \sin 2\eta),$$

$$\alpha_2 = \int_0^t d\tau (-\partial_\tau \zeta \sin^2 \eta + \Delta \cos 2\eta + \Omega \cos \zeta \sin 2\eta).$$
(14)

Therefore, the system's free evolution operator can be explicitly written as

$$U_{\mathcal{S}}(t) = \sum_{k=1,2} e^{i\alpha_k(t)} |\psi_k(t)\rangle \langle \psi_k(0)|$$
(15)

with either Δ , Ω or ζ , η .

The driven two-level system is coupled to a bosonic reservoir, which can be characterized by the reservoir Hamiltonian in the laser-adapted interaction picture:

$$H_B = \sum_k \Omega_k b_k^{\dagger} b_k.$$

Here, $\Omega_k = \omega_k - \omega_L$, where b_k and ω_k represent the annihilation operator and the eigenfrequency of the *k*th mode of the bosonic reservoir, respectively. Furthermore, we consider the interaction Hamiltonian as

$$H_I = \sigma_y \otimes B_y.$$

Here, $B_y = i \sum_k g_k^y (b_k^{\dagger} - b_k)$, where g_k^y denotes the coupling strength of the driven two-level system to the *k*th bosonic mode.

Using the system evolution operator given by Eq. (15), the system operator σ_v in the interaction picture is

$$\tilde{\sigma}_{y}(t) = \sum_{m,n=1}^{2} e^{i\theta_{mn}^{y}(t)} \xi_{mn}^{y}(t) \tilde{F}_{mn}.$$
(16)

Here, the coefficients are defined as follows:

$$\begin{aligned} \xi_{11}^{y} &= \xi_{22}^{y} = \sin 2\eta \sin \zeta, \\ \xi_{12}^{y} &= \xi_{21}^{y} = \sqrt{1 - \sin^{2} 2\eta \sin^{2} \zeta} \end{aligned}$$

and

$$\begin{aligned} \theta_{12}^{y} &= -\theta_{21}^{y} = \alpha_{2} - \alpha_{1} + \varphi_{12}, \\ \theta_{11}^{y} &= \pi, \ \theta_{22}^{y} = 0. \end{aligned}$$

Here, α_1 and α_2 are the global phases as given by Eq. (14), and $\tan \varphi_{12} = \cos \zeta / \cos 2\eta \sin \zeta$. The instantaneous frequencies read

$$\begin{aligned} \alpha_0 &\equiv \alpha_{12}^y = -\alpha_{21}^y \\ &= \partial_t \zeta \cos 2\eta + 2\Delta \cos 2\eta + 2\Omega \cos \zeta \sin 2\eta \\ &+ \frac{\partial_t \eta \sin 2\eta \sin 2\zeta + \partial_t \zeta \cos 2\eta}{1 - \sin^2 2\eta \cos^2 \zeta}. \end{aligned}$$

We redefine the decoherence operators as $\tilde{\Sigma}_{+} = \tilde{F}_{21}$, $\tilde{\Sigma}_{-} = \tilde{F}_{12}$, and $\tilde{\Sigma}_{z} = \tilde{F}_{22} - \tilde{F}_{11}$, satisfying $\tilde{\Sigma}_{+} = \tilde{\Sigma}_{-}^{\dagger}$, $[\tilde{\Sigma}_{z}, \tilde{\Sigma}_{+}] = 2\tilde{\Sigma}_{+}$, and $[\tilde{\Sigma}_{z}, \tilde{\Sigma}_{-}] = -2\tilde{\Sigma}_{-}$. By relabeling the indices in Eq. (16) and replacing 11, 22 with *z*, 21 with +, and 12 with -, it yields

$$ilde{\sigma}_{y}(t) = \sum_{k=+,-,z} e^{i heta_{k}^{y}(t)} \xi_{k}^{y}(t) ilde{\Sigma}_{k}$$

with $\theta_z^y = 0$ and $\xi_z^y = \xi_{22}^y$. Thus, the coarse-grained master equation for the driven two-level system can be expressed explicitly as follows:

$$\begin{split} \dot{\tilde{\rho}}_{\mathrm{S}}(t) &= -i[\langle \tilde{S} \rangle_{\Delta t}, \, \tilde{\rho}_{\mathrm{S}}(t)] \\ &+ \sum_{k,k'=+,-,z} \Gamma_{kk'}^{\Delta t}(t) \bigg(\tilde{\Sigma}_{k} \tilde{\rho}_{\mathrm{S}}(t) \tilde{\Sigma}_{k'}^{\dagger} - \frac{1}{2} \{ \tilde{\Sigma}_{k'}^{\dagger} \tilde{\Sigma}_{k}, \, \tilde{\rho}_{\mathrm{S}}(t) \} \bigg). \end{split}$$

The decoherence rates are given by

$$\Gamma_{kk'}^{\Delta t}(t) = \frac{\Delta t}{2\pi} \xi_{k'}^{y}(t) \xi_{k}^{y}(t)$$

$$\times e^{i[\theta_{k}^{y}(t) - \theta_{k'}^{y}(t)]} e^{i[\alpha_{k}^{y}(t) - \alpha_{k'}^{y}(t)]\Delta t/2}$$

$$\times \int_{-\infty}^{+\infty} \gamma(\omega) \operatorname{sinc}\left[\frac{[\omega + \alpha_{k'}^{y}(t)]\Delta t}{2}\right]$$

$$\times \operatorname{sinc}\left[\frac{[\omega + \alpha_{k}^{y}(t)]\Delta t}{2}\right] d\omega, \qquad (17)$$

and the Lamb shift is

$$\langle \tilde{S} \rangle_{\Delta t} = \sum_{kk'} S_{kk'}^{\Delta t}(t) \tilde{\Sigma}_{k'}^{\dagger} \tilde{\Sigma}_k,$$

where

$$S_{kk'}^{\Delta t}(t) = \frac{\Delta t}{4\pi i} \xi_{k'}^{y}(t) \xi_{k}^{y}(t)$$

$$\times e^{i[\theta_{k}^{y}(t) - \theta_{k'}^{y}(t)]} e^{i[\alpha_{k}^{y}(t) - \alpha_{k'}^{y}(t)]\Delta t/2}$$

$$\times \int_{-\infty}^{+\infty} \sigma(\omega) \operatorname{sinc}\left[\frac{\left[\omega + \alpha_{k'}^{y}(t)\right]\Delta t}{2}\right]$$

$$\times \operatorname{sinc}\left[\frac{\left[\omega + \alpha_{k}^{y}(t)\right]\Delta t}{2}\right] d\omega. \quad (18)$$

In the Schrödinger picture, the coarse-graining master equation is expressed as

$$\dot{\rho}_{S}(t) \equiv \mathcal{L}[\rho_{S}(t)]$$
$$= \mathcal{H}[\rho_{S}(t)] + \mathcal{D}[\rho_{S}(t)]$$
(19)

where the Hamiltonian part is

$$\mathcal{H}[\rho_{\mathrm{S}}(t)] = -i[H_{\mathrm{S}} + \langle S \rangle_{\Delta t}, \rho_{\mathrm{S}}(t)]$$

and the dissipative part is given by

$$\mathcal{D}[\rho_{\rm S}] = \sum_{k,k'} \Gamma_{kk'}^{\Delta t}(t) \bigg(\Sigma_k \rho_{\rm S} \Sigma_{k'}^{\dagger} - \frac{1}{2} \big\{ \Sigma_{k'}^{\dagger} \Sigma_k, \rho_{\rm S} \big\} \bigg). \quad (20)$$

The time-dependent decoherence operators in the Schrödinger picture, denoted by $\{\Sigma_k\}$, satisfy $\tilde{\Sigma}_k = U_S(t)\Sigma_k U_S^{\dagger}(t)$.

III. LEOS METHOD FOR DYNAMICAL LEAKAGE-FREE PATHS

In this section, we demonstrate the effectiveness of the LEO method [29,35] in protecting quantum states encoded within the DLFPs.

A. One-component dynamical equation

In this subsection, we will derive a simplified dynamical equation for the quantum state in the DLFP [27,30]. First, we present a matrix-to-vector mapping for two-level systems. The master equation Eq. (19) can be converted into superoperator form using the "bra-ket" notation for the superoperator [41,42]:

$$\mathcal{L}[\rho_{S}(t)] \leftrightarrow \hat{\mathcal{L}}|\rho_{S}(t)\rangle\rangle,$$

$$\mathrm{Tr}\{X^{\dagger}Y\} \leftrightarrow \langle\langle X|Y\rangle\rangle,$$

$$X\rho_{S}(t)Y^{\dagger} \leftrightarrow (X\otimes Y^{*})|\rho_{S}(t)\rangle\rangle,$$

where Y^* denotes the complex conjugate of the operator Y. In this superoperator notation, the density matrix can be expanded into a " 4×1 " vector:

$$|\rho_{S}(t)\rangle\rangle = \sum_{m,n=1}^{2} \rho_{mn}(t)|\psi_{m}(t)\rangle \otimes |\psi_{n}^{*}(t)\rangle.$$

Here, $\{|\psi_m(t)\rangle\}$ are DLFPs which were defined in Eq. (2). Thus, the coarse-graining master equation Eq. (19) becomes

$$|\dot{\rho}_{S}(t)\rangle\rangle = \sum_{m,n=1}^{2} \rho_{mn}(t)(\hat{\mathcal{H}} + \hat{\mathcal{D}})|\psi_{m}(t)\rangle \otimes |\psi_{n}^{*}(t)\rangle, \quad (21)$$

with

$$\hat{\mathcal{H}} = -i[(H_S + \langle S \rangle_{\Delta t}) \otimes I - I \otimes (H_S + \langle S \rangle_{\Delta t})^*]$$

and

$$\begin{split} \hat{\mathcal{D}} &= \sum_{k,k'} \Gamma_{kk'}^{\Delta t}(t) \bigg\{ \Sigma_k \otimes \Sigma_{k'}^* \\ &- \frac{1}{2} \big[\Sigma_{k'}^{\dagger} \Sigma_k \otimes I + I \otimes \big(\Sigma_{k'}^{\dagger} \Sigma_k \big)^T \big] \bigg\}, \end{split}$$

where A^T denotes the transpose of A. Due to $(\langle \psi_{m'} | \otimes \langle \psi_{n'}^* |) [|\psi_m(t)\rangle \otimes |\psi_n^*(t)\rangle] = \delta_{m'm} \delta_{n'n}$ and $|\dot{\psi}_m(t)\rangle = -iH_S(t)|\psi_m(t)\rangle$, we use $\langle \psi_{m'} | \otimes \langle \psi_{n'}^* |$ on the left of Eq. (21) and obtain

$$\dot{\rho}_{m'n'}(t) = \sum_{m,n=1}^{2} [\langle \psi_{m'} | \otimes \langle \psi_{n'}^* | \hat{S} | \psi_m(t) \rangle \otimes | \psi_n^*(t) \rangle + \langle \psi_{m'} | \otimes \langle \psi_{n'}^* | \hat{D} | \psi_m(t) \rangle \otimes | \psi_n^*(t) \rangle] \rho_{mn}(t),$$

with $\hat{S} = -i(\langle S \rangle_{\Delta t} \otimes I - I \otimes \langle S \rangle_{\Delta t}^*)$. Furthermore, we define $|\Psi_i\rangle\rangle = |\psi_m(t)\rangle \otimes |\psi_n^*(t)\rangle$ with i = m + 2(n-1), so that it yields

$$\dot{\rho}_{i'}(t) = \sum_{i=1}^{4} (\langle \langle \Psi_{i'} | \hat{\mathcal{S}} | \Psi_i \rangle \rangle + \langle \langle \Psi_{i'} | \hat{\mathcal{D}} | \Psi_i \rangle \rangle) \rho_i(t).$$

We rewrite the above equation into a vector equation

$$\vec{\rho} = \vec{\mathcal{L}}\vec{\rho} \tag{22}$$

with the density operator vector $\vec{\rho} = [\rho_1, \rho_2, \rho_3, \rho_4]^T$ and the Liouvillian matrix $\bar{\mathcal{L}}_{i'i} = \langle \langle \Psi_{i'} | \hat{\mathcal{S}} | \Psi_i \rangle \rangle + \langle \langle \Psi_{i'} | \hat{\mathcal{D}} | \Psi_i \rangle \rangle$ [41].

To derive an exact one-component dynamical equation for ρ_i , we employ the Feshbach *P-Q* partitioning technique. This involves dividing the vector $\vec{\rho}$ into two parts: a onedimensional vector of interest *P*(*t*), referred to as the

$$\vec{\rho} = \begin{bmatrix} P(t) \\ Q(t) \end{bmatrix}, \quad \vec{\mathcal{L}} = \begin{bmatrix} h(t) & R(t) \\ W(t) & D(t) \end{bmatrix}.$$
(23)

Here, h(t) is a 1 × 1 matrix acting on the subspace defined by P(t), and D(t) is a 3 × 3 matrix that only acts on Q(t). The matrices R(t) and W(t) represent off-diagonal contributions, with dimensions 1 × 3 and 3 × 1, respectively. Suppose that the quantum state is initially prepared on one of DLFPs ρ_i for i = 1 or 4, leading to P(0) = 1 and $Q(0) = [0]_{3\times 1}$. Equation (22) could be decomposed into

$$\dot{P}(t) = h(t)P(t) + R(t)Q(t),$$

 $\dot{Q}(t) = D(t)Q(t) + W(t)P(t).$ (24)

Using Eq. (22), the formal solution for P(t) is given by

$$\dot{P}(t) = h(t)P(t) + \int_0^t dt'g(t,t')P(t'),$$
(25)

where g(t, t') = R(t)G(t, t')W(t') and $G(t, t') = \mathcal{T}_{\leftarrow} \exp[\int_{t'}^{t} D(s)ds]$. To obtain a more concise formal solution, we define

$$p(t) = \exp\left[-\int_0^t h(t')dt'\right]P(t),$$

which satisfies

$$\dot{p}(t) = \exp\left[-\int_0^t h(s)ds\right]$$
$$\times \int_0^t dt'g(t,t') \exp\left[\int_0^{t'} h(s)ds\right]p(t'). \quad (26)$$

This integrodifferential equation represents the exact onecomponent dynamical equation for $\rho_i(t)$.

B. LEOs for open quantum systems

Our objective is to protect the free evolution along with the dynamical leakage-free paths using the LEOs. Specifically, we consider a scenario where the detuning $\Delta(t)$ in the system Hamiltonian [Eq. (11)] decreases from a constant Δ_0 to Δ_f , while the driving strength $\Omega(t)$ increases from zero to Ω_0 . Without loss of generality, we choose

$$\Omega = \frac{3\pi}{2t_{f}^{3}} \frac{t(t-t_{f})}{\sin\left(\frac{\pi}{2} - \frac{\pi t}{2t_{f}}\right)},$$

$$\Delta = \frac{3\pi t(t-t_{f})}{2t_{f}^{3}} \tan\left(\frac{\pi t}{2t_{f}}\right) \cot\left(\frac{\pi t^{2}(2t-3t_{f})}{2t_{f}^{3}}\right) + \frac{\pi}{4t_{f}}.$$
(27)

The one-component dynamical equation [Eq. (26)] shows that if $\dot{\rho}_1(t) = 0$, meaning

$$\int_{0}^{t} dt' g(t, t') \exp\left[\int_{0}^{t'} h(s) ds\right] \rho_{1}(t') = 0, \qquad (28)$$

then the open two-level system will evolve into $|\psi_1(t_f)\rangle$ along the decoherence path $|\psi_1(t)\rangle$ in the Hilbert space.

We examine a driven two-level system interacting with a bosonic heat reservoir at temperature T_B and in its equilibrium state ρ_B . The correlation functions of the heat reservoir operators are delineated by

$$Tr\{b_{k'}b_{k}^{\dagger}\rho_{B}\} = \frac{\delta_{k'k}}{1 - \exp(-\beta\Omega_{k})},$$
$$Tr\{b_{k'}^{\dagger}b_{k}\rho_{B}\} = \frac{\delta_{k'k}}{\exp(\beta\Omega_{k}) - 1},$$
$$Tr\{b_{k'}b_{k}\rho_{B}\} = 0, \quad Tr\{b_{k'}^{\dagger}b_{k}^{\dagger}\rho_{B}\} = 0$$

where $\beta = T_B^{-1}$. In the continuum limit, the summation over $(g_k^y)^2$ is substituted with an integral:

$$\sum_{k} \left(g_{k}^{v}\right)^{2} \to \int_{0}^{\infty} d\omega J(\omega).$$

Thus, the correlation function of $B_{y}(t)$ takes the form

$$C_{yy}(\tau) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{2\pi J(|\omega|)}{|1 - \exp(-\beta\omega)|} \exp(-i\omega\tau) d\omega,$$

yielding

$$\gamma(\omega) = \frac{2\pi J(|\omega|)}{|1 - \exp(-\beta\omega)|}.$$

Without loss of generality, we consider an Ohmic spectral density with an exponential frequency cutoff at the cutoff frequency ω_c :

$$J(\omega) = \mu \omega \exp\left(-\frac{\omega}{\omega_c}\right),\,$$

where μ represents a dimensionless coupling constant.

To implement the desired dynamical leakage-free path, we apply a LEO pulse to the system. Mathematically, this is achieved by introducing the term

$$H_{\text{LEO}}(t) = c(t)(|\psi_1(t)\rangle\langle\psi_1(t)| - |\psi_2(t)\rangle\langle\psi_2(t)|),$$

into the original system Hamiltonian $H_S^0(t)$ [refer to Eq. (11)], which is diagonal in the DLFP frame. Here, c(t) represents the control function governing the sequence of pulses, while $|\psi_1(t)\rangle$ and $|\psi_2(t)\rangle$ denote the DLFPs. Thus, the updated system Hamiltonian becomes

$$H_{\mathcal{S}}(t) = H_{\mathcal{S}}^0(t) + H_{\text{LEO}}(t).$$

In the experimental frame, the modified system Hamiltonian can be explicitly expressed as

$$H_{S}(t) = \Delta'(t)\sigma_{z} + \Omega'_{x}(t)\sigma_{x} + \Omega'_{y}(t)\sigma_{y},$$

where

$$\begin{aligned} \Omega'_x(t) &= (2\partial_t \eta + c\,\sin 2\eta\,\sin 2\zeta)/\sin\zeta,\\ \Omega'_y(t) &= -2c\,\sin 2\eta\,\sin\zeta,\\ \Delta'(t) &= 2c\,\cos 2\eta + 2\partial_t \eta\cot 2\eta\cot\zeta - \partial_t\zeta \end{aligned}$$

We may have concerns regarding the impact of integrating LEOs into the system Hamiltonian on the validity of the coarse-graining master equation (19). However, it is crucial to note that the LEO Hamiltonian does not affect the DLFPs, as

demonstrated by the fact that the DLFPs are the eigenstates of the LEO Hamiltonian. Therefore, the structure of the coarsegraining master equation (19) remains intact, except for the adjusted global phases:

$$\alpha_1(t) = \int_0^t d\tau [-\dot{\zeta}(\tau)\cos^2\eta(\tau) - \Delta(\tau)\cos 2\eta(\tau) - \Omega(\tau)\cos\zeta(\tau)\sin 2\eta(\tau) - c(\tau)],$$

$$\alpha_2(t) = \int_0^t d\tau [-\dot{\zeta}(\tau)\sin^2\eta(\tau) + \Delta(\tau)\cos 2\eta(\tau) + \Omega(\tau)\cos\zeta(\tau)\sin 2\eta(\tau) + c(\tau)].$$

Consequently, there is a corresponding adjustment in the instantaneous frequencies:

$$\begin{aligned} \alpha_c &\equiv \alpha_0 + 2c \\ &= \partial_t \zeta \cos 2\eta + 2\Delta \cos 2\eta + 2\Omega \cos \zeta \sin 2\eta \\ &+ \frac{\partial_t \eta \sin 2\eta \sin 2\zeta + \partial_t \zeta \cos 2\eta}{1 - \sin^2 2\eta \cos^2 \zeta} + 2c. \end{aligned}$$
(29)

More precisely speaking, the instantaneous frequencies read

$$\alpha_{-}^{y} = \partial_{t}\zeta\cos 2\eta + 2\Delta\cos 2\eta + 2\Omega\cos\zeta\sin 2\eta + \frac{\partial_{t}\eta\sin 2\eta\sin 2\zeta + \partial_{t}\zeta\cos 2\eta}{1 - \sin^{2}2\eta\cos^{2}\zeta} + 2c, \alpha_{+}^{y} = -\partial_{t}\zeta\cos 2\eta + 2\Delta\cos 2\eta + 2\Omega\cos\zeta\sin 2\eta - \frac{\partial_{t}\eta\sin 2\eta\sin 2\zeta + \partial_{t}\zeta\cos 2\eta}{1 - \sin^{2}2\eta\cos^{2}\zeta} - 2c.$$

In essence, while the addition of the LEO Hamiltonian does not alter the decoherence operators $\{\Sigma_k(t)\}$, it does affect the decoherence rates $\{\Gamma_{kk'}^{\Delta t}(t)\}$ and the Lamb shift strengths $\{S_{kk'}^{\Delta t}(t)\}$.

In the context of the LEO method for closed quantum systems, achieving $\dot{p}(t) = 0$ implies that $\exp[\int_0^{t'} h(s)ds]$ contains rapidly oscillating functions, or equivalently, that $g(t, t') \rightarrow 0$ can be fulfilled. To demonstrate this, let us examine the expression for the elements of the Liouvillian matrix $\bar{\mathcal{L}}$:

$$\bar{\mathcal{L}}_{i'i} = \langle \langle \Psi_{i'} | \hat{\mathcal{H}}_{\text{LEO}} | \Psi_i \rangle \rangle + \langle \langle \Psi_{i'} | \hat{\mathcal{S}} | \Psi_i \rangle \rangle + \langle \langle \Psi_{i'} | \hat{\mathcal{D}} | \Psi_i \rangle \rangle, \quad (30)$$

where $\hat{\mathcal{H}}_{\text{LEO}}$ represents the LEO superoperator

$$\hat{\mathcal{H}}_{\text{LEO}} = -i(H_{\text{LEO}} \otimes I - I \otimes H_{\text{LEO}}^*).$$

This gives us the expression for h(t):

$$h(t) = \bar{\mathcal{H}}_{11}^{\text{LEO}} + \bar{\mathcal{S}}_{11} + \bar{\mathcal{D}}_{11}$$

where $\bar{\mathcal{H}}_{11}^{\text{LEO}} = \langle \langle \Psi_1 | \hat{\mathcal{H}}_{\text{LEO}} | \Psi_1 \rangle \rangle$, $\bar{\mathcal{S}}_{11} = \langle \langle \Psi_1 | \hat{\mathcal{S}} | \Psi_1 \rangle \rangle$, and $\bar{\mathcal{D}}_{11} = \langle \langle \Psi_1 | \hat{\mathcal{D}} | \Psi_1 \rangle \rangle$. Since $\langle S \rangle_{\Delta t}$ and H_{LEO} are Hermitian operators, both $\bar{\mathcal{S}}_{11}$ and $\bar{\mathcal{H}}_{11}^{\text{LEO}}$ are equal to zero. Considering the dissipator given by Eq. (20), we find $h(t) = \bar{\mathcal{D}}_{11} = -\Gamma_{--}^{\Delta t}$. Hence, the LEO pulse does not introduce rapid oscillations in $\exp[\int_0^{t'} h(s) ds]$, which distinguishes it from closed systems [31,34,35]. Moreover, based on the definition of p(t) as shown in Eq. (25), P(t) decays rapidly to zero if $\Gamma_{--}^{\Delta t}$ greatly exceeds the other decoherence rates and Lamb shift strengths in the coarse-graining master equation. This rapid decay is facilitated by the dissipator, where the term corresponding to $\Gamma_{--}^{\Delta t}$ describes the decay from $|\psi_2(t)\rangle$ to $|\psi_1(t)\rangle$. As a result, the decoherence path is naturally shielded by decoherence, as we will discuss further.

Next, let us analyze the term g(t, t') in Eq. (28). We aim to demonstrate that the LEO pulse effectively protects the quantum state on the decoherence path by inducing modifications to the decoherence rates and Lamb shift strengths. Substituting Eq. (19) into Eq. (30), we find

$$R^{T} = \begin{bmatrix} \frac{1}{2} (2\Gamma_{z+}^{\Delta t} - \Gamma_{+z}^{\Delta t} + \Gamma_{z-}^{\Delta t}) + i(S_{+z}^{\Delta t} - S_{z-}^{\Delta t}) \\ \frac{1}{2} (\Gamma_{+z}^{\Delta t} + \Gamma_{z-}^{\Delta t}) - i(S_{+z}^{\Delta t} - S_{z-}^{\Delta t}) \\ \Gamma_{++}^{\Delta t} \end{bmatrix},$$

$$W = \begin{bmatrix} \frac{1}{2} (2\Gamma_{z-}^{\Delta t} - \Gamma_{z+}^{\Delta t} + \Gamma_{-z}^{\Delta t}) + i(S_{z+}^{\Delta t} - S_{-z}^{\Delta t}) \\ \frac{1}{2} (3\Gamma_{-z}^{\Delta t} - \Gamma_{z+}^{\Delta t}) - i(S_{z+}^{\Delta t} - S_{-z}) \\ \Gamma_{--}^{\Delta t} \end{bmatrix},$$

$$D = \begin{bmatrix} -\Gamma_{d} + iS_{d} - 2ic & \Gamma_{+-}^{\Delta t} \\ \Gamma_{-+}^{\Delta t} & -\Gamma_{d} - iS_{d} + 2ic & \frac{1}{2} (\Gamma_{z-}^{\Delta t} - \Gamma_{+z}^{\Delta t}) - iS_{n} \\ \frac{1}{2} (\Gamma_{-z}^{\Delta t} - \Gamma_{z+}^{\Delta t}) - iS_{n}^{*} & \frac{1}{2} (\Gamma_{-z}^{\Delta t} - \Gamma_{z+}^{\Delta t} - 2\Gamma_{z+}^{\Delta t}) + iS_{n} \end{bmatrix},$$

where $\Gamma_d = (\Gamma_{++}^{\Delta t} + \Gamma_{--}^{\Delta t} + 2\Gamma_{zz}^{\Delta t})/2$, $S_n = S_{+z}^{\Delta t} - S_{z-}^{\Delta t}$, and $S_d = S_{++}^{\Delta t} - S_{--}^{\Delta t}$. Upon inspection of Eqs. (31) and (32), we notice that both the decoherence rates and Lamb shifts involve nonzero phase factors, such as $\exp\{i[\theta_k^y(t) - \theta_{k'}^y(t)] + i[\alpha_k^y(t) - \alpha_{k'}^y(t)]\Delta t/2\}$ for $k \neq k'$ (the antirotating wave terms), which depend on the LEO pulse strength c(t) as illustrated by Eq. (29). If the LEO pulse strength significantly exceeds the other parameters in the coarse-graining master equation, these antirotating wave terms will incorporate rapidly oscillating functions, such as

 $\exp(\pm 4i \int_0^{t'} c(s)ds)$ or $\exp(\pm 2i \int_0^{t'} c(s)ds)$. For instance, one of the decoherence rates is

$$\Gamma_{+-}^{\Delta t}(t) = \frac{\Delta t}{2\pi} \xi_{-}^{y}(t) \xi_{+}^{y}(t) e^{i\{-2\int_{0}^{t} [\alpha_{0}(t') + c(t')]dt' + [\alpha_{0}(t) + c(t)]\Delta t\}} \\ \times \int_{-\infty}^{+\infty} \gamma(\omega) \operatorname{sinc}\left[\frac{[\omega + \alpha_{-}^{y}(t)]\Delta t}{2}\right] \\ \times \operatorname{sinc}\left[\frac{[\omega + \alpha_{+}^{y}(t)]\Delta t}{2}\right] d\omega,$$
(31)



FIG. 1. The decoherence rates as a function of the dimensionless time $\omega_e t$ for the dynamics governed by $H_S^0(t)$ (red dashed lines) and $H_S(t)$ (blue solid lines). The parameters are chosen as $\Delta t = 0.1t_f$, $\tau = 0.02t_f$, $\Delta \tau = 0.6\tau$, $c_0 = -100t_f^{-1}$, $\beta = 0.1t_f$, $\omega_c = 1 \times 10^3 t_f^{-1}$, and $\mu = 10(\omega_c t_f)^{-1}$. We set $t_f = 1$ as a unit for the other parameters.

and the corresponding Lamb shift strength reads

$$S_{+-}^{\Delta t}(t) = \frac{\Delta t}{4\pi i} \xi_{-}^{y}(t) \xi_{+}^{y}(t) e^{i\left\{-2\int_{0}^{t} [\alpha_{0}(t') + c(t')]dt' + [\alpha_{0}(t) + c(t)]\Delta t\right\}} \\ \times \int_{-\infty}^{+\infty} \sigma(\omega) \operatorname{sinc}\left[\frac{\left[\omega + \alpha_{-}^{y}(t)\right]\Delta t}{2}\right] \\ \times \operatorname{sinc}\left[\frac{\left[\omega + \alpha_{+}^{y}(t)\right]\Delta t}{2}\right] d\omega.$$
(32)

[It is worth noting that when the spectral function $J(\omega)$ takes the Breit-Wigner form [43], $C(\tau)$ and the integrals in Eqs. (31) and (32) can be expressed analytically.] Therefore, all of the antirotating wave terms will approximate to zero within the single pulse time interval $\Delta \tau$, indicating that the rotating wave approximation can be applied during this interval. For our analysis, we consider a bang-bang control, with the control function chosen as

$$c(t) = \begin{cases} c_0, & n\tau < t < n\tau + \Delta\tau, \text{ for } n \ge 0, \\ 0, & \text{otherwise.} \end{cases}$$

Here, c_0 is the pulse strength, and τ denotes the single control time interval. As illustrated in Fig. 1(a), the nonsecular terms in the coarse-graining master equation, such as $\Gamma_{+-}^{\Delta t}(t)$, are effectively suppressed by the LEO in the time interval $\Delta \tau$. Since the nondiagonal terms in the matrix *D* can be neglected, we have

$$G = \operatorname{diag}\{e^{\int_{t'}^{t} ds[-\Gamma_d(s) + iS_d(s) - 2ic(s)]}, e^{\int_{t'}^{t} ds[-\Gamma_d(s) - iS_d(s) + 2ic(s)]}, e^{-\int_{t'}^{t} ds\Gamma_{++}^{\Delta t}(s)}\},$$
$$R = [0, 0, \Gamma_{++}^{\Delta t}(t)], \quad W^T = [0, 0, \Gamma_{--}^{\Delta t}(t)].$$



FIG. 2. The fidelity as a function of the dimensionless time t/t_f for the dynamics governed by $H_S^0(t)$ (red dotted lines and black dashed lines) and $H_S(t)$ (blue solid lines and green dot-dashed lines) with (a) $\beta = 10t_f$ and (b) $\beta = 0.1t_f$. The parameters are chosen as $\tau = 0.02t_f$, $\Delta \tau = 0.6\tau$, $c_0 = -100t_f^{-1}$, $\omega_c = 1 \times 10^3 t_f^{-1}$, and $\mu = 10(\omega_c t_f)^{-1}$. We set $t_f = 1$ as a unit for the other parameters.

This simplifies the expression for g(t, t'):

$$g(t,t') = \Gamma_{++}^{\Delta t}(t)\Gamma_{--}^{\Delta t}(t')e^{-\int_{t'}^{t'} ds \Gamma_{++}^{\Delta t}(s)},$$
(33)

where the decoherence rates are given by

$$\Gamma_{++}^{\Delta t}(t) = \frac{\Delta t}{2\pi} (1 - \sin^2 2\eta \sin^2 \zeta) \int_{-\infty}^{+\infty} \gamma(\omega) \\ \times \operatorname{sinc}^2 \left[\frac{(\omega - \alpha_c) \Delta t}{2} \right] d\omega,$$
$$\Gamma_{--}^{\Delta t}(t) = \frac{\Delta t}{2\pi} (1 - \sin^2 2\eta \sin^2 \zeta) \int_{-\infty}^{+\infty} \gamma(\omega) \\ \times \operatorname{sinc}^2 \left[\frac{(\omega + \alpha_c) \Delta t}{2} \right] d\omega.$$
(34)

In the low-temperature limit, as β tends to positive infinity, the function $\gamma(\omega)$ converges to $2\pi J(|\omega|)$ for $\omega > 0$ and zero for $\omega < 0$. Thus, $\Gamma_{++}^{\Delta t}(t)$ tends to zero. Utilizing Eq. (33), we find g(t, t') = 0, indicating that the time derivative of ρ_1 must be zero according to Eq. (28). This observation aligns with the behavior predicted by the coarse-graining master equation. At zero reservoir temperature, the decoherence rate $\Gamma_{--}^{\Delta t}(t)$ persists, while $\Gamma_{++}^{\Delta t}(t)$ is negligible. The other decoherence rates are suppressed by H_{LEO} . Hence, in this scenario, the instantaneous steady state of the coarse-graining master equation is $|\psi_1(t)\rangle$, thereby ensuring the protection of ρ_1 by both the LEO Hamiltonian and the decoherence process.

In Fig. 2(a), we depict the evolution of the fidelity $F_1 = \langle \psi_1(t) | \rho(t) | \psi_1(t) \rangle$ concerning the reservoir temperature $\beta = 10t_f$. For a lengthy coarse-graining period ($\Delta t = 10t_f$), during which the rotating wave effects are negligible, both the

Hamiltonian incorporating the LEO pulse, $H_S(t)$ (represented by the green solid line), and the Hamiltonian without the LEO pulse, $H_S^0(t)$ (depicted by the black dashed line), achieve satisfactory final fidelities. However, for a brief coarse-graining period ($\Delta t = 0.1t_f$), where the antirotating wave terms cannot be disregarded, the fidelity diminishes rapidly when the LEO pulse is not employed (illustrated by the red dotted line). In contrast, the blue solid line indicates that the LEO pulse efficiently mitigates the rotating wave effect, showcasing superior performance compared to the control scenario without the LEO pulse.

In Fig. 2(b), we examine the scenario of finite reservoir temperature with $\beta = 0.1t_f$, a value comparable to α_0 . The effectiveness of the LEO pulse persists in suppressing leakage for both short and long coarse-graining times. This effectiveness can be attributed to alterations in the decoherence rates induced by the leakage elimination pulse. According to Eq. (34), the driven two-level system couples to the heat reservoir with an instantaneous frequency of $\pm \alpha_c$. The integrations in Eq. (34) are chiefly influenced by the reservoir frequency around α_c . This effect becomes more apparent when considering the limit of a large coarse-graining time, i.e., $\Delta t \rightarrow \infty$. Due to

we have

$$\Gamma_{++}^{\Delta t}(t) = \pi \left(1 - \sin^2 2\eta \sin^2 \zeta\right) \frac{\mu |\alpha_c| \exp\left(-\frac{|\alpha_c|}{\omega_c}\right)}{|1 - \exp(-\beta\alpha_c)|},$$

$$\Gamma_{--}^{\Delta t}(t) = \pi \left(1 - \sin^2 2\eta \sin^2 \zeta\right) \frac{\mu |\alpha_c| \exp\left(-\frac{|\alpha_c|}{\omega_c}\right)}{|1 - \exp(\beta\alpha_c)|}$$

 $\lim_{\Delta t \to \infty} \Delta t \operatorname{sinc}^2(\omega + \alpha_k^{y}) = \pi \,\delta(\omega + \alpha_k^{y}),$

with $\alpha_c(t) = \alpha_0(t) + 2c(t)$. In this limit, the decoherence rates satisfy $\Gamma_{++}^{\Delta t} \propto |\alpha_c|/|1 - \exp(\beta \alpha_c)|$ and $\Gamma_{--}^{\Delta t} \propto |\alpha_c|/|1 \exp(-\beta\alpha_c)$, where $\alpha_c < 0$ has been considered. If the pulse strength $|c_0|$ exceeds the instantaneous frequency $|\alpha_0|$ significantly, then $|1 - \exp[\beta \alpha_c]|^{-1} \ll |1 - \exp[\beta \alpha_0]|^{-1}$, leading to the suppression of $\Gamma_{++}^{\Delta t}(t)$ in the time interval $\Delta \tau$. Thus, g(t', t) = 0 can be attained if $c/\alpha_0 \to \infty$ [see Eq. (33)], resulting in $\dot{\rho}_1(t) = 0$. Moreover, $|1 - \exp(-\beta \alpha_c)|^{-1}$ approaches 1 with increasing c_0/α_0 . Due to $\Gamma_{--}^{\Delta t} \propto |\alpha_c|$, the LEO pulse significantly enhances $\Gamma_{--}^{\Delta t}(t)$ in the time interval $\Delta \tau$, indicating a rapid decay of $\exp[\int_0^{t'} h(s) ds]$. As a result, the instantaneous steady state of the coarse-graining master equation undergoes a change accordingly. This phenomenon is confirmed by the plots of $\Gamma_{++}^{\Delta t}(t)$ and $\Gamma_{--}^{\Delta t}(t)$ in Figs. 1(b) and 1(c) for $\beta = 0.1t_f$. The prevalence of population on eigenstate $|\psi_1(t)\rangle$ in the instantaneous steady state suggests an improved performance of the free evolution along with the DLFP using the LEO pulse.

The fidelity for the case of finite reservoir temperature $(\beta \sim \alpha_0)$ can be further enhanced by increasing the ratio $\Delta \tau / \tau$ and the pulse strength c_0 , as illustrated in Figs. 3(a) and 3(b). In this scenario, we adopt dynamical coarse graining, wherein the coarse-graining time dynamically aligns with the physical time, i.e., $\Delta t = t$. As seen in both Figs. 3(a) and 3(b), there is a rapid initial drop in fidelity, which can be attributed to the small coarse-graining time. However, as time progresses, fidelity gradually increases. This is because,



FIG. 3. (a) The fidelity as a function of the dimensionless time t/t_f for different $\Delta \tau$ with $c_0 t_f = -100$. (b) The fidelity as a function of the dimensionless time t/t_f for different c_0 with $\Delta \tau = 0.6\tau$. The parameters are chosen as $\tau = 0.02t_f$, $\beta = 0.1t_f \omega_c = 1 \times 10^3 t_f^{-1}$, and $\mu = 10(\omega_c t_f)^{-1}$. We set $t_f = 1$ as a unit for the other parameters.

with the evolution, the coarse-graining time increases, thereby enhancing the transition intensity to the DLFP. As depicted in Fig. 3(a), the ratio $\Delta \tau / \tau$ notably impacts LEO control. When $\Delta \tau / \tau = 0$, the dynamics revert to the case without LEO control. The final fidelity improves with an increase in the pulse time interval $\Delta \tau$. Similar outcomes are observed when augmenting the pulse strength c_0 . A stronger bang-bang pulse yields a superior final fidelity [see Fig. 3(b)]. Moreover, Figs. 3(a) and 3(b) reveal that fidelities oscillate nonsmoothly during evolution, primarily due to instantaneous swapping between different instantaneous steady states. This observation aligns with our discussion on how the LEO pulse enhances $\Gamma_{--}^{\Delta t}$ and suppresses $\Gamma_{++}^{\Delta t}$. Therefore, with a sufficiently strong LEO pulse and a properly chosen ratio $\Delta \tau / \tau$, we can consistently anticipate satisfactory performance by utilizing the DLFP

Notably, the LEO pulse can be used to protect the quantum state encoded in $|\psi_2\rangle$, the other leakage-free path, or the DLFPs, if we apply the LEO pulse with $c_0 > 0$. Here, we maintain the assumptions $|c_0| \gg |\alpha_0|$. The numerical results are presented in Fig. 4, considering a long coarse-graining time and ultralow reservoir temperature, with $\Delta t = 10t_f$ and $\beta = 10t_f$, respectively. In Fig. 4(a), we present the fidelity $F_2 = \langle \psi_2(t) | \rho(t) | \psi_2(t) \rangle$ as a function of t/t_f for the open quantum systems dynamics with the Hamiltonian $H_{S}(t)$ (the blue solid line) and $H_{S}^{0}(t)$ (the red dotted line). When the LEO pulse is absent, the instantaneous steady state of the coarsegraining master equation is $|\psi_1(t)\rangle$ due to $\alpha_0 < 0$. The initial state undergoes decay into the instantaneous steady state, resulting in a rapid decrease of fidelity [see the red dotted line in Fig. 4(a)]. In contrast, when the LEO pulse with $c_0 > 0$ is applied, the instantaneous frequency must satisfy $\alpha_c > 0$ in the time interval $\Delta \tau$ if $|c_0| \gg \alpha_0$. At this time, the tran-



FIG. 4. The fidelities (a) and the decoherence rates (b) as a function of the dimensionless time t/t_f with $\Delta \tau = 0.6\tau$. The parameters are chosen as $\tau = 0.02t_f$, $\Delta t = 10t_f$, $c_0 = 100t_f^{-1}$, $\beta = 10t_f$, $\omega_c = 1 \times 10^3 t_f^{-1}$, and $\mu = 10(\omega_c t_f)^{-1}$. We set $t_f = 1$ as a unit for the other parameters.

sition direction caused by decoherence will overturn, and the instantaneous steady state in the time interval $\Delta \tau$ is $|\psi_2(t)\rangle$, as illustrated by the decoherence rates plotted in Fig. 4(b). Therefore, the LEO method can still be employed to protect quantum states encoded in the $|\psi_2(t)\rangle$, which is illustrated by the red dotted line in Fig. 4(a).

IV. CONCLUSION

The ability to achieve quantum state engineering in the presence of uncontrollable coupling between a quantum system and its surroundings is crucial for quantum information processing. In this paper, we combine the coarse-graining averaging technique and the LEO method [27] to study the effect of the dynamical decoupling pulse on the open quantum system. First, we derive a comprehensive coarse-grained master equation to examine the impact of rotating wave terms. Through the utilization of an LEO Hamiltonian that is diagonal in the frame of the DLFPs, we establish that the quantum state encoded in the DLFPs can be protected.

This protection is because the decoherence rates and Lamb shifts undergo modification with the addition of the LEO pulse, effectively canceling rotating wave terms and enabling the use of the rotating wave approximation. Therefore, it seems that the combination of the coarse-graining approach and LEO operators appears promising. Due to the presence of rapidly oscillating parts in the counter-rotating wave terms, these terms approximate to zero within a single pulse time interval, which is similar to the principle of the LEO method in closed systems [28,30]. But different from the LEO method in closed systems, the transition towards the protected DLFPs induced by decoherence is enhanced, while other transitions are suppressed by the leakage elimination pulse. Therefore, the quantum state evolving along the DLFP remains well protected even at finite reservoir temperatures.

It is worth emphasizing that our method is applicable to the unitary evolution initially from an arbitrary state of a time-dependent quantum system. This demonstrates the effectiveness of our approach for various control methods. Our results coincide with tracking eigenstates of system Hamiltonians in open quantum systems, particularly at zero environment temperature [18], providing insights into achieving adiabatic quantum computation. On the other hand, our method might also be helpful in designing shortcuts to adiabaticity [39], when the initial and final states are set as eigenstates of the system's time-dependent Hamiltonians.

Although in this paper we only discuss examples of open two-level systems, for systems with higher-dimensional Hilbert spaces, we can directly derive conclusions based on the coarse-graining master equation [Eq. (10)] and the one component dynamical equation [Eq. (26)]. For an Ndimensional quantum system, the Liouvillian matrix and the density matrix vector can still be decomposed according to Eq. (23). Similar to the two-level case, in the Liouvillian matrix $\overline{\mathcal{L}}$, h remains a real number, and all the off-diagonal elements depend only on $\Gamma^{\Delta t}_{mn,m'n'}$ and $S_{mn,m'n'}$ with $mn \neq m'n'$. When we apply LEO pulses to the DLFP, the phase term $e^{i \int_0^t [\alpha_{mn}^i(s) - \alpha_{m'n'}^j(s)] ds}$ in $\Gamma_{mn,m'n'}^{\Delta t}$ and $S_{mn,m'n'}^{\Delta t}$ contains rapid oscillation terms, such as $\exp[\pm 4i \int_0^{t'} c(s) ds]$ or $\exp[\pm 2i \int_0^{t'} c(s) ds]$. Here, we have considered that $\alpha_{mn}(t) =$ $\alpha_{mn}^0(t) \pm c(t)$, which can be obtained by the same procedure for obtaining Eq. (29). Therefore, all the terms will approach zero due to the rapid oscillations except $\Gamma_{mn,mn}^{\Delta t}$ terms. Since $\Gamma_{mn,mn}^{\Delta t}$ depends on the Einstein distribution $|1 - \exp(-\beta \omega_{mn})|^{-1}$, the LEO pulse can effectively suppress transitions from the DLFP to the other state which is orthogonal to the DLFP, while increasing the transition rate of reverse transitions. Therefore, for multidimensional quantum systems, the DLFP can still be effectively protected. However, this conclusion may not hold for all of the DLFPs, as the successful protection of DLFPs using LEO pulses still not only depends on the Hamiltonian of the quantum system but also on the strength of the pulses.

At last, we would like to emphasize that our method proposes a control scheme specifically for Markovian environments. It is well known that quantum systems coupled to non-Markovian environments are controllable. By reducing the overlap between the environmental correlation function and the spectral density, decoherence can be suppressed [44,45]. These methods are particularly effective in suppressing environmental thermal noise. When the environment is Markovian, the environmental spectrum is flat, causing any characteristic frequency of the system to resonantly couple with the environment. Our method provides some attempts to suppress decoherence caused by Markovian environments, demonstrating that decoherence induced by Markovian environments can also be mitigated. On the other hand, similar to other dynamical decoupling methods, the application of the LEO method is subject to several limitations. For example, the LEO method assumes perfect control pulses,

meaning they are instantaneous and error free. In reality, pulses suffer from errors and finite width, which can reduce the effectiveness of the LEO method [46]. Complex pulse sequences require precise timing control and high-fidelity pulse generation, demanding significant computational and experimental resources. Optimizing these sequences also necessitates substantial computational effort, which can be challenging for today's computer technology.

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APPENDIX: GENERAL FORM OF THE COARSE-GRAINING MASTER EQUATION

In the interaction picture, the von Neumann equation becomes

$$\dot{\tilde{\rho}}(t) = -i[\tilde{H}_{\rm I}(t), \,\tilde{\rho}(t)].\tag{A1}$$

The formal solution to the above equation can be written as $\tilde{\rho}(t) = \tilde{U}(t, t_0)\tilde{\rho}(t_0)\tilde{U}^{\dagger}(t, t_0)$ with the evolution operator

$$\tilde{U}(t,t_0) = \mathcal{T} \exp\left(-i \int_{t_0}^t \tilde{H}_{\mathrm{I}}(t') dt'\right),$$

where T is a time ordering operator. Here, we consider the weak-coupling limit $\lambda \ll 1$. Equation (A1) can be formally integrated to yield

$$\tilde{\rho}(t) = -i \int_{t_0}^t dt_1[\tilde{H}_1(t_1), \tilde{\rho}(t_1)]$$

and reinserting this result in Eq. (A1) one obtains the following exact equation:

$$\dot{\tilde{\rho}}(t) = -i[\tilde{H}_{\mathrm{I}}(t), \tilde{\rho}(t)] - \int_{t_0}^t dt_1[\tilde{H}_{\mathrm{I}}(t), [\tilde{H}_{\mathrm{I}}(t_1), \tilde{\rho}(t_1)]] + O(\lambda^3).$$

Let us consider assumptions that $\tilde{\rho}(t) = \tilde{\rho}_{\rm S}(t) \otimes \rho_{\rm B}$ (the Born approximation) and $\text{Tr}_{\rm B}(\rho_{\rm B}B_k) = 0$, where $\rho_{\rm B}$ is the thermal equilibrium state

$$\rho_{\rm B} = \frac{\exp(-\beta H_{\rm B})}{\operatorname{Tr}_{\rm B} \{\exp(-\beta H_{\rm B})\}}$$

at the inverse environment temperature $\beta = (k_B T_B)^{-1}$. Under the usual assumptions of initially factorizing the density matrix and ignoring any changes in the reservoir part of the density matrix, we obtain

$$\tilde{\rho}_{S}(t) = -i \operatorname{Tr}_{B} \{ [\tilde{H}_{I}(t), \tilde{\rho}_{S}(t) \otimes \rho_{B}] \} - \int_{t_{0}}^{t} dt_{1} \operatorname{Tr}_{B} \{ [\tilde{H}_{I}(t), [\tilde{H}_{I}(t_{1}), \tilde{\rho}_{S}(t_{1}) \otimes \rho_{B}]] \} + O(\lambda^{3})$$

where $Tr_B\{...\}$ denotes the trace over the reservoir degrees of freedom. Evaluating the traces leads to the definition of the reservoir correlation functions

$$C_{ij}(\tau) = \operatorname{Tr}_{\mathrm{B}}\{e^{iH_{\mathrm{B}}\tau}B_{i}^{\dagger}e^{-iH_{\mathrm{B}}\tau}B_{j}\rho_{\mathrm{B}}\} = C_{ji}^{*}(-\tau),$$

and omitting the higher-order terms of the coupling coefficient λ we obtain with $\langle B_i \rangle_{\rm B} = 0$

$$\dot{\tilde{\rho}}_{\rm S}(t) = -\lambda^2 \sum_{i,j} \int_{t_0}^t dt_1 C_{ij}(t-t_1) [\tilde{A}_{\rm j}(t_1) \tilde{\rho}_{\rm S}(t_1), \tilde{A}_{\rm i}(t)] + \text{H.c.},$$

which is the Redfield master equation in the interaction picture. By formally integrating the Redfield master equation, we have

$$\begin{split} \tilde{\rho}_{\rm S}(t) &\equiv \tilde{\rho}_{\rm S}(t_0) + \Delta t \, \mathcal{L}^{\Delta t} \, \tilde{\rho}_{\rm S}(t_0) \\ &= \tilde{\rho}_{\rm S}(t_0) - i \frac{\lambda^2}{2i} \sum_{i,j} \int_{t_0}^t \int_{t_0}^t C_{ij}(t_2 - t_1) \text{sgn}(t_2 - t_1) \\ &\times [\tilde{A}_i^{\dagger}(t_2) \tilde{A}_j(t_1), \, \tilde{\rho}_{\rm S}(t_0)] dt_1 dt_2 \\ &+ \lambda^2 \sum_{i,j} \int_{t_0}^t \int_{t_0}^t C_{ij}(t_2 - t_1) [\tilde{A}_j(t_1) \tilde{\rho}_{\rm S}(t_0) \tilde{A}_i^{\dagger}(t_2)] \\ &- \frac{1}{2} \{ \tilde{A}_i^{\dagger}(t_2) \tilde{A}_j(t_1), \, \tilde{\rho}_{\rm S}(t_0) \} dt_1 dt_2. \end{split}$$

The even and odd Fourier transforms of the reservoir correlation function read

. . .

$$C_{ij}(\tau) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \gamma_{ij}(\omega) e^{-i\omega\tau} d\omega,$$
$$C_{ij}(\tau) \operatorname{sgn}(\tau) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \sigma_{ij}(\omega) e^{-i\omega\tau} d\omega$$

with

$$\begin{aligned} \gamma_{ij}(\omega) &= K_{ij}(\omega) + K_{ij}^*(\omega), \\ \sigma_{ij}(\omega) &= K_{ij}(\omega) - K_{ij}^*(\omega), \end{aligned}$$

where $K_{ij}(\omega) = \int_0^{+\infty} C_{ij}(\tau) e^{i\omega\tau} d\tau$ is the one-sided Fourier transform of the correlation function.

Here we define a coarse-graining timescale $\Delta t = t - t_0$ which corresponds to the timescale after which the reservoir has effectively "reset." By defining time averaging of an operator O(t) over the coarse-graining timescale Δt as

$$\langle O(t) \rangle_{\Delta t} = \frac{1}{\Delta t} \int_{t_0}^t O(t') dt',$$

we arrive at

$$\langle \dot{\tilde{\rho}}_{\mathrm{S}}(t) \rangle_{\Delta t} = \frac{\tilde{\rho}_{\mathrm{S}}(t) - \tilde{\rho}_{\mathrm{S}}(t_0)}{\Delta t} = \mathcal{L}^{\Delta t} \tilde{\rho}_{\mathrm{S}}(t_0).$$
(A2)

In the above equation, the assumption $\tau_c \ll \Delta t \ll \tau_s$ is made, where τ_c is the inverse of the high-frequency cutoff ω_c in the reservoir spectral density, and τ_s corresponds to the characteristic time for significant changes of $\tilde{\rho}_{\rm S}(t)$. Equation (A2) may not be suitable for determining the next discretization step of Δt . To address this, assuming that the reservoir resets in the time Δt such that the reservoir interacts with the system in the same manner at each time step Δt , we can replace $\tilde{\rho}_{\rm S}(t_0)$ in the right-hand side of Eq. (A2) by $\tilde{\rho}_{\rm S}(t)$ approximately. This leads to a Markovian approximation and the following coarse-graining master equation:

$$\dot{\tilde{\rho}}_{\mathrm{S}}(t) = -i[\langle \tilde{S} \rangle_{\Delta t}, \, \tilde{\rho}_{\mathrm{S}}(t)] + \frac{\lambda^2 \Delta t}{2\pi} \sum_{i,j} \int_{-\infty}^{+\infty} d\omega \gamma_{ij}(\omega) \bigg(\langle \tilde{A}_j^{\omega} \rangle_{\Delta t} \, \tilde{\rho}_{\mathrm{S}}(t) \langle \tilde{A}_i^{\omega} \rangle_{\Delta t}^{\dagger} - \frac{1}{2} \big\{ \langle \tilde{A}_i^{\omega} \rangle_{\Delta t}^{\dagger} \langle \tilde{A}_j^{\omega} \rangle_{\Delta t}, \, \tilde{\rho}_{\mathrm{S}}(t) \big\} \bigg),$$

where the coarse-graining decoherence operators are given by

$$\left\langle \tilde{A}_{i}^{\omega} \right\rangle_{\Delta t} = \frac{1}{\Delta t} \int_{t}^{t+\Delta t} \tilde{A}_{i}(\tau) e^{i\omega\tau} d\tau \tag{A3}$$

and the Lamb shift operator is defined as

$$\langle \tilde{S} \rangle_{\Delta t} = \frac{\lambda^2 \Delta t}{4\pi i} \sum_{i,j} \int_{-\infty}^{+\infty} d\omega \sigma_{ij}(\omega) \langle \tilde{A}_i^{\omega} \rangle_{\Delta t}^{\dagger} \langle \tilde{A}_j^{\omega} \rangle_{\Delta t}.$$

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